```
*******
space group: 1 {'Hall': 'P 1', 'HM': 'P 1'}
Crystal system: Triclinic
+x,+y,+z
. . . . . . . . . . . . . . . . . . . .
        Seitz
                  | Jones
| \{1|(0.0,0.0,0.0)\} | +x,+y,+z |
. . . . . . . . . . . . . . . . . . .
*******
space group: 2 {'Hall': '-P 1', 'HM': 'P -1'}
Crystal system: Triclinic
+x,+y,+z
. . . . . . . . . . . . . . . . . . .
     Seitz |
                        Jones
| \{1 | (0.0,0.0,0.0)\} | +x,+y,+z |
| \{-1|(0.0,0.0,0.0)\} | -x,-y,-z |
*******
space group: 3:b {'Hall': 'P 2y', 'HM': 'P 1 2 1'}
Crystal system: Monoclinic
Setting: b
+x,+y,+z
-x,+y,-z
         Seitz
                         Jones
 \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z \mid
| {2_0y0|(0.0,0.0,0.0)} | -x,+y,-z |
******
space group: 3:c {'Hall': 'P 2', 'HM': 'P 1 1 2'}
Crystal system: Monoclinic
Setting: c
+x,+y,+z
-x,-y,+z
                         Jones
         Seitz
\{1|(0.0,0.0,0.0)\} |+x,+y,+z|
| {2_00z|(0.0,0.0,0.0)} | -x,-y,+z |
```

```
space group: 3:a {'Hall': 'P 2x', 'HM': 'P 2 1 1'}
Crystal system: Monoclinic
Setting: a
+x,+y,+z
+x,-y,-z
| Seitz | Jones |
\{1|(0.0,0.0,0.0)\} +x,+y,+z 
| \{2_x00|(0.0,0.0,0.0)\} | +x,-y,-z |
. . . . . . . . . . . . . . . . . . . .
******
space group: 4:b {'Hall': ' P 2yb', 'HM': 'P 1 21 1'}
Crystal system: Monoclinic
Setting: b
+x,+y,+z
-x,+y+1/2,-z
   Seitz | Jones |
| {1|(0.0,0.0,0.0)} | +x,+y,+z |
| \{2_0y0|(0.0,0.5,0.0)\} | -x,+y+1/2,-z |
. . . . . . . . . . . . . . . . . . .
******
space group: 4:c {'Hall': ' P 2c', 'HM': 'P 1 1 21'}
Crystal system: Monoclinic
Setting: c
+x,+y,+z
-x,-y,+z+1/2
. . . . . . . . . . . . . . . . . . . .
| Seitz | Jones |
\{1 \mid (0.0,0.0,0.0)\} + x,+y,+z \mid
| \{2_{00z} | (0.0,0.0,0.5)\} | -x,-y,+z+1/2 |
. . . . . . . . . . . . . . . . . . . .
******
space group: 4:a {'Hall': ' P 2xa', 'HM': 'P 21 1 1'}
Crystal system: Monoclinic
Setting: a
+x,+y,+z
+x+1/2,-y,-z
. . . . . . . . . . . . . . . . . . . .
```

```
Seitz
                             Jones
    \{1 \mid (0.0,0.0,0.0)\} + x,+y,+z
  \{2_x00|(0.5,0.0,0.0)\} \mid +x+1/2,-y,-z \mid
*******
space group: 5:b1 {'Hall': 'C 2y', 'HM': ' C 1 2 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
-x,+y,-z
          Seitz
                               Jones
 \{1 \mid (0.0,0.0,0.0)\} \mid +x,+y,+z \\ \{2\_0y0 \mid (0.0,0.0,0.0)\} \mid -x,+y,-z \}
    \{1|(0.5,0.5,0.0)\} | +x+1/2,+y+1/2,+z |
| \{2_0y0|(0.5,0.5,0.0)\} | -x+1/2,+y+1/2,-z |
******
space group: 5:b2 {'Hall': 'A 2y', 'HM': ' A 1 2 1'}
Crystal system: Monoclinic
Setting: b2
+X,+Y,+Z
-x,+y,-z
          Seitz
                              Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
-x,+y,-z
 {2_0y0|(0.0,0.0,0.0)} |
    \{1|(0.0,0.5,0.5)\} +x,+y+1/2,+z+1/2 |
  \{2_0y0|(0.0,0.5,0.5)\} \mid -x,+y+1/2,-z+1/2 \mid
*******
space group: 5:b3 {'Hall': 'I 2y', 'HM': ' I 1 2 1'}
Crystal system: Monoclinic
Setting: b3
+x,+y,+z
-x,+y,-z
          Seitz
                                  Jones
   {1|(0.0,0.0,0.0)}
                                +x,+y,+z
| {2_0y0|(0.0,0.0,0.0)} |
                            -x,+y,-z
    \{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2 |
```

```
| \{2_0y0|(0.5,0.5,0.5)\} | -x+1/2,+y+1/2,-z+1/2 |
. . . . . . . . . . . . . . . . . . .
*******
space group: 5:c1 {'Hall': 'A 2', 'HM': ' A 1 1 2'}
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
-x,-y,+z
         Seitz
                            Jones
\{1 \mid (0.0, 0.5, 0.5)\} \mid +x, +y+1/2, +z+1/2 \mid
 \{2\_00z \mid (0.0,0.5,0.5)\} \mid -x,-y+1/2,+z+1/2 \mid
******
space group: 5:c2 {'Hall': 'B 2', 'HM': ' B 1 1 2'}
Crystal system: Monoclinic
Setting: c2
+x,+y,+z
-x,-y,+z
                           Jones
         Seitz
\{1|(0.5,0.0,0.5)\} | +x+1/2,+y,+z+1/2 |
| \{2_{00z} | (0.5,0.0,0.5)\} | -x+1/2,-y,+z+1/2 |
. . . . . . . . . . . . . . . . . . . .
*******
space group: 5:c3 {'Hall': 'I 2', 'HM': ' I 1 1 2'}
Crystal system: Monoclinic
Setting: c3
+x,+y,+z
-x,-y,+z
         Seitz
                            Jones
{1|(0.0,0.0,0.0)} |
                            +x,+y,+z
 \{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2 |
| \{2_{00z} | (0.5, 0.5, 0.5)\} | -x+1/2, -y+1/2, +z+1/2 |
```

```
space group: 5:a1 {'Hall': 'B 2x', 'HM': ' B 2 1 1'}
Crystal system: Monoclinic
Setting: a1
+x,+y,+z
+x,-y,-z
        Seitz | Jones
\{1|(0.5,0.0,0.5)\} | +x+1/2,+y,+z+1/2 |
\{2_x00|(0.5,0.0,0.5)\}\ |\ +x+1/2,-y,-z+1/2\ |
*******
space group: 5:a2 {'Hall': 'C 2x', 'HM': ' C 2 1 1'}
Crystal system: Monoclinic
Setting: a2
+x,+y,+z
+x,-y,-z
        Seitz | Jones
\{1|(0.5,0.5,0.0)\} +x+1/2,+y+1/2,+z |
\{2_x00|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,-z \mid
*******
space group: 5:a3 {'Hall': 'I 2x', 'HM': ' I 2 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
+x,-y,-z
                    Jones
        Seitz
\{1 \mid (0.5,0.5,0.5)\} \mid +x+1/2,+y+1/2,+z+1/2 \mid \{2_x00 \mid (0.5,0.5,0.5)\} \mid +x+1/2,-y+1/2,-z+1/2 \mid
*******
space group: 6:b {'Hall': 'P -2y', 'HM': 'P 1 m 1'}
```

```
Crystal system: Monoclinic
Setting: b
+x,+y,+z
+x,-y,+z
          Seitz
                            Jones
  {1|(0.0,0.0,0.0)}
                         | +x,+y,+z |
| {m_x0z|(0.0,0.0,0.0)} | +x,-y,+z |
******
space group: 6:c {'Hall': 'P -2', 'HM': 'P 1 1 m'}
Crystal system: Monoclinic
Setting: c
+x,+y,+z
+x,+y,-z
      . . . . . . . . . . . . .
          Seitz
                           Jones
   {1|(0.0,0.0,0.0)}
                         | +x,+y,+z |
| \{m_xy0 | (0.0,0.0,0.0)\} | +x,+y,-z |
******
space group: 6:a {'Hall': 'P -2x', 'HM': 'P m 1 1'}
Crystal system: Monoclinic
Setting: a
+x,+y,+z
-x,+y,+z
          Seitz
                            Jones
   {1|(0.0,0.0,0.0)}
                         | +x,+y,+z |
| \{m_0yz | (0.0,0.0,0.0)\} | -x,+y,+z |
. . . . . . . . . . . . . . . . . . .
******
space group: 7:b1 {'Hall': 'P -2yc', 'HM': ' P 1 c 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
+x,-y,+z+1/2
   . . . . . . . . . . . . . . . .
          Seitz
                              Jones
   \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
```

```
| \{m_x0z|(0.0,0.0,0.5)\} | +x,-y,+z+1/2 |
. . . . . . . . . . . . . . . . . . .
*******
space group: 7:b2 {'Hall': 'P -2yac', 'HM': ' P 1 n 1'}
Crystal system: Monoclinic
Setting: b2
+x,+y,+z
+x+1/2,-y,+z+1/2
 Seitz | Jones
\{1|(0.0,0.0,0.0)\} +x,+y,+z
| \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2 |
. . . . . . . . . . . . . . . . . . .
*******
space group: 7:b3 {'Hall': 'P -2ya', 'HM': ' P 1 a 1'}
Crystal system: Monoclinic
Setting: b3
+x,+y,+z
+x+1/2,-y,+z
. . . . . . . . . . . . . . . . . . .
         Seitz | Jones
{1|(0.0,0.0,0.0)} | +x,+y,+z
| \{m_x 0z | (0.5, 0.0, 0.0)\} | +x+1/2, -y, +z |
. . . . . . . . . . . . . . . . . . .
*******
space group: 7:c1 {'Hall': 'P -2a', 'HM': ' P 1 1 a'}
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
+x+1/2, +y, -z
   .....
         Seitz |
                            Jones
\{1|(0.0,0.0,0.0)\} +x,+y,+z
| \{m_xy0 | (0.5,0.0,0.0)\} | +x+1/2,+y,-z |
. . . . . . . . . . . . . . . . . . . .
*******
space group: 7:c2 {'Hall': 'P -2ab', 'HM': ' P 1 1 n'}
Crystal system: Monoclinic
Setting: c2
+x,+y,+z
```

```
+x+1/2, +y+1/2, -z
         Seitz
                              Jones
   {1|(0.0,0.0,0.0)}
                             +x,+y,+z
| \{m_xy0|(0.5,0.5,0.0)\} | +x+1/2,+y+1/2,-z |
*******
space group: 7:c3 {'Hall': 'P -2b', 'HM': ' P 1 1 b'}
Crystal system: Monoclinic
Setting: c3
+x,+y,+z
+x,+y+1/2,-z
         Seitz
                            Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
| \{m_xy0 | (0.0,0.5,0.0)\} | +x,+y+1/2,-z |
*******
space group: 7:a1 {'Hall': 'P -2xb', 'HM': ' P b 1 1'}
Crystal system: Monoclinic
Setting: a1
+x,+y,+z
-x,+y+1/2,+z
         Seitz
                            Jones
   {1|(0.0,0.0,0.0)}
                         +x,+y,+z
 \{m_0yz \mid (0.0,0.5,0.0)\} \mid -x,+y+1/2,+z
*******
space group: 7:a2 {'Hall': 'P -2xbc', 'HM': ' P n 1 1'}
Crystal system: Monoclinic
Setting: a2
+x,+y,+z
-x, +y+1/2, +z+1/2
         Seitz
                              Jones
    {1|(0.0,0.0,0.0)}
                             +x,+y,+z
| \{m_0yz | (0.0,0.5,0.5)\} | -x,+y+1/2,+z+1/2 |
```

```
*******
space group: 7:a3 {'Hall': 'P -2xc', 'HM': ' P c 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
-x,+y,+z+1/2
. . . . . . . . . . . . . . . . . . . .
   Seitz | Jones
\{1|(0.0,0.0,0.0)\} +x,+y,+z
| \{m_0yz | (0.0,0.0,0.5)\} | -x,+y,+z+1/2 |
*******
space group: 8:b1 {'Hall': 'C -2y', 'HM': ' C 1 m 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
+x,-y,+z
   Seitz | Jones
\{1 \mid (0.5, 0.5, 0.0)\} \mid +x+1/2, +y+1/2, +z \mid
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z |
******
space group: 8:b2 {'Hall': 'A -2y', 'HM': ' A 1 m 1'}
Crystal system: Monoclinic
Setting: b2
+x,+y,+z
+x,-y,+z
        Seitz | Jones |
| \{m_x \dot{0}z | (0.0, 0.5, 0.5)\} | +x,-y+1/2,+z+1/2 |
. . . . . . . . . . . . . . . . . . .
*******
space group: 8:b3 {'Hall': 'I -2y', 'HM': ' I 1 m 1'}
```

Crystal system: Monoclinic

Setting: b3

```
+x,+y,+z
+x,-y,+z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
| {m_x0z|(0.0,0.0,0.0)} |
                                 +x,-y,+z
    \{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2 |
*******
space group: 8:c1 {'Hall': 'A -2', 'HM': ' A 1 1 m'}
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
+x,+y,-z
       . . . . . . . . . . . . .
          Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 \{m_xy0 \mid (0.0,0.0,0.0)\} \mid +x,+y,-z
    \{1|(0.0,0.5,0.5)\} | +x,+y+1/2,+z+1/2 |
  \{m_xy0 \mid (0.0,0.5,0.5)\} \mid +x,+y+1/2,-z+1/2 \mid
*******
space group: 8:c2 {'Hall': 'B -2', 'HM': ' B 1 1 m'}
Crystal system: Monoclinic
Setting: c2
+x,+y,+z
+x,+y,-z
          Seitz
                                 Jones
 \{1 \mid (0.0,0.0,0.0)\} \mid +x,+y,+z \\ \{m_xy0 \mid (0.0,0.0,0.0)\} \mid +x,+y,-z \}
 \{1|(0.5,0.0,0.5)\} +x+1/2,+y,+z+1/2 |
| {m_xy0|(0.5,0.0,0.5)} | +x+1/2,+y,-z+1/2 |
******
space group: 8:c3 {'Hall': 'I -2', 'HM': ' I 1 1 m'}
Crystal system: Monoclinic
Setting: c3
+x,+y,+z
+x,+y,-z
```

```
Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  \{m_xy0 | (0.0,0.0,0.0)\} \mid
                                +x,+y,-z
    {1|(0.5,0.5,0.5)}
                         | +x+1/2, +y+1/2, +z+1/2
 \{m_xy0|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,-z+1/2
*******
space group: 8:a1 {'Hall': 'B -2x', 'HM': ' B m 1 1'}
Crystal system: Monoclinic
Setting: a1
+x,+y,+z
-x,+y,+z
          Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
 \{m_0yz \mid (0.0,0.0,0.0)\} \mid
                              -x,+y,+z
    \{1 \mid (0.5, 0.0, 0.5)\}
                         | +x+1/2, +y, +z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\} \mid -x+1/2,+y,+z+1/2
*******
space group: 8:a2 {'Hall': 'C -2x', 'HM': ' C m 1 1'}
Crystal system: Monoclinic
Setting: a2
+x,+y,+z
-x,+y,+z
          Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 \{m_0yz | (0.0,0.0,0.0)\} \mid
                              -x,+y,+z
    \{1|(0.5,0.5,0.0)\} +x+1/2,+y+1/2,+z
  \{m_0yz \mid (0.5, 0.5, 0.0)\} \mid -x+1/2, +y+1/2, +z
*******
space group: 8:a3 {'Hall': 'I -2x', 'HM': ' I m 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
-x,+y,+z
          Seitz
                                  Jones
```

```
{1|(0.0,0.0,0.0)}
                               +x,+y,+z
  \{m_0yz \mid (0.0,0.0,0.0)\} \mid
                               -x,+y,+z
    \{1 \mid (0.5, 0.5, 0.5)\} \mid +x+1/2, +y+1/2, +z+1/2 \mid
  \{m_0yz \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, +y+1/2, +z+1/2 \mid
*******
space group: 9:b1 {'Hall': 'C -2yc', 'HM': ' C 1 c 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
+x,-y,+z+1/2
         Seitz
                                Jones
 {1|(0.0,0.0,0.0)}
| \{m_x0z | (0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2 |
******
space group: 9:b2 {'Hall': 'A -2yac', 'HM': ' A 1 n 1'}
Crystal system: Monoclinic
Setting: b2
+X,+Y,+Z
+x+1/2,-y,+z+1/2
. . . . . . . . . . . . . . . . . . .
         Seitz
                              Jones
   \{1 \mid (0.0,0.0,0.0)\} \mid +x,+y,+z
 \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
   \{1|(0.0,0.5,0.5)\} +x,+y+1/2,+z+1/2 |
  \{m_x0z|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,+z \mid
*******
space group: 9:b3 {'Hall': 'I -2ya', 'HM': ' I 1 a 1'}
Crystal system: Monoclinic
Setting: b3
+x,+y,+z
+x+1/2,-y,+z
         Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
                          +x+1/2,-y,+z
| \{m_x0z|(0.5,0.0,0.0)\} |
   \{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2 |
```

```
|\{m_x0z|(0.0,0.5,0.5)\}| +x,-y+1/2,+z+1/2
*******
space group: 9:-b1 {'Hall': 'A -2ya', 'HM': 'A 1 a 1'}
Crystal system: Monoclinic
Setting: -b1
+x,+y,+z
+x+1/2,-y,+z
         Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
                           +x+1/2,-y,+z
 \{m_x0z|(0.5,0.0,0.0)\}
                        +x,+y+1/2,+z+1/2
   {1|(0.0,0.5,0.5)}
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
******
space group: 9:-b2 {'Hall': 'C -2ybc', 'HM': 'C 1 n 1'}
Crystal system: Monoclinic
Setting: -b2
+x,+y,+z
+x,-y+1/2,+z+1/2
                             Jones
         Seitz
   \{1 \mid (0.0, 0.0, 0.0)\}
                           +x,+y,+z
 \{m_x0z|(0.0,0.5,0.5)\} \mid +x,-y+1/2,+z+1/2
  \{1|(0.5,0.5,0.0)\} +x+1/2,+y+1/2,+z
| \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
*******
space group: 9:-b3 {'Hall': 'I -2yc', 'HM': 'I 1 c 1'}
Crystal system: Monoclinic
Setting: -b3
+x,+y,+z
+x,-y,+z+1/2
         Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                             +x,+y,+z
                        +x,-y,+z+1/2
 \{m_x0z|(0.0,0.0,0.5)\}
   \{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2 |
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z
```

```
space group: 9:c1 {'Hall': 'A -2a', 'HM': ' A 1 1 a'}
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
+x+1/2, +y, -z
        Seitz
                          Jones
| \{m_xy0 | (0.5,0.5,0.5)\} | +x+1/2,+y+1/2,-z+1/2 |
*******
space group: 9:c2 {'Hall': 'B -2bc', 'HM': ' B 1 1 n'}
Crystal system: Monoclinic
Setting: c2
+x,+y,+z
+x,+y+1/2,-z+1/2
        Seitz
                    l Jones
  \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
| \{m_xy0|(0.0,0.5,0.5)\} | +x,+y+1/2,-z+1/2 |
  \{1|(0.5,0.0,0.5)\} +x+1/2,+y,+z+1/2 |
| {m_xy0|(0.5,0.5,0.0)} | +x+1/2,+y+1/2,-z |
*******
space group: 9:c3 {'Hall': 'I -2b', 'HM': ' I 1 1 b'}
Crystal system: Monoclinic
Setting: c3
+x,+y,+z
+x,+y+1/2,-z
        Seitz
                          Jones
   {1|(0.0,0.0,0.0)}
                          +x,+y,+z
\{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2
 \{m_xy0 | (0.5,0.0,0.5)\} \mid +x+1/2,+y,-z+1/2
*******
```

space group: 9:-c1 {'Hall': 'B -2b', 'HM': 'B 1 1 b'}

```
Crystal system: Monoclinic
Setting: -c1
+x,+y,+z
+x, +y+1/2, -z
. . . . . . . . . . . . . . . . . . .
         Seitz
                               Jones
 {1|(0.0,0.0,0.0)}
 \{m_xy0|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,-z+1/2
*******
space group: 9:-c2 {'Hall': 'A -2ac', 'HM': 'A 1 1 n'}
Crystal system: Monoclinic
Setting: -c2
+x,+y,+z
+x+1/2, +y, -z+1/2
. . . . . . . . . . . . . . . . . . .
         Seitz
                             Jones
   {1|(0.0,0.0,0.0)} |
                          +x,+y,+z
| \{m_xy0|(0.5,0.0,0.5)\} | +x+1/2,+y,-z+1/2
   \{1|(0.0,0.5,0.5)\} | +x,+y+1/2,+z+1/2 |
| {m_xy0|(0.5,0.5,0.0)} | +x+1/2,+y+1/2,-z |
******
space group: 9:-c3 {'Hall': 'I -2a', 'HM': 'I 1 1 a'}
Crystal system: Monoclinic
Setting: -c3
+x,+y,+z
+x+1/2, +y, -z
         Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 \{m_xy0|(0.5,0.0,0.0)\}
                           +x+1/2,+y,-z
   \{1|(0.5,0.5,0.5)\} +x+1/2,+y+1/2,+z+1/2 |
 \{m_xy0|(0.0,0.5,0.5)\} +x,+y+1/2,-z+1/2
*******
space group: 9:a1 {'Hall': 'B -2xb', 'HM': ' B b 1 1'}
Crystal system: Monoclinic
Setting: a1
```

+x,+y,+z

```
-x,+y+1/2,+z
         Seitz
                              Jones
 \{m_0yz \mid (0.5,0.5,0.5)\} \mid -x+1/2,+y+1/2,+z+1/2 \mid
*******
space group: 9:a2 {'Hall': 'C -2xbc', 'HM': ' C n 1 1'}
Crystal system: Monoclinic
Setting: a2
+x,+y,+z
-x, +y+1/2, +z+1/2
. . . . . . . . . . . . . . . . . . . .
         Seitz
                      Jones
   \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
 \{m_0yz \mid (0.0,0.5,0.5)\} \mid -x,+y+1/2,+z+1/2 \mid
   \{1|(0.5,0.5,0.0)\} +x+1/2,+y+1/2,+z |
 \{m_0yz \mid (0.5,0.0,0.5)\} \mid -x+1/2,+y,+z+1/2 \mid
*******
space group: 9:a3 {'Hall': 'I -2xc', 'HM': ' I c 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
-x,+y,+z+1/2
         Seitz
                             Jones
\{1 \mid (0.5, 0.5, 0.5)\} \mid +x+1/2, +y+1/2, +z+1/2
| \{m_0yz | (0.5,0.5,0.0)\} | -x+1/2,+y+1/2,+z
*******
space group: 9:-a1 {'Hall': 'C -2xc', 'HM': 'C c 1 1'}
Crystal system: Monoclinic
Setting: -a1
+x,+y,+z
-x,+y,+z+1/2
```

```
Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                              -x, +y, +z+1/2
    {1|(0.5,0.5,0.0)}
                             +x+1/2,+y+1/2,+z
 \{m_0yz \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, +y+1/2, +z+1/2 \mid
******
space group: 9:-a2 {'Hall': 'B -2xbc', 'HM': 'B n 1 1'}
Crystal system: Monoclinic
Setting: -a2
+x,+y,+z
-x, +y+1/2, +z+1/2
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
  \{m_0yz \mid (0.0,0.5,0.5)\}\
                           -x, +y+1/2, +z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                           +x+1/2,+y,+z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}\
                           -x+1/2, +y+1/2, +z
******
space group: 9:-a3 {'Hall': 'I -2xb', 'HM': 'I b 1 1'}
Crystal system: Monoclinic
Setting: -a3
+x,+y,+z
-x,+y+1/2,+z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{m_0yz \mid (0.0, 0.5, 0.0)\} \mid
                               -x, +y+1/2, +z
    {1|(0.5,0.5,0.5)}
                         +x+1/2,+y+1/2,+z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}\
                             -x+1/2,+y,+z+1/2
*******
space group: 10:b {'Hall': ' -P 2y', 'HM': 'P 1 2/m 1'}
Crystal system: Monoclinic
Setting: b
+x,+y,+z
-x,+y,-z
          Seitz
                            Jones
    {1|(0.0,0.0,0.0)}
                         +x,+y,+z
```

```
\{2_0y0 \mid (0.0,0.0,0.0)\} \mid -x,+y,-z \mid
    \{-1 \mid (0.0,0.0,0.0)\} \mid -x,-y,-z \mid
  \{m_x0z|(0.0,0.0,0.0)\} \mid +x,-y,+z \mid
*******
space group: 10:c {'Hall': ' -P 2', 'HM': 'P 1 1 2/m'}
Crystal system: Monoclinic
Setting: c
+x,+y,+z
-x,-y,+z
                          | Jones
          Seitz
   {1|(0.0,0.0,0.0)}
                          +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\} \mid -x,-y,+z \mid
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z \mid
| {m_xy0|(0.0,0.0,0.0)} | +x,+y,-z |
*******
space group: 10:a {'Hall': ' -P 2x', 'HM': 'P 2/m 1 1'}
Crystal system: Monoclinic
Setting: a
+x,+y,+z
+x,-y,-z
                             Jones
          Seitz
   {1|(0.0,0.0,0.0)}
                         +x,+y,+z
  \{2_x00 \mid (0.0,0.0,0.0)\} \mid +x,-y,-z \mid
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z \mid
| {m_0yz|(0.0,0.0,0.0)} | -x,+y,+z |
******
space group: 11:b {'Hall': '-P 2yb', 'HM': 'P 1 21/m 1'}
Crystal system: Monoclinic
Setting: b
+x,+y,+z
-x,+y+1/2,-z
          Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
| \{2_0y0|(0.0,0.5,0.0)\} | -x,+y+1/2,-z |
    \{-1 \mid (0.0, 0.0, 0.0)\}
                            -x,-y,-z
 \{m_x0z|(0.0,0.5,0.0)\} \mid +x,-y+1/2,+z \mid
```

```
*******
space group: 11:c {'Hall': '-P 2c', 'HM': 'P 1 1 21/m'}
Crystal system: Monoclinic
Setting: c
+x,+y,+z
-x,-y,+z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                              Jones
   \{1 \mid (0.0,0.0,0.0)\} \mid +x,+y,+z
| \{2_{00z} | (0.0,0.0,0.5)\} | -x,-y,+z+1/2 |
   \{-1 \mid (0.0, 0.0, 0.0)\}
                           -x,-y,-z
| \{m_xy0|(0.0,0.0,0.5)\} | +x,+y,-z+1/2 |
*******
space group: 11:a {'Hall': '-P 2xa', 'HM': 'P 21/m 1 1'}
Crystal system: Monoclinic
Setting: a
+x,+y,+z
+x+1/2,-y,-z
                            Jones
          Seitz
   {1|(0.0,0.0,0.0)} |
                          +x,+y,+z
\{2_{x00}|(0.5,0.0,0.0)\} \mid +x+1/2,-y,-z
    \{-1 \mid (0.0,0.0,0.0)\} \mid -x,-y,-z
  \{m_0yz \mid (0.5,0.0,0.0)\} \mid -x+1/2,+y,+z \mid
*******
space group: 12:b1 {'Hall': ' -C 2y', 'HM': ' C 1 2/m 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
-x,+y,-z
                               Jones
          Seitz
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
  {2_0y0|(0.0,0.0,0.0)} |
                               -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid
                               -x,-y,-z
                            +x,-y,+z
  \{m_x0z | (0.0,0.0,0.0)\}
    \{1|(0.5,0.5,0.0)\} +x+1/2,+y+1/2,+z |
  \{2_0y0|(0.5,0.5,0.0)\} \mid -x+1/2,+y+1/2,-z \mid
    \{-1 \mid (0.5, 0.5, 0.0)\} \mid -x+1/2, -y+1/2, -z \mid
```

```
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z |
 . . . . . . . . . . . . . . . . . . .
*******
space group: 12:b2 {'Hall': ' -A 2y', 'HM': ' A 1 2/m 1'}
Crystal system: Monoclinic
Setting: b2
+x,+y,+z
-x,+y,-z
                                Seitz
                                                         | Jones
\{1 \mid (0.0,0.5,0.5)\} \mid +x,+y+1/2,+z+1/2 \mid \{2_0y0 \mid (0.0,0.5,0.5)\} \mid -x,+y+1/2,-z+1/2 \mid [2_0y0 \mid (0.0,0.5,0.5)] \mid -x,+y+1/2,-z+1/2 \mid -x,+y+1/2,
             \{-1 \mid (0.0, 0.5, 0.5)\} \mid -x, -y+1/2, -z+1/2 \mid
 |\{m_x0z|(0.0,0.5,0.5)\}| +x,-y+1/2,+z+1/2|
*******
space group: 12:b3 {'Hall': ' -I 2y', 'HM': ' I 1 2/m 1'}
Crystal system: Monoclinic
Setting: b3
+x,+y,+z
-x,+y,-z
                                Seitz | Jones
         {2_0y0|(0.0,0.0,0.0)} |
      {m_x0z|(0.0,0.0,0.0)} |
      \{-1 \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, -y+1/2, -z+1/2 \mid
 | \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2 |
*******
space group: 12:c1 {'Hall': ' -A 2', 'HM': ' A 1 1 2/m'}
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
-x,-y,+z
 . . . . . . . . . . . . . . . . . . . .
```

```
Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  {2_00z|(0.0,0.0,0.0)} |
                               -x,-y,+z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  {m_xy0|(0.0,0.0,0.0)} |
                               +x,+y,-z
    {1|(0.0,0.5,0.5)}
                          | +x,+y+1/2,+z+1/2 |
  \{2\_00z \mid (0.0,0.5,0.5)\} \mid -x,-y+1/2,+z+1/2
    \{-1 \mid (0.0, 0.5, 0.5)\}
                          | -x, -y+1/2, -z+1/2
 \{m_xy0|(0.0,0.5,0.5)\} \mid +x,+y+1/2,-z+1/2 \mid
*******
space group: 12:c2 {'Hall': ' -B 2', 'HM': ' B 1 1 2/m'}
Crystal system: Monoclinic
Setting: c2
+x,+y,+z
-x,-y,+z
```

Seitz	Jones
{1 (0.0,0.0,0.0)} {2_00z (0.0,0.0,0.0)} {-1 (0.0,0.0,0.0)} {m_xy0 (0.0,0.0,0.0)} {1 (0.5,0.0,0.5)} {2_00z (0.5,0.0,0.5)} {-1 (0.5,0.0,0.5)} {m_xy0 (0.5,0.0,0.5)}	+x,+y,+z -x,-y,+z -x,-y,-z +x,+y,-z +x+1/2,+y,+z+1/2 -x+1/2,-y,+z+1/2 -x+1/2,-y,-z+1/2 +x+1/2,+y,-z+1/2

space group: 12:c3 {'Hall': ' -I 2', 'HM': ' I 1 1 2/m'}

Crystal system: Monoclinic

Setting: c3 +x,+y,+z-x,-y,+z

	·
Seitz	Jones
{1 (0.0,0.0,0.0)} {2_00z (0.0,0.0,0.0)} {-1 (0.0,0.0,0.0)} {m_xy0 (0.0,0.0,0.0)} {1 (0.5,0.5,0.5)} {2_00z (0.5,0.5,0.5)} {-1 (0.5,0.5,0.5)} {m_xy0 (0.5,0.5,0.5)}	+x,+y,+z -x,-y,+z -x,-y,-z +x,+y,-z +x+1/2,+y+1/2,+z+1/2 -x+1/2,-y+1/2,+z+1/2 -x+1/2,-y+1/2,-z+1/2 +x+1/2,+y+1/2,-z+1/2

```
space group: 12:a1 {'Hall': ' -B 2x', 'HM': ' B 2/m 1 1'}
Crystal system: Monoclinic
Setting: a1
+x,+y,+z
+x,-y,-z
           Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                                +X,+Y,+Z
 {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
 {m_0yz|(0.0,0.0,0.0)} |
                               -x,+y,+z
    {1|(0.5,0.0,0.5)}
                          +x+1/2,+y,+z+1/2
  \{2_x00|(0.5,0.0,0.5)\} \mid +x+1/2,-y,-z+1/2
    \{-1 \mid (0.5, 0.0, 0.5)\} \mid -x+1/2, -y, -z+1/2 \mid
  \{m_0yz \mid (0.5,0.0,0.5)\} \mid -x+1/2,+y,+z+1/2 \mid
*******
space group: 12:a2 {'Hall': ' -C 2x', 'HM': ' C 2/m 1 1'}
Crystal system: Monoclinic
Setting: a2
+x,+y,+z
+x,-y,-z
           Seitz
                                 Jones
                                +x,+y,+z
   {1|(0.0,0.0,0.0)}
 \{2 \times 00 \mid (0.0, 0.0, 0.0)\} \mid
                                +x,-y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\} \mid
                                -x,+y,+z
    \{1|(0.5,0.5,0.0)\} +x+1/2,+y+1/2,+z |
  \{2_x00|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,-z \mid
    \{-1 \mid (0.5, 0.5, 0.0)\}
                          | -x+1/2, -y+1/2, -z |
 \{m_0yz \mid (0.5, 0.5, 0.0)\} \mid -x+1/2, +y+1/2, +z \mid
*******
space group: 12:a3 {'Hall': ' -I 2x', 'HM': ' I 2/m 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
+x,-y,-z
    . . . . . . . . . . . . . . . .
           Seitz
                                   Jones
  {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
```

```
{2_x00|(0.0,0.0,0.0)} |
                                  +x,-y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\} \mid
                                  -x,+y,+z
    \{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2
  \{2_x00|(0.5,0.5,0.5)\} \mid +x+1/2,-y+1/2,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, -y+1/2, -z+1/2 \mid
 \{m_0yz \mid (0.5,0.5,0.5)\} \mid -x+1/2,+y+1/2,+z+1/2 \mid
*******
space group: 13:b1 {'Hall': ' -P 2yc', 'HM': ' P 1 2/c 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
-x,+y,-z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                               Jones
    {1|(0.0,0.0,0.0)}
                             +x,+y,+z
 \{2_0y0|(0.0,0.0,0.5)\} \mid -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                            -x,-y,-z
 \{m_x0z|(0.0,0.0,0.5)\} | +x,-y,+z+1/2
*******
space group: 13:b2 {'Hall': ' -P 2yac', 'HM': ' P 1 2/n 1'}
Crystal system: Monoclinic
Setting: b2
+x,+y,+z
-x+1/2,+y,-z+1/2
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
 \{2_0y0|(0.5,0.0,0.5)\} \mid -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
 \{m_x0z|(0.5,0.0,0.5)\} \mid +x+1/2,-y,+z+1/2 \mid
*******
space group: 13:b3 {'Hall': ' -P 2ya', 'HM': ' P 1 2/a 1'}
Crystal system: Monoclinic
Setting: b3
+x,+y,+z
-x+1/2,+y,-z
          Seitz
                               Jones
```

```
{1|(0.0,0.0,0.0)}
                           +x,+y,+z
  \{2_0y0|(0.5,0.0,0.0)\} \mid -x+1/2,+y,-z \mid
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z
  \{m_x0z|(0.5,0.0,0.0)\} \mid +x+1/2,-y,+z \mid
*******
space group: 13:c1 {'Hall': ' -P 2a', 'HM': ' P 1 1 2/a'}
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
-x+1/2,-y,+z
          Seitz
                               Jones
    \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
  \{2\_00z \mid (0.5,0.0,0.0)\} \mid -x+1/2,-y,+z
  \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z
| \{m_xy0|(0.5,0.0,0.0)\} | +x+1/2,+y,-z |
******
space group: 13:c2 {'Hall': ' -P 2ab', 'HM': ' P 1 1 2/n'}
Crystal system: Monoclinic
Setting: c2
+X,+Y,+Z
-x+1/2, -y+1/2, +z
. . . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 \{2\_00z | (0.5,0.5,0.0)\} \mid -x+1/2,-y+1/2,+z \mid
    \{-1 \mid (0.0, 0.0, 0.0)\}
                             -x,-y,-z
  \{m_xy0|(0.5,0.5,0.0)\} \mid +x+1/2,+y+1/2,-z \mid
*******
space group: 13:c3 {'Hall': ' -P 2b', 'HM': ' P 1 1 2/b'}
Crystal system: Monoclinic
Setting: c3
+x,+y,+z
-x,-y+1/2,+z
    . . . . . . . . . . . . . . . .
          Seitz
                               Jones
                          | +x,+y,+z
   {1|(0.0,0.0,0.0)}
| \{2_{00z} | (0.0, 0.5, 0.0)\} | -x, -y+1/2, +z
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z
```

```
| \{m_xy0|(0.0,0.5,0.0)\} | +x,+y+1/2,-z |
. . . . . . . . . . . . . . . . . . . .
*******
space group: 13:a1 {'Hall': ' -P 2xb', 'HM': ' P 2/b 1 1'}
Crystal system: Monoclinic
Setting: a1
+x,+y,+z
+x,-y+1/2,-z
          Seitz
                               Jones
   \{1 \mid (0.0, 0.0, 0.0)\} + x, +y, +z
| \{2_x00|(0.0,0.5,0.0)\} | +x,-y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z
  \{m_0yz \mid (0.0,0.5,0.0)\} \mid -x,+y+1/2,+z \mid
******
space group: 13:a2 {'Hall': ' -P 2xbc', 'HM': ' P 2/n 1 1'}
Crystal system: Monoclinic
Setting: a2
+x,+y,+z
+x,-y+1/2,-z+1/2
          Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
\{2_x00|(0.0,0.5,0.5)\} \mid +x,-y+1/2,-z+1/2 \mid
  \overline{\{-1 \mid (0.0,0.0,0.0)\}} \quad | \quad -x,-y,-z
| \{m_0yz | (0.0,0.5,0.5)\} | -x,+y+1/2,+z+1/2 |
 . . . . . . . . . . . . . . . . . . .
*******
space group: 13:a3 {'Hall': ' -P 2xc', 'HM': ' P 2/c 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
+x,-y,-z+1/2
                            Jones
          Seitz
   \{1 \mid (0.0, 0.0, 0.0)\} + x, +y, +z
  {2_x00|(0.0,0.0,0.5)} |
                            +x,-y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z
| \{m_0yz | (0.0,0.0,0.5)\} | -x,+y,+z+1/2 |
```

```
*******
space group: 14:b1 {'Hall': '-P 2ybc', 'HM': ' P 1 21/c 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
-x, +y+1/2, -z+1/2
. . . . . . . . . . . . . . . . . . . .
                      Jones
  \{1 \mid (0.0,0.0,0.0)\} + x,+y,+z
| \{2_0y0|(0.0,0.5,0.5)\} | -x,+y+1/2,-z+1/2 |
\{-1 \mid (0.0,0.0,0.0)\} \mid -x,-y,-z
| \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2 |
*******
space group: 14:b2 {'Hall': '-P 2yn', 'HM': ' P 1 21/n 1'}
Crystal system: Monoclinic
Setting: b2
+x,+y,+z
-x+1/2,+y+1/2,-z+1/2
         Seitz | Jones
 \{1 \mid (0.0, 0.0, 0.0)\} + x, +y, +z
| \{m_x0z | (0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2 |
*******
space group: 14:b3 {'Hall': '-P 2yab', 'HM': ' P 1 21/a 1'}
Crystal system: Monoclinic
Setting: b3
+x,+y,+z
-x+1/2,+y+1/2,-z
         Seitz | Jones
   \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
| \{2_0y0|(0.5,0.5,0.0)\} | -x+1/2,+y+1/2,-z |
   \{-1 \mid (0.0,0.0,0.0)\} \mid -x,-y,-z
 \{m_x0z|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,+z \mid
```

space group: 14:c1 {'Hall': '-P 2ac', 'HM': ' P 1 1 21/a'}

```
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
-x+1/2, -y, +z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                               +x,+y,+z
\{2\_00z|(0.5,0.0,0.5)\}\ |\ -x+1/2,-y,+z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z
  \{m_xy0 \mid (0.5,0.0,0.5)\} \mid +x+1/2,+y,-z+1/2 \mid
*******
space group: 14:c2 {'Hall': '-P 2n', 'HM': ' P 1 1 21/n'}
Crystal system: Monoclinic
Setting: c2
+x,+y,+z
-x+1/2, -y+1/2, +z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                  Jones
   {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
| {2_00z|(0.5,0.5,0.5)} | -x+1/2,-y+1/2,+z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid
                               -x,-y,-z
| \{m_xy0 | (0.5, 0.5, 0.5)\} | +x+1/2, +y+1/2, -z+1/2 |
******
space group: 14:c3 {'Hall': '-P 2bc', 'HM': ' P 1 1 21/b'}
Crystal system: Monoclinic
Setting: c3
+x,+y,+z
-x,-y+1/2,+z+1/2
          Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 \{2_{00z} | (0.0, 0.5, 0.5)\} \mid
                           -x,-y+1/2,+z+1/2
   \{-1 \mid (0.0, 0.0, 0.0)\}
                            -x,-y,-z
 \{m_xy0|(0.0,0.5,0.5)\} \mid +x,+y+1/2,-z+1/2
*******
space group: 14:a1 {'Hall': '-P 2xab', 'HM': ' P 21/b 1 1'}
Crystal system: Monoclinic
Setting: a1
```

+x,+y,+z

```
+x+1/2,-y+1/2,-z
 . . . . . . . . . . . . . . . . . . .
         Seitz
                         Jones
  \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
\{2_x00|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,-z \mid
  \{-1 \mid (0.0,0.0,0.0)\} \mid -x,-y,-z
| {m_0yz|(0.5,0.5,0.0)} | -x+1/2,+y+1/2,+z |
*******
space group: 14:a2 {'Hall': '-P 2xn', 'HM': ' P 21/n 1 1'}
Crystal system: Monoclinic
Setting: a2
+x,+y,+z
+x+1/2,-y+1/2,-z+1/2
Seitz
                 | Jones
   \{1 \mid (0.0, 0.0, 0.0)\} + x, +y, +z
| \{2_x00|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,-z+1/2 |
  \{-1 \mid (0.0,0.0,0.0)\} \mid -x,-y,-z
|\{m_0yz|(0.5,0.5,0.5)\}|-x+1/2,+y+1/2,+z+1/2|
*******
space group: 14:a3 {'Hall': '-P 2xac', 'HM': ' P 21/c 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
+x+1/2,-y,-z+1/2
. . . . . . . . . . . . . . . . . . . .
                 | Jones
         Seitz
  \{1 \mid (0.0, 0.0, 0.0)\} \mid +x,+y,+z
\{2_x00|(0.5,0.0,0.5)\} \mid +x+1/2,-y,-z+1/2 \mid
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid -x, -y, -z
| \{m_0yz | (0.5,0.0,0.5)\} | -x+1/2,+y,+z+1/2 |
*******
space group: 15:b1 {'Hall': ' -C 2yc', 'HM': ' C 1 2/c 1'}
Crystal system: Monoclinic
Setting: b1
+x,+y,+z
-x,+y,-z+1/2
```

```
Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  {2_0y0|(0.0,0.0,0.5)} |
                               -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid
                                 -x,-y,-z
  \{m_x0z | (0.0,0.0,0.5)\}
                               +x,-y,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                             +x+1/2,+y+1/2,+z
  \{2_0y0|(0.5,0.5,0.5)\} \mid -x+1/2,+y+1/2,-z+1/2 \mid
    \{-1 \mid (0.5, 0.5, 0.0)\}
                             -x+1/2,-y+1/2,-z
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 15:b2 {'Hall': ' -A 2yac', 'HM': ' A 1 2/n 1'}
Crystal system: Monoclinic
```

Setting: b2 +x,+y,+z

-x+1/2,+y,-z+1/2

Seitz	Jones
{1 (0.0,0.0,0.0)}	+x,+y,+z
{2_0y0 (0.5,0.0,0.5)}	-x+1/2,+y,-z+1/2
{-1 (0.0,0.0,0.0)}	-x,-y,-z
{m_x0z (0.5,0.0,0.5)}	+x+1/2,-y,+z+1/2
{1 (0.0,0.5,0.5)}	+x,+y+1/2,+z+1/2
{2_0y0 (0.5,0.5,0.0)}	-x+1/2,+y+1/2,-z
{-1 (0.0,0.5,0.5)}	-x,-y+1/2,-z+1/2
{m_x0z (0.5,0.5,0.0)}	+x+1/2,-y+1/2,+z

.

space group: 15:b3 {'Hall': ' -I 2ya', 'HM': ' I 1 2/a 1'}

Crystal system: Monoclinic

Setting: b3 +x,+y,+z-x+1/2,+y,-z

· · · · · · · · · · · · · · · · · · ·	·
Seitz	Jones
{1 (0.0,0.0,0.0)} {2_0y0 (0.5,0.0,0.0)} {-1 (0.0,0.0,0.0)} {m_x0z (0.5,0.0,0.0)} {1 (0.5,0.5,0.5)} {2_0y0 (0.0,0.5,0.5)} {-1 (0.5,0.5,0.5)} {m_x0z (0.0,0.5,0.5)}	+x,+y,+z -x+1/2,+y,-z -x,-y,-z +x+1/2,-y,+z +x+1/2,+y+1/2,+z+1/2 -x,+y+1/2,-z+1/2 -x+1/2,-y+1/2,-z+1/2 +x,-y+1/2,+z+1/2

```
space group: 15:-b1 {'Hall': ' -A 2ya', 'HM': 'A 1 2/a 1'}
Crystal system: Monoclinic
Setting: -b1
+x,+y,+z
-x+1/2,+y,-z
                                Jones
   {1|(0.0,0.0,0.0)}
                               +x,+y,+z
 {2_0y0|(0.5,0.0,0.0)} |
                             -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{m_x0z|(0.5,0.0,0.0)\}
                             +x+1/2,-y,+z
                           +x,+y+1/2,+z+1/2
    {1|(0.0,0.5,0.5)}
  \{2_0y0|(0.5,0.5,0.5)\}
                          -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.5, 0.5)\} \mid -x, -y+1/2, -z+1/2
  \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 15:-b2 {'Hall': ' -C 2ybc', 'HM': 'C 1 2/n 1'}
Crystal system: Monoclinic
Setting: -b2
+x,+y,+z
-x, +y+1/2, -z+1/2
  . . . . . . . . . . . . . . . . . .
          Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                             +x,+y,+z
  {2 0y0|(0.0,0.5,0.5)} |
                          -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid
                           -x,-y,-z
  \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
    {1|(0.5,0.5,0.0)}
                        +x+1/2,+y+1/2,+z
  \{2_0y0|(0.5,0.0,0.5)\} \mid -x+1/2,+y,-z+1/2 \mid
    \{-1 \mid (0.5, 0.5, 0.0)\}
                        | -x+1/2, -y+1/2, -z |
 \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2 |
*******
space group: 15:-b3 {'Hall': ' -I 2yc', 'HM': 'I 1 2/c 1'}
Crystal system: Monoclinic
Setting: -b3
+x,+y,+z
-x,+y,-z+1/2
    Seitz
                                Jones
  {1|(0.0,0.0,0.0)}
                                +x,+y,+z
```

```
{2_0y0|(0.0,0.0,0.5)} |
                                 -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                 +x,-y,+z+1/2
                            +x+1/2, +y+1/2, +z+1/2
    \{1 \mid (0.5, 0.5, 0.5)\}
  {2_0y0|(0.5,0.5,0.0)}
                               -x+1/2,+y+1/2,-z
    \{-1 \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, -y+1/2, -z+1/2
  \{m_x0z|(0.5,0.5,0.0)\}
                               +x+1/2,-y+1/2,+z
*******
space group: 15:c1 {'Hall': ' -A 2a', 'HM': ' A 1 1 2/a'}
Crystal system: Monoclinic
Setting: c1
+x,+y,+z
-x+1/2, -y, +z
. . . . . . . . . . . . . .
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {2_00z|(0.5,0.0,0.0)} |
                                 -x+1/2,-y,+z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  {m_xy0|(0.5,0.0,0.0)}
                                 +x+1/2,+y,-z
    \{1 \mid (0.0, 0.5, 0.5)\}
                               +x, +y+1/2, +z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\} \mid
                            -x+1/2,-y+1/2,+z+1/2
    \{-1 \mid (0.0, 0.5, 0.5)\}
                               -x,-y+1/2,-z+1/2
 \{m_xy0|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,-z+1/2
******
space group: 15:c2 {'Hall': ' -B 2bc', 'HM': ' B 1 1 2/n'}
Crystal system: Monoclinic
Setting: c2
+x,+y,+z
-x,-y+1/2,+z+1/2
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +X,+Y,+Z
  {2_00z|(0.0,0.5,0.5)} |
                            -x,-y+1/2,+z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.0,0.5,0.5)\}
                            +x, +y+1/2, -z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2,+y,+z+1/2
  \{2_{00z}|(0.5,0.5,0.0)\}
                            -x+1/2,-y+1/2,+z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                            -x+1/2,-y,-z+1/2
  \{m_xy0|(0.5,0.5,0.0)\} | +x+1/2,+y+1/2,-z
```

space group: 15:c3 {'Hall': ' -I 2b', 'HM': ' I 1 1 2/b'}

```
Crystal system: Monoclinic
Setting: c3
+x,+y,+z
-x,-y+1/2,+z
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{2\_00z \mid (0.0, 0.5, 0.0)\}
                                 -x,-y+1/2,+z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                                 +x,+y+1/2,-z
    \{1|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, +z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                              -x+1/2,-y,+z+1/2
    \{-1 \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, -y+1/2, -z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                              +x+1/2,+y,-z+1/2
*******
space group: 15:-c1 {'Hall': ' -B 2b', 'HM': 'B 1 1 2/b'}
Crystal system: Monoclinic
Setting: -c1
+x,+y,+z
-x,-y+1/2,+z
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {2_00z|(0.0,0.5,0.0)} |
                                 -x,-y+1/2,+z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                                 +x,+y+1/2,-z
    \{1 \mid (0.5, 0.0, 0.5)\}
                              +x+1/2,+y,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, -y+1/2, +z+1/2
    \{-1 \mid (0.5, 0.0, 0.5)\}
                              -x+1/2, -y, -z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2,+y+1/2,-z+1/2
******
space group: 15:-c2 {'Hall': ' -A 2ac', 'HM': 'A 1 1 2/n'}
Crystal system: Monoclinic
Setting: -c2
+x,+y,+z
-x+1/2,-y,+z+1/2
```

_		L	ı
į	Seitz	Jones	ļ
+	{1 (0.0,0.0,0.0)} {2_00z (0.5,0.0,0.5)}	+x,+y,+z -x+1/2,-y,+z+1/2	<u> </u>
	{-1 (0.0,0.0,0.0)} {m xv0 (0.5.0.0.0.5)}	-x,-y,-z +x+1/2.+vz+1/2	

```
| +x,+y+1/2,+z+1/2 |
    {1|(0.0,0.5,0.5)}
  \{2\_00z \mid (0.5,0.5,0.0)\} \mid -x+1/2,-y+1/2,+z \mid
    \{-1 \mid (0.0, 0.5, 0.5)\} \mid -x, -y+1/2, -z+1/2 \mid
  \{m_xy0|(0.5,0.5,0.0)\} \mid +x+1/2,+y+1/2,-z \mid
*******
space group: 15:-c3 {'Hall': '-I 2a', 'HM': 'I 1 1 2/a'}
Crystal system: Monoclinic
Setting: -c3
+x,+y,+z
-x+1/2,-y,+z
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{2_{00z}|(0.5,0.0,0.0)\}
                                -x+1/2,-y,+z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                                +x+1/2,+y,-z
    \{1 \mid (0.5, 0.5, 0.5)\}
                          +x+1/2,+y+1/2,+z+1/2
  \{2_{00z} | (0.0, 0.5, 0.5)\}
                             -x,-y+1/2,+z+1/2
    \{-1 \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, -y+1/2, -z+1/2
                              +x,+y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
*******
space group: 15:a1 {'Hall': ' -B 2xb', 'HM': ' B 2/b 1 1'}
Crystal system: Monoclinic
Setting: a1
+x,+y,+z
+x,-y+1/2,-z
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
  \{2_{x00}|(0.0,0.5,0.0)\}
                                 +x,-y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_0yz \mid (0.0, 0.5, 0.0)\}
                                -x,+y+1/2,+z
    \{1|(0.5,0.0,0.5)\}
                              +x+1/2,+y,+z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
                              -x+1/2,-y,-z+1/2
    \{-1 \mid (0.5, 0.0, 0.5)\}
  \{m_0yz \mid (0.5, 0.5, 0.5)\} \mid
                            -x+1/2, +y+1/2, +z+1/2
*******
space group: 15:a2 {'Hall': ' -C 2xbc', 'HM': ' C 2/n 1 1'}
Crystal system: Monoclinic
Setting: a2
```

+x,+y,+z

```
+x,-y+1/2,-z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2_x00|(0.0,0.5,0.5)\} \mid +x,-y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_0yz \mid (0.0, 0.5, 0.5)\}
                              -x, +y+1/2, +z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                              +x+1/2,+y+1/2,+z
  \{2_{\times}00 \mid (0.5, 0.0, 0.5)\}
                              +x+1/2,-y,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                              -x+1/2, -y+1/2, -z
 \{m_0yz \mid (0.5,0.0,0.5)\} \mid -x+1/2,+y,+z+1/2 \mid
*******
space group: 15:a3 {'Hall': ' -I 2xc', 'HM': ' I 2/c 1 1'}
Crystal system: Monoclinic
Setting: a3
+x,+y,+z
+x,-y,-z+1/2
           Seitz
                                      Jones
    {1|(0.0,0.0,0.0)}
                                     +x,+y,+z
  {2_x00|(0.0,0.0,0.5)} |
                                  +x,-y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                     -x,-y,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}\ |
                                  -x,+y,+z+1/2
    \{1 \mid (0.5, 0.5, 0.5)\}
                              +x+1/2, +y+1/2, +z+1/2
  \{2_{\times}00 \mid (0.5, 0.5, 0.0)\}\ \mid
                              +x+1/2,-y+1/2,-z
    \{-1 \mid (0.5, 0.5, 0.5)\}
                              -x+1/2, -y+1/2, -z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\} \mid
                                -x+1/2,+y+1/2,+z
*******
space group: 15:-a1 {'Hall': ' -C 2xc', 'HM': 'C 2/c 1 1'}
Crystal system: Monoclinic
Setting: -a1
+X,+Y,+Z
+x,-y,-z+1/2
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                     +x,+y,+z
  \{2_{x00}|(0.0,0.0,0.5)\}
                                  +x,-y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                     -x,-y,-z
  \{m_0yz \mid (0.0,0.0,0.5)\} \mid
                                  -x,+y,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                                +x+1/2,+y+1/2,+z
  \{2_{x00} | (0.5, 0.5, 0.5)\}
                              +x+1/2,-y+1/2,-z+1/2
```

-x+1/2,-y+1/2,-z

 $\{-1 \mid (0.5, 0.5, 0.0)\}$

```
| \{m_0yz | (0.5,0.5,0.5)\} | -x+1/2,+y+1/2,+z+1/2 |
. . . . . . . . . . . . . . . . . . .
*******
space group: 15:-a2 {'Hall': ' -B 2xbc', 'HM': 'B 2/n 1 1'}
Crystal system: Monoclinic
Setting: -a2
+x,+y,+z
+x,-y+1/2,-z+1/2
    . . . . . . . . . . . . . . . .
                                 Jones
          Seitz
   \{1 \mid (0.0, 0.0, 0.0)\} + x, +y, +z
 \{2_x00|(0.0,0.5,0.5)\} \mid +x,-y+1/2,-z+1/2 \mid
    \{-1 \mid (0.0,0.0,0.0)\} \mid -x,-y,-z
  \{m_0yz \mid (0.0,0.5,0.5)\} \mid -x,+y+1/2,+z+1/2
  \{1|(0.5,0.0,0.5)\}\ | +x+1/2,+y,+z+1/2 | \{2_x00|(0.5,0.5,0.0)\}\ | +x+1/2,-y+1/2,-z |
    \{-1 \mid (0.5, 0.0, 0.5)\} \mid -x+1/2, -y, -z+1/2 \mid
| \{m_0yz | (0.5,0.5,0.0)\} | -x+1/2,+y+1/2,+z |
*******
space group: 15:-a3 {'Hall': ' -I 2xb', 'HM': 'I 2/b 1 1'}
Crystal system: Monoclinic
Setting: -a3
+x,+y,+z
+x,-y+1/2,-z
          Seitz
                          | Jones
   {1|(0.0,0.0,0.0)} |
                               +x,+y,+z
  {2_x00|(0.0,0.5,0.0)} |
                               +x,-y+1/2,-z
   \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
                             -x, +y+1/2, +z
  {m_0yz|(0.0,0.5,0.0)} |
    \{1|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,+z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\} | +x+1/2,-y,-z+1/2
    \{-1|(0.5,0.5,0.5)\} | -x+1/2,-y+1/2,-z+1/2
| \{m_0yz | (0.5,0.0,0.5)\} | -x+1/2,+y,+z+1/2
******
space group: 16 {'Hall': 'P 2 2', 'HM': 'P 2 2 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z
. . . . . . . . . . . . . . . . . . . .
```

```
Seitz
                           Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                          +x,+y,+z
  {2_00z|(0.0,0.0,0.0)} |
                          -x,-y,+z
 \{2_x00|(0.0,0.0,0.0)\} \mid +x,-y,-z \mid
| \{2_0y0|(0.0,0.0,0.0)\} | -x,+y,-z |
******
space group: 17 {'Hall': ' P 2c 2', 'HM': 'P 2 2 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z+1/2
+x,-y,-z
          Seitz
                             Jones
    {1|(0.0,0.0,0.0)}
                           +x,+y,+z
 {2_00z|(0.0,0.0,0.5)} |
                          -x,-y,+z+1/2
| {2_x00|(0.0,0.0,0.0)} |
                           +x,-y,-z
 \{2_0y0|(0.0,0.0,0.5)\} \mid -x,+y,-z+1/2
******
space group: 17:cab {'Hall': ' P 2a 2a', 'HM': 'P 21 2 2'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2, -y, +z
+x+1/2,-y,-z
          Seitz
                             Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
| \{2_{00z} | (0.5, 0.0, 0.0)\} | -x+1/2, -y, +z
| \{2_x00|(0.5,0.0,0.0)\} | +x+1/2,-y,-z
  {2_0y0|(0.0,0.0,0.0)} |
                            -x,+y,-z
*******
space group: 17:bca {'Hall': ' P 2 2b', 'HM': 'P 2 21 2'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y,+z
+x,-y+1/2,-z
. . . . . . . . . . . . . . . . . . .
                             Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                           +x,+y,+z
 \{2\_00z \mid (0.0,0.0,0.0)\} \mid -x,-y,+z
 \{2_x00|(0.0,0.5,0.0)\} \mid +x,-y+1/2,-z
| \{2_0y0|(0.0,0.5,0.0)\} | -x,+y+1/2,-z |
. . . . . . . . . . . . . . . . . . . .
*******
space group: 18 {'Hall': 'P 2 2ab', 'HM': 'P 21 21 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x+1/2,-y+1/2,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                               +x,+y,+z
                            -x,-y,+z
  {2_00z|(0.0,0.0,0.0)} |
| {2_x00|(0.5,0.5,0.0)} | +x+1/2,-y+1/2,-z |
\{2_0y0|(0.5,0.5,0.0)\} \mid -x+1/2,+y+1/2,-z \mid
*******
space group: 18:cab {'Hall': 'P 2bc 2', 'HM': 'P 2 21 21'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
| {2_00z|(0.0,0.5,0.5)} | -x,-y+1/2,+z+1/2 |
 {2_x00|(0.0,0.0,0.0)} |
                           +x,-y,-z
| \{2_0y0|(0.0,0.5,0.5)\} | -x,+y+1/2,-z+1/2
*******
space group: 18:bca {'Hall': 'P 2ac 2ac', 'HM': 'P 21 2 21'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x+1/2, -y, +z+1/2
+x+1/2,-y,-z+1/2
          Seitz
                                 Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
 \{2\_00z \mid (0.5,0.0,0.5)\} \mid -x+1/2,-y,+z+1/2 \mid
| \{2_x00|(0.5,0.0,0.5)\} | +x+1/2,-y,-z+1/2 |
| \{2_0y0|(0.0,0.0,0.0)\} | -x,+y,-z
*******
space group: 19 {'Hall': ' P 2ac 2ab', 'HM': 'P 21 21 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2, -y, +z+1/2
+x+1/2,-y+1/2,-z
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\} + x, +y, +z
\{2\_00z|(0.5,0.0,0.5)\} | -x+1/2,-y,+z+1/2
| \{2_x00|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,-z |
\{2_0y0|(0.0,0.5,0.5)\}\ |\ -x,+y+1/2,-z+1/2\ |
******
space group: 20 {'Hall': ' C 2c 2', 'HM': 'C 2 2 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z+1/2
+x,-y,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
 \{2\_00z \mid (0.0,0.0,0.5)\}\
                               -x,-y,+z+1/2
 {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
 {2_0y0|(0.0,0.0,0.5)} |
                               -x,+y,-z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                             +x+1/2,+y+1/2,+z
| \{2_{00z} | (0.5, 0.5, 0.5)\} | -x+1/2, -y+1/2, +z+1/2
| \{2_x00|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,-z
| \{2_0y0|(0.5,0.5,0.5)\} | -x+1/2,+y+1/2,-z+1/2
. . . . . . . . . . . . . . . . . . .
*******
space group: 20:cab {'Hall': ' A 2a 2a', 'HM': 'A 21 2 2'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2,-y,+z
+x+1/2,-y,-z
. . . . . . . . . . . . . . . . . . . .
```

```
Seitz
                                     Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
  \{2\ 00z \mid (0.5,0.0,0.0)\}
                                 -x+1/2, -y, +z
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                                 +x+1/2,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                   -x,+y,-z
    \{1 \mid (0.0, 0.5, 0.5)\}
                               +x, +y+1/2, +z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, +z+1/2
  \{2_{x00} | (0.5, 0.5, 0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
  \{2_0y0|(0.0,0.5,0.5)\}
                               -x,+y+1/2,-z+1/2
*******
space group: 20:bca {'Hall': ' B 2 2b', 'HM': 'B 2 21 2'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y,+z
+x,-y+1/2,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                   -x,-y,+z
  \{2_{x00} | (0.0, 0.5, 0.0)\}
                                 +x,-y+1/2,-z
  {2_0y0|(0.0,0.5,0.0)}
                                 -x,+y+1/2,-z
    \{1 \mid (0.5, 0.0, 0.5)\}
                               +x+1/2,+y,+z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                               -x+1/2,-y,+z+1/2
                             +x+1/2,-y+1/2,-z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
  {2_0y0|(0.5,0.5,0.5)}
                             -x+1/2,+y+1/2,-z+1/2
*******
space group: 21 {'Hall': 'C 2 2', 'HM': 'C 2 2 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z
           Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
  \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
    \{1 \mid (0.5, 0.5, 0.0)\}
                             +x+1/2, +y+1/2, +z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                             -x+1/2, -y+1/2, +z
  \{2_{x00}|(0.5,0.5,0.0)\}
                             +x+1/2,-y+1/2,-z
  {2_0y0|(0.5,0.5,0.0)}
                             -x+1/2,+y+1/2,-z
```

.

```
******
```

space group: 21:cab {'Hall': 'A 2 2', 'HM': 'A 2 2 2'}

Crystal system: Orthorhombic

Setting: cab +x,+y,+z -x,-y,+z +x,-y,-z

.......

++ Seitz	Jones
{1 (0.0,0.0,0.0)}	+x,+y,+z
{2_00z (0.0,0.0,0.0)}	-x,-y,+z
{2_x00 (0.0,0.0,0.0)}	+x,-y,-z
{2_0y0 (0.0,0.0,0.0)}	-x,+y,-z
{1 (0.0,0.5,0.5)}	+x,+y+1/2,+z+1/2
{2_00z (0.0,0.5,0.5)}	-x,-y+1/2,+z+1/2
{2_x00 (0.0,0.5,0.5)}	+x,-y+1/2,-z+1/2
{2_0y0 (0.0,0.5,0.5)}	-x,+y+1/2,-z+1/2

.......

space group: 21:bca {'Hall': 'B 2 2', 'HM': 'B 2 2 2'}

Crystal system: Orthorhombic

Setting: bca +x,+y,+z -x,-y,+z +x,-y,-z

.

+	Jones
{1 (0.0,0.0,0.0)} {2_00z (0.0,0.0,0.0)} {2_x00 (0.0,0.0,0.0)} {2_0y0 (0.0,0.0,0.0)} {1 (0.5,0.0,0.5)} {2_00z (0.5,0.0,0.5)} {2_x00 (0.5,0.0,0.5)} {2_0y0 (0.5,0.0,0.5)}	+x,+y,+z -x,-y,+z +x,-y,-z -x,+y,-z +x+1/2,+y,+z+1/2 -x+1/2,-y,+z+1/2 +x+1/2,-y,-z+1/2 -x+1/2,+y,-z+1/2

```
******
```

space group: 22 {'Hall': 'F 2 2', 'HM': 'F 2 2 2'}

Crystal system: Orthorhombic

+x,+y,+z

-x,-y,+z +x,-y,-z

+----+

```
Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  {2 00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
  \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
    \{1|(0.0,0.5,0.5)\}
                             +x, +y+1/2, +z+1/2
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                             -x,-y+1/2,+z+1/2
  \{2_{x00} | (0.0, 0.5, 0.5)\}
                             +x,-y+1/2,-z+1/2
  \{2_0y0|(0.0,0.5,0.5)\}
                             -x, +y+1/2, -z+1/2
                             +x+1/2, +y, +z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
  \{2_{00z} | (0.5, 0.0, 0.5)\}
                             -x+1/2, -y, +z+1/2
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                             +x+1/2,-y,-z+1/2
  \{2\_0y0|(0.5,0.0,0.5)\}
                             -x+1/2,+y,-z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                             +x+1/2, +y+1/2, +z
                             -x+1/2, -y+1/2, +z
  \{2_{00z} | (0.5, 0.5, 0.0)\}
  \{2_{x00}|(0.5,0.5,0.0)\}
                             +x+1/2,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\}
                             -x+1/2,+y+1/2,-z
******
space group: 23 {'Hall': 'I 2 2', 'HM': 'I 2 2 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                    -x,-y,+z
  \{2 \times 00 \mid (0.0, 0.0, 0.0)\}
                                    +x,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                    -x,+y,-z
                             +x+1/2, +y+1/2, +z+1/2
    \{1 \mid (0.5, 0.5, 0.5)\}
  {2_00z|(0.5,0.5,0.5)}
                             -x+1/2,-y+1/2,+z+1/2
  \{2_{x00} | (0.5, 0.5, 0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.5,0.5,0.5)}
                             -x+1/2,+y+1/2,-z+1/2
*******
space group: 24 {'Hall': ' I 2b 2c', 'HM': 'I 21 21 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z+1/2
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +X,+Y,+Z
```

-x,-y+1/2,+z

{2_00z|(0.0,0.5,0.0)} |

```
{2_x00|(0.0,0.0,0.5)} |
                            +x,-y,-z+1/2
 {2_0y0|(0.0,0.5,0.5)} |
                           -x,+y+1/2,-z+1/2
                         +x+1/2, +y+1/2, +z+1/2
    {1|(0.5,0.5,0.5)}
 \{2\_00z \mid (0.5,0.0,0.5)\}\
                          -x+1/2,-y,+z+1/2
 \{2_{x00} | (0.5, 0.5, 0.0)\} \mid
                           +x+1/2,-y+1/2,-z
                            -x+1/2,+y,-z
| {2_0y0|(0.5,0.0,0.0)} |
******
space group: 25 {'Hall': 'P 2 -2', 'HM': 'P m m 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z
         Seitz
                          Jones
   {1|(0.0,0.0,0.0)}
                        | +x,+y,+z |
 {2_00z|(0.0,0.0,0.0)}
                       |-x,-y,+z|
| {m_0yz|(0.0,0.0,0.0)} |
                         -x,+y,+z
| \{m_x0z|(0.0,0.0,0.0)\} | +x,-y,+z |
******
space group: 25:cab {'Hall': 'P -2 2', 'HM': 'P 2 m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y,-z
+x,-y,-z
         Seitz
                          Jones
   {1|(0.0,0.0,0.0)}
                        +x,+y,+z
| {m_xy0|(0.0,0.0,0.0)} | +x,+y,-z |
| \{2_x00|(0.0,0.0,0.0)\} | +x,-y,-z |
| {m_x0z|(0.0,0.0,0.0)} | +x,-y,+z |
*******
space group: 25:bca {'Hall': 'P -2 -2', 'HM': 'P m 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z
-x,+y,+z
         Seitz
                          Jones
```

```
\{1 \mid (0.0,0.0,0.0)\} \mid +x,+y,+z \mid
  \{m_xy0 | (0.0,0.0,0.0)\} \mid +x,+y,-z \mid
 \{m_0yz | (0.0,0.0,0.0)\} \mid -x,+y,+z \mid
| \{2_0y0|(0.0,0.0,0.0)\} | -x,+y,-z |
******
space group: 26 {'Hall': ' P 2c -2', 'HM': 'P m c 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z+1/2
-x,+y,+z
          Seitz
                              Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
                           -x,-y,+z+1/2
  {2_00z|(0.0,0.0,0.5)} |
| \{m_0yz | (0.0,0.0,0.0)\} | -x,+y,+z
| \{m_x0z|(0.0,0.0,0.5)\} | +x,-y,+z+1/2
*******
space group: 26:ba-c {'Hall': ' P 2c -2c', 'HM': ' P c m 21'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z+1/2
-x,+y,+z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                              Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                            +x,+y,+z
| \{2_{00z} | (0.0,0.0,0.5)\} | -x,-y,+z+1/2
| \{m_0yz | (0.0,0.0,0.5)\} | -x,+y,+z+1/2
| \{m_x 0z | (0.0, 0.0, 0.0)\} | +x,-y,+z
*******
space group: 26:cab {'Hall': ' P -2a 2a', 'HM': 'P 21 m a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x+1/2, +y, -z
+x+1/2,-y,-z
          Seitz
                              Jones
```

```
{1|(0.0,0.0,0.0)}
                           +x,+y,+z
 \{m_xy0|(0.5,0.0,0.0)\} \mid +x+1/2,+y,-z \mid
| {2_x00|(0.5,0.0,0.0)} | +x+1/2,-y,-z |
| \{m_x0z|(0.0,0.0,0.0)\} | +x,-y,+z
*******
space group: 26:-cba {'Hall': ' P -2 2a', 'HM': ' P 21 a m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x,+y,-z
+x+1/2,-y,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                            Jones
                           +x,+y,+z
+x,+y,-z
  {1|(0.0,0.0,0.0)}
| {m_xy0|(0.0,0.0,0.0)} |
\{2_x00|(0.5,0.0,0.0)\} \mid +x+1/2,-y,-z \mid
| \{m_x0z|(0.5,0.0,0.0)\} | +x+1/2,-y,+z |
*******
space group: 26:bca {'Hall': ' P -2 -2b', 'HM': 'P b 21 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z
-x,+y+1/2,+z
. . . . . . . . . . . . . . . . . . .
          Seitz
                              Jones
    \{1 \mid (0.0, 0.0, 0.0)\} \mid +x, +y, +z
| {m_xy0|(0.0,0.0,0.0)} |
                            +x,+y,-z
| \{m_0yz | (0.0,0.5,0.0)\} | -x,+y+1/2,+z |
| \{2_0y0|(0.0,0.5,0.0)\} | -x,+y+1/2,-z |
. . . . . . . . . . . . . . . . . . .
*******
space group: 26:a-cb {'Hall': ' P -2b -2', 'HM': ' P m 21 b'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x,+y+1/2,-z
-x,+y,+z
          Seitz
                              Jones
```

```
{1|(0.0,0.0,0.0)}
                          +x,+y,+z
 {m_xy0|(0.0,0.5,0.0)} |
                         +x,+y+1/2,-z
                         -x,+y,+z
| {m_0yz|(0.0,0.0,0.0)} |
 {2_0y0|(0.0,0.5,0.0)} |
                         -x,+y+1/2,-z
*******
space group: 27 {'Hall': 'P 2 -2c', 'HM': 'P c c 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z+1/2
         Seitz
                            Jones
   \{1 \mid (0.0, 0.0, 0.0)\}
                         +x,+y,+z
| {2_00z|(0.0,0.0,0.0)} |
                         -x,-y,+z
\{ m_0yz | (0.0,0.0,0.5) \} | -x,+y,+z+1/2 
| \{m_x0z|(0.0,0.0,0.5)\} | +x,-y,+z+1/2 |
******
space group: 27:cab {'Hall': 'P -2a 2', 'HM': 'P 2 a a'}
Crystal system: Orthorhombic
Setting: cab
+X,+Y,+Z
+x+1/2,+y,-z
+x,-y,-z
         Seitz
                            Jones
   {1|(0.0,0.0,0.0)}
                         +x,+y,+z
| \{m_xy0|(0.5,0.0,0.0)\} | +x+1/2,+y,-z
 {2_x00|(0.0,0.0,0.0)} |
                          +x,-y,-z
| {m_x0z|(0.5,0.0,0.0)} | +x+1/2,-y,+z
*******
space group: 27:bca {'Hall': 'P -2b -2b', 'HM': 'P b 2 b'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y+1/2,-z
-x,+y+1/2,+z
  . . . . . . . . . . . . . . . .
         Seitz
                            Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
```

```
| \{m_xy0|(0.0,0.5,0.0)\} | +x,+y+1/2,-z |
 \{m_0yz \mid (0.0,0.5,0.0)\} \mid -x,+y+1/2,+z \mid
\{2_0y0|(0.0,0.0,0.0)\} \mid -x,+y,-z
. . . . . . . . . . . . . . . . . . . .
*******
space group: 28 {'Hall': 'P 2 -2a', 'HM': 'P m a 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x+1/2, +y, +z
          Seitz
                             Jones
   {1|(0.0,0.0,0.0)}
                            +x,+y,+z
| {2_00z|(0.0,0.0,0.0)} |
                           -x,-y,+z
| {m_0yz|(0.5,0.0,0.0)} |
                          -x+1/2, +y, +z
| \{m_x0z|(0.5,0.0,0.0)\} | +x+1/2,-y,+z |
*******
space group: 28:ba-c {'Hall': 'P 2 -2b', 'HM': ' P b m 2'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-X,-Y,+Z
-x,+y+1/2,+z
. . . . . . . . . . . . . . . . . . .
          Seitz
                            Jones
   {1|(0.0,0.0,0.0)}
                            +x,+y,+z
| {2_00z|(0.0,0.0,0.0)} |
                           -x,-y,+z
| \{m_0yz | (0.0,0.5,0.0)\} | -x,+y+1/2,+z
| {m_x0z|(0.0,0.5,0.0)} | +x,-y+1/2,+z |
*******
space group: 28:cab {'Hall': 'P -2b 2', 'HM': 'P 2 m b'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y+1/2,-z
+x,-y,-z
          Seitz
                              Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
| \{m_xy0|(0.0,0.5,0.0)\} | +x,+y+1/2,-z |
```

```
| \{2_x00 | (0.0,0.0,0.0)\} | +x,-y,-z
| \{m_x0z|(0.0,0.5,0.0)\} | +x,-y+1/2,+z |
*******
space group: 28:-cba {'Hall': 'P -2c 2', 'HM': ' P 2 c m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x,+y,-z+1/2
+x,-y,-z
         Seitz
                            Jones
   {1|(0.0,0.0,0.0)}
                         +x,+y,+z
| \{m_xy0|(0.0,0.0,0.5)\} |
                         +x,+y,-z+1/2
| \{2_x00|(0.0,0.0,0.0)\} | +x,-y,-z
| \{m_x0z|(0.0,0.0,0.5)\} | +x,-y,+z+1/2 |
*******
space group: 28:bca {'Hall': 'P -2c -2c', 'HM': 'P c 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z+1/2
-x,+y,+z+1/2
. . . . . . . . . . . . . . . . . . .
         Seitz
                         Jones
   {1|(0.0,0.0,0.0)}
                         +x,+y,+z
| \{m_xy0|(0.0,0.0,0.5)\} | +x,+y,-z+1/2
| \{m_0yz | (0.0,0.0,0.5)\} | -x,+y,+z+1/2
| {2_0y0|(0.0,0.0,0.0)} |
                         -x,+y,-z
*******
space group: 28:a-cb {'Hall': 'P -2a -2a', 'HM': ' P m 2 a'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x+1/2, +y, -z
-x+1/2,+y,+z
         Seitz
                            Jones
   \{1|(0.0,0.0,0.0)\} +x,+y,+z
|\{m_xy0|(0.5,0.0,0.0)\}| +x+1/2,+y,-z|
```

```
| \{m_0yz | (0.5,0.0,0.0)\} | -x+1/2,+y,+z |
  {2_0y0|(0.0,0.0,0.0)} |
                            -x,+y,-z
*******
space group: 29 {'Hall': ' P 2c -2ac', 'HM': 'P c a 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z+1/2
-x+1/2,+y,+z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 {2_00z|(0.0,0.0,0.5)} |
                            -x,-y,+z+1/2
| \{m_0yz | (0.5,0.0,0.5)\} |
                          -x+1/2,+y,+z+1/2
  \{m_x0z|(0.5,0.0,0.0)\}
                            +x+1/2,-y,+z
*******
space group: 29:ba-c {'Hall': ' P 2c -2b', 'HM': ' P b c 21'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z+1/2
-x,+y+1/2,+z
          Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                             +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.5)\}
                            -x,-y,+z+1/2
| {m_0yz|(0.0,0.5,0.0)} |
                            -x,+y+1/2,+z
| \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
******
space group: 29:cab {'Hall': ' P -2b 2a', 'HM': 'P 21 a b'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x, +y+1/2, -z
+x+1/2,-y,-z
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
| {m_xy0|(0.0,0.5,0.0)}
                            +x,+y+1/2,-z
| {2_x00|(0.5,0.0,0.0)} |
                            +x+1/2,-y,-z
```

```
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z |
. . . . . . . . . . . . . . . . . . .
*******
space group: 29:-cba {'Hall': ' P -2ac 2a', 'HM': ' P 21 c a'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x+1/2,+y,-z+1/2
+x+1/2,-y,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
| \{m_xy0|(0.5,0.0,0.5)\} | +x+1/2,+y,-z+1/2
| {2_x00|(0.5,0.0,0.0)} |
                           +x+1/2,-y,-z
| \{m_x0z|(0.0,0.0,0.5)\} |
                             +x,-y,+z+1/2
*******
space group: 29:bca {'Hall': ' P -2bc -2c', 'HM': 'P c 21 b'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y+1/2,-z+1/2
-x, +y, +z+1/2
                                Jones
          Seitz
    {1|(0.0,0.0,0.0)}
                          +x,+y,+z
 \{m_xy0|(0.0,0.5,0.5)\}
                          +x,+y+1/2,-z+1/2
| \{m_0yz | (0.0,0.0,0.5)\} | -x,+y,+z+1/2
| {2_0y0|(0.0,0.5,0.0)} |
                             -x,+y+1/2,-z
******
space group: 29:a-cb {'Hall': ' P -2a -2ab', 'HM': ' P b 21 a'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x+1/2, +y, -z
-x+1/2,+y+1/2,+z
   . . . . . . . . . . . . . . . .
          Seitz
                                Jones
                             +x,+y,+z
   {1|(0.0,0.0,0.0)}
| {m_xy0|(0.5,0.0,0.0)} |
                           +x+1/2,+y,-z
| \{m_0yz|(0.5,0.5,0.0)\} | -x+1/2,+y+1/2,+z |
```

```
| \{2_0y0|(0.0,0.5,0.0)\} | -x,+y+1/2,-z
. . . . . . . . . . . . . . . . . . . .
*******
space group: 30 {'Hall': 'P 2 -2bc', 'HM': 'P n c 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x, +y+1/2, +z+1/2
   Seitz
                               Jones
                           +x,+y,+z
-x,-y,+z
   {1|(0.0,0.0,0.0)}
| {2_00z|(0.0,0.0,0.0)} |
\{m_0yz \mid (0.0,0.5,0.5)\} \mid -x,+y+1/2,+z+1/2 \mid
| {m_x0z|(0.0,0.5,0.5)} | +x,-y+1/2,+z+1/2 |
******
space group: 30:ba-c {'Hall': 'P 2 -2ac', 'HM': ' P c n 2'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z
-x+1/2, +y, +z+1/2
 . . . . . . . . . . . . . . . . . . .
          Seitz
                              Jones
  {1|(0.0,0.0,0.0)}
                            +x,+y,+z
                         -x,-y,+z
| {2 00z|(0.0,0.0,0.0)} | |
| \{m_0yz | (0.5,0.0,0.5)\} | -x+1/2,+y,+z+1/2 |
|\{m_x0z|(0.5,0.0,0.5)\}| +x+1/2,-y,+z+1/2|
******
space group: 30:cab {'Hall': 'P -2ac 2', 'HM': 'P 2 n a'}
Crystal system: Orthorhombic
Setting: cab
+X,+Y,+Z
+x+1/2, +y, -z+1/2
+x,-y,-z
         Seitz
                              Jones
 \{1|(0.0,0.0,0.0)\} +x,+y,+z
| \{m_xy0|(0.5,0.0,0.5)\} | +x+1/2,+y,-z+1/2 |
| {2_x00|(0.0,0.0,0.0)} |
                          +x,-y,-z
| {m_x0z|(0.5,0.0,0.5)} | +x+1/2,-y,+z+1/2 |
```

```
*******
space group: 30:-cba {'Hall': 'P -2ab 2', 'HM': ' P 2 a n'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x+1/2, +y+1/2, -z
+x,-y,-z
         Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                            +x,+y,+z
| \{m_xy0|(0.5,0.5,0.0)\} | +x+1/2,+y+1/2,-z
| {2_x00|(0.0,0.0,0.0)} |
                            +x,-y,-z
| {m_x0z|(0.5,0.5,0.0)} | +x+1/2,-y+1/2,+z |
******
space group: 30:bca {'Hall': 'P -2ab -2ab', 'HM': 'P b 2 n'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x+1/2, +y+1/2, -z
-x+1/2,+y+1/2,+z
  . . . . . . . . . . . . . . . . . .
         Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                            +x,+y,+z
| \{m_xy0|(0.5,0.5,0.0)\} | +x+1/2,+y+1/2,-z |
| \{m_0yz | (0.5, 0.5, 0.0)\} | -x+1/2, +y+1/2, +z
| {2_0y0|(0.0,0.0,0.0)} |
                             -x,+y,-z
******
space group: 30:a-cb {'Hall': 'P -2bc -2bc', 'HM': ' P n 2 b'}
Crystal system: Orthorhombic
Setting: a-cb
+X,+Y,+Z
+x,+y+1/2,-z+1/2
-x, +y+1/2, +z+1/2
         Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                             +x,+y,+z
| \{m_xy0|(0.0,0.5,0.5)\} | +x,+y+1/2,-z+1/2 |
| \{m_0yz | (0.0,0.5,0.5)\} | -x,+y+1/2,+z+1/2 |
| {2_0y0|(0.0,0.0,0.0)} |
                            -x,+y,-z
```

```
*******
space group: 31 {'Hall': ' P 2ac -2', 'HM': 'P m n 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2,-y,+z+1/2
-x,+y,+z
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +X,+Y,+Z
 {2_00z|(0.5,0.0,0.5)} |
                          -x+1/2,-y,+z+1/2
  \{m_0yz \mid (0.0,0.0,0.0)\}
                              -x,+y,+z
| \{m_x0z | (0.5,0.0,0.5)\} |
                          +x+1/2,-y,+z+1/2
*******
space group: 31:ba-c {'Hall': ' P 2bc -2bc', 'HM': ' P n m 21'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y+1/2,+z+1/2
-x, +y+1/2, +z+1/2
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
| {2_00z|(0.0,0.5,0.5)} |
                          -x,-y+1/2,+z+1/2
 \{m_0yz \mid (0.0,0.5,0.5)\} \mid
                          -x, +y+1/2, +z+1/2
| {m_x0z|(0.0,0.0,0.0)} |
                               +x,-y,+z
*******
space group: 31:cab {'Hall': ' P -2ab 2ab', 'HM': 'P 21 m n'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x+1/2, +y+1/2, -z
+x+1/2,-y+1/2,-z
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
 \{m_xy0|(0.5,0.5,0.0)\}
                          +x+1/2, +y+1/2, -z
| {2_x00|(0.5,0.5,0.0)}
                          +x+1/2,-y+1/2,-z
 \{m_x0z|(0.0,0.0,0.0)\}
                               +x,-y,+z
```

.....

```
******
```

space group: 31:-cba {'Hall': ' P -2 2ac', 'HM': ' P 21 n m'}

Crystal system: Orthorhombic

Setting: -cba

+x,+y,+z

+x,+y,-z

+x+1/2,-y,-z+1/2

Seitz	Jones
{1 (0.0,0.0,0.0)}	+x,+y,+z
{m_xy0 (0.0,0.0,0.0)}	+x,+y,-z
{2_x00 (0.5,0.0,0.5)}	+x+1/2,-y,-z+1/2
{m_x0z (0.5,0.0,0.5)}	+x+1/2,-y,+z+1/2

.

space group: 31:bca {'Hall': ' P -2 -2bc', 'HM': 'P n 21 m'}

Crystal system: Orthorhombic

Setting: bca

+x,+y,+z

+x,+y,-z

-x,+y+1/2,+z+1/2

+	
Seitz	Jones
{1 (0.0,0.0,0.0)} {m_xy0 (0.0,0.0,0.0)} {m_0yz (0.0,0.5,0.5)} {2_0y0 (0.0,0.5,0.5)}	+x,+y,+z

space group: 31:a-cb {'Hall': ' P -2ab -2', 'HM': ' P m 21 n'}

Crystal system: Orthorhombic

Setting: a-cb

+x,+y,+z

+x+1/2, +y+1/2, -z

-x,+y,+z

±	L
Seitz	Jones
{1 (0.0,0.0,0.0)} {m_xy0 (0.5,0.5,0.0)} {m_0yz (0.0,0.0,0.0)} {2_0y0 (0.5,0.5,0.0)}	+x,+y,+z

.

```
******
```

space group: 32 {'Hall': 'P 2 -2ab', 'HM': 'P b a 2'}

Crystal system: Orthorhombic

+x,+y,+z

-x,-y,+z

-x+1/2, +y+1/2, +z

......

l Coit-	Jones I
Seitz	
—	+x,+y,+z

.

space group: 32:cab {'Hall': 'P -2bc 2', 'HM': 'P 2 c b'}

Crystal system: Orthorhombic

Setting: cab +x,+y,+z

+x,+y+1/2,-z+1/2

+x,-y,-z

.

	- · · · · ·
Seitz	Jones
{1 (0.0,0.0,0.0)} {m_xy0 (0.0,0.5,0.5)} {2_x00 (0.0,0.0,0.0)} {m_x0z (0.0,0.5,0.5)}	+x,+y,+z +x,+y+1/2,-z+1/2 +x,-y,-z +x,-y+1/2,+z+1/2

......

space group: 32:bca {'Hall': 'P -2ac -2ac', 'HM': 'P c 2 a'}

Crystal system: Orthorhombic

Setting: bca +x,+y,+z +x+1/2,+y,-z+1/2

-x+1/2, +y, +z+1/2

.

+	Jones
{1 (0.0,0.0,0.0)}	+x,+y,+z
{m_xy0 (0.5,0.0,0.5)}	+x+1/2,+y,-z+1/2
{m_0yz (0.5,0.0,0.5)}	-x+1/2,+y,+z+1/2
{2_0y0 (0.0,0.0,0.0)}	-x,+y,-z

.

```
space group: 33 {'Hall': ' P 2c -2n', 'HM': 'P n a 21'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z+1/2
-x+1/2,+y+1/2,+z+1/2
. . . . . . . . . . . . . . . . . . .
                                Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
                           -x,-y,+z+1/2
 {2_00z|(0.0,0.0,0.5)} |
| \{m_0yz | (0.5, 0.5, 0.5)\} | -x+1/2, +y+1/2, +z+1/2
|\{m_x0z|(0.5,0.5,0.0)\}| +x+1/2,-y+1/2,+z
*******
space group: 33:ba-c {'Hall': ' P 2c -2ab', 'HM': ' P b n 21'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z+1/2
-x+1/2,+y+1/2,+z
. . . . . . . . . . . . . . . . . . .
         Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
| \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 33:cab {'Hall': ' P -2bc 2a', 'HM': 'P 21 n b'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y+1/2,-z+1/2
+x+1/2,-y,-z
         Seitz
                                Jones
   \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
| {m_xy0|(0.0,0.5,0.5)} |
                           +x,+y+1/2,-z+1/2
                         +x+1/2,-y,-z
 {2_x00|(0.5,0.0,0.0)} |
|\{m_x0z|(0.5,0.5,0.5)\}| +x+1/2,-y+1/2,+z+1/2|
```

```
*******
space group: 33:-cba {'Hall': ' P -2n 2a', 'HM': ' P 21 c n'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x+1/2, +y+1/2, -z+1/2
+x+1/2,-y,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +X,+Y,+Z
 \{m_xy0|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,-z+1/2
| {2_x00|(0.5,0.0,0.0)} |
                            +x+1/2,-y,-z
| \{m_x0z|(0.0,0.5,0.5)\} |
                           +x,-y+1/2,+z+1/2
*******
space group: 33:bca {'Hall': ' P -2n -2ac', 'HM': 'P c 21 n'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x+1/2, +y+1/2, -z+1/2
-x+1/2,+y,+z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
\{m_xy0|(0.5,0.5,0.5)\} +x+1/2,+y+1/2,-z+1/2
| {m_0yz|(0.5,0.0,0.5)} |
                           -x+1/2,+y,+z+1/2
| {2_0y0|(0.0,0.5,0.0)} |
                              -x,+y+1/2,-z
*******
space group: 33:a-cb {'Hall': ' P -2ac -2n', 'HM': ' P n 21 a'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x+1/2,+y,-z+1/2
-x+1/2, +y+1/2, +z+1/2
          Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{m_xy0|(0.5,0.0,0.5)\}
                           +x+1/2,+y,-z+1/2
 \{m_0yz \mid (0.5, 0.5, 0.5)\} \mid
                           -x+1/2, +y+1/2, +z+1/2
| {2_0y0|(0.0,0.5,0.0)} |
                               -x,+y+1/2,-z
```

```
*******
space group: 34 {'Hall': 'P 2 -2n', 'HM': 'P n n 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x+1/2, +y+1/2, +z+1/2
         Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
                          -x,-y,+z
 {2_00z|(0.0,0.0,0.0)} |
| \{m_0yz | (0.5,0.5,0.5)\} | -x+1/2,+y+1/2,+z+1/2 |
\{m_x0z|(0.5,0.5,0.5)\} +x+1/2,-y+1/2,+z+1/2 \}
*******
space group: 34:cab {'Hall': 'P -2n 2', 'HM': 'P 2 n n'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x+1/2,+y+1/2,-z+1/2
+x,-y,-z
         Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                               +x,+y,+z
\{m_xy0|(0.5,0.5,0.5)\} +x+1/2,+y+1/2,-z+1/2
| {2_x00|(0.0,0.0,0.0)} |
                          +x,-y,-z
| \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 34:bca {'Hall': 'P -2n -2n', 'HM': 'P n 2 n'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x+1/2, +y+1/2, -z+1/2
-x+1/2,+y+1/2,+z+1/2
  . . . . . . . . . . . . . . . .
         Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                               +x,+y,+z
 \{m_xy0|(0.5,0.5,0.5)\} \mid +x+1/2,+y+1/2,-z+1/2
 \{m_0yz \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, +y+1/2, +z+1/2
| {2_0y0|(0.0,0.0,0.0)} |
                               -x,+y,-z
```

```
space group: 35 {'Hall': 'C 2 -2', 'HM': 'C m m 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +X,+Y,+Z
 {2_00z|(0.0,0.0,0.0)} |
                                -x,-y,+z
  \{m_0yz \mid (0.0,0.0,0.0)\} \mid
                                -x,+y,+z
  \{m_x0z | (0.0,0.0,0.0)\} \mid
                                +x,-y,+z
    {1|(0.5,0.5,0.0)}
                          +x+1/2,+y+1/2,+z
  \{2\_00z \mid (0.5,0.5,0.0)\} \mid -x+1/2,-y+1/2,+z \mid
  \{m_0yz \mid (0.5, 0.5, 0.0)\}\
                            -x+1/2,+y+1/2,+z
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z |
*******
space group: 35:cab {'Hall': 'A -2 2', 'HM': 'A 2 m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y,-z
+x,-y,-z
           Seitz
                                  Jones
    \{1|(0.0,0.0,0.0)\}
                                +x,+y,+z
| {m_xy0|(0.0,0.0,0.0)} |
                                +x,+y,-z
  \{2_{x00} | (0.0, 0.0, 0.0)\}
                                +x,-y,-z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                +x,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                          +x,+y+1/2,+z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                          +x,+y+1/2,-z+1/2
  \{2_{x00} | (0.0, 0.5, 0.5)\}
                            +x,-y+1/2,-z+1/2
  \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
*******
space group: 35:bca {'Hall': 'B -2 -2', 'HM': 'B m 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z
-x,+y,+z
   . . . . . . . . . . . . . . . .
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
```

```
{m_xy0|(0.0,0.0,0.0)} |
                                 +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                 -x,+y,+z
  {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2, +y, +z+1/2
  \{m_xy0 | (0.5,0.0,0.5)\}
                            +x+1/2,+y,-z+1/2
 \{m_0yz \mid (0.5,0.0,0.5)\}\
                            -x+1/2,+y,+z+1/2
  \{2_0y0|(0.5,0.0,0.5)\} \mid -x+1/2,+y,-z+1/2
*******
space group: 36 {'Hall': ' C 2c -2', 'HM': 'C m c 21'}
Crystal system: Orthorhombic
+X,+Y,+Z
-x,-y,+z+1/2
-x,+y,+z
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{2_{00z}|(0.0,0.0,0.5)\}
                                 -x,-y,+z+1/2
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                   -x,+y,+z
  \{m_x0z|(0.0,0.0,0.5)\}
                                 +x,-y,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                               +x+1/2, +y+1/2, +z
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, -y+1/2, +z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,+y+1/2,+z
\{m_x0z|(0.5,0.5,0.5)\} +x+1/2,-y+1/2,+z+1/2
*******
space group: 36:ba-c {'Hall': ' C 2c -2c', 'HM': ' C c m 21'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z+1/2
-x,+y,+z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.5)\}
                                 -x,-y,+z+1/2
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                 -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                   +x,-y,+z
    \{1 \mid (0.5, 0.5, 0.0)\}
                               +x+1/2,+y+1/2,+z
  \{2_{00z} | (0.5, 0.5, 0.5)\}
                            -x+1/2,-y+1/2,+z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, +y+1/2, +z+1/2
                               +x+1/2,-y+1/2,+z
  \{m_x0z|(0.5,0.5,0.0)\}
```

```
space group: 36:cab {'Hall': ' A -2a 2a', 'HM': 'A 21 m a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x+1/2, +y, -z
+x+1/2,-y,-z
          Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{m_xy0|(0.5,0.0,0.0)\}
                                +x+1/2,+y,-z
 {2_x00|(0.5,0.0,0.0)} |
                                +x+1/2,-y,-z
 {m_x0z|(0.0,0.0,0.0)} |
                                  +x,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
  \{m \times v0 \mid (0.5, 0.5, 0.5)\}
                           +x+1/2, +y+1/2, -z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                           +x+1/2,-y+1/2,-z+1/2
  \{m_x0z|(0.0,0.5,0.5)\}
                              +x,-y+1/2,+z+1/2
******
space group: 36:-cba {'Hall': ' A -2 2a', 'HM': ' A 21 a m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x,+y,-z
+x+1/2,-y,-z
          Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{m \times y0 \mid (0.0, 0.0, 0.0)\} \mid
                                 +x,+y,-z
  {2_x00|(0.5,0.0,0.0)} |
                                +x+1/2,-y,-z
  \{m_x0z | (0.5,0.0,0.0)\} \mid
                               +x+1/2,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x,+y+1/2,+z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                              +x,+y+1/2,-z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,-z+1/2
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 36:bca {'Hall': ' B -2 -2b', 'HM': 'B b 21 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z
-x, +y+1/2, +z
          Seitz
                                   Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{m_xy0|(0.0,0.0,0.0)\}
                                  +x,+y,-z
  {m_0yz|(0.0,0.5,0.0)}
                                -x,+y+1/2,+z
  \{2 \text{ 0y0} | (0.0, 0.5, 0.0)\}
                                -x,+y+1/2,-z
    \{1 \mid (0.5, 0.0, 0.5)\}
                              +x+1/2,+y,+z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                              +x+1/2, +y, -z+1/2
 \{m_0yz | (0.5, 0.5, 0.5)\} \mid
                            -x+1/2,+y+1/2,+z+1/2
                            -x+1/2, +y+1/2, -z+1/2
  {2_0y0|(0.5,0.5,0.5)} |
*******
space group: 36:a-cb {'Hall': ' B -2b -2', 'HM': ' B m 21 b'}
Crystal system: Orthorhombic
Setting: a-cb
+X,+V,+Z
+x, +y+1/2, -z
-x,+y,+z
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
                                +x,+y+1/2,-z
  \{m_xy0|(0.0,0.5,0.0)\}
 {m_0yz|(0.0,0.0,0.0)} |
                                  -x,+y,+z
  {2_0y0|(0.0,0.5,0.0)} |
                                -x,+y+1/2,-z
    \{1|(0.5,0.0,0.5)\}
                              +x+1/2,+y,+z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
 \{m \ 0yz | (0.5,0.0,0.5)\}
                             -x+1/2,+y,+z+1/2
 \{2_0y0|(0.5,0.5,0.5)\} \mid -x+1/2,+y+1/2,-z+1/2
******
space group: 37 {'Hall': 'C 2 -2c', 'HM': 'C c c 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {2_00z|(0.0,0.0,0.0)} |
                                  -x,-y,+z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y,+z+1/2
  \{m_x0z|(0.0,0.0,0.5)\}
                                +x,-y,+z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                              +x+1/2,+y+1/2,+z
  \{2_{00z} | (0.5, 0.5, 0.0)\}
                              -x+1/2,-y+1/2,+z
  \{m_0yz \mid (0.5, 0.5, 0.5)\}\
                            -x+1/2, +y+1/2, +z+1/2
| \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
```

```
space group: 37:cab {'Hall': 'A -2a 2', 'HM': 'A 2 a a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x+1/2,+y,-z
+x,-y,-z
          Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +X,+Y,+Z
 \{m_xy0|(0.5,0.0,0.0)\}
                             +x+1/2,+y,-z
| {2_x00|(0.0,0.0,0.0)} |
                               +x,-y,-z
| {m_x0z|(0.5,0.0,0.0)} |
                             +x+1/2,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                           +x,+y+1/2,+z+1/2
 \{m_xy0|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,-z+1/2
 \{2_x00|(0.0,0.5,0.5)\} \mid +x,-y+1/2,-z+1/2
  \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 37:bca {'Hall': 'B -2b -2b', 'HM': 'B b 2 b'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y+1/2,-z
-x,+y+1/2,+z
          Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  \{m_xy0|(0.0,0.5,0.0)\}
                              +x,+y+1/2,-z
 \{m_0yz \mid (0.0, 0.5, 0.0)\} \mid
                              -x,+y+1/2,+z
  {2_0y0|(0.0,0.0,0.0)} |
                                 -x,+y,-z
    {1|(0.5,0.0,0.5)}
                            +x+1/2,+y,+z+1/2
  \{m_xy0|(0.5,0.5,0.5)\} | +x+1/2,+y+1/2,-z+1/2
 \{m_0yz \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, +y+1/2, +z+1/2
  {2_0y0|(0.5,0.0,0.5)} |
                            -x+1/2,+y,-z+1/2
*******
space group: 38 {'Hall': 'A 2 -2', 'HM': 'A m m 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z
          Seitz
                                Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                -x,-y,+z
 {m_0yz|(0.0,0.0,0.0)} |
                                -x,+y,+z
                            +x,-y,+z
+x,+y+1/2,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.0)\}
    \{1 \mid (0.0, 0.5, 0.5)\}
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                          |-x,-y+1/2,+z+1/2|
 \{m_0yz \mid (0.0,0.5,0.5)\} \mid -x,+y+1/2,+z+1/2
  \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
*******
space group: 38:ba-c {'Hall': 'B 2 -2', 'HM': ' B m m 2'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z
-x,+y,+z
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
  {2_00z|(0.0,0.0,0.0)} |
                                -x,-y,+z
| {m_0yz|(0.0,0.0,0.0)} |
                                -x,+y,+z
  \{m_x0z|(0.0,0.0,0.0)\}
                                +x,-y,+z
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2, +y, +z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\} \mid -x+1/2,-y,+z+1/2
 \{m_0yz \mid (0.5,0.0,0.5)\} \mid -x+1/2,+y,+z+1/2
| \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
******
space group: 38:cab {'Hall': 'B -2 2', 'HM': 'B 2 m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y,-z
+x,-y,-z
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
  \{m_xy0|(0.0,0.0,0.0)\}
                                +x,+y,-z
 {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
  \{m_x0z|(0.0,0.0,0.0)\}
                                +x,-y,+z
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2, +y, +z+1/2
  {m_xy0|(0.5,0.0,0.5)}
                            +x+1/2, +y, -z+1/2
 \{2_{x00}|(0.5,0.0,0.5)\} \mid +x+1/2,-y,-z+1/2
| {m_x0z|(0.5,0.0,0.5)} | +x+1/2,-y,+z+1/2 |
```

```
space group: 38:-cba {'Hall': 'C -2 2', 'HM': ' C 2 m m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x,+y,-z
+x,-y,-z
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 \{m_xy0|(0.0,0.0,0.0)\}
                                +x,+y,-z
| {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
  \{m_x0z | (0.0,0.0,0.0)\} |
                                +x,-y,+z
    \{1|(0.5,0.5,0.0)\} | +x+1/2,+y+1/2,+z
  \{m_xy0|(0.5,0.5,0.0)\} | +x+1/2,+y+1/2,-z
  \{2_x00|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,-z \mid
| {m_x0z|(0.5,0.5,0.0)} | +x+1/2,-y+1/2,+z |
*******
space group: 38:bca {'Hall': 'C -2 -2', 'HM': 'C m 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+X,+Y,-Z
-x,+y,+z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
  \{m_xy0|(0.0,0.0,0.0)\}
                                +x,+y,-z
 {m_0yz|(0.0,0.0,0.0)} |
                                -x,+y,+z
  {2_0y0|(0.0,0.0,0.0)} |
                                -x,+y,-z
    {1|(0.5,0.5,0.0)}
                          +x+1/2,+y+1/2,+z
 \{m_xy0 \mid (0.5, 0.5, 0.0)\} \mid +x+1/2, +y+1/2, -z
| \{m_0yz | (0.5,0.5,0.0)\} | -x+1/2,+y+1/2,+z |
| \{2_0y0|(0.5,0.5,0.0)\} | -x+1/2,+y+1/2,-z
. . . . . . . . . . . . . . . . . . .
*******
space group: 38:a-cb {'Hall': 'A -2 -2', 'HM': ' A m 2 m'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x,+y,-z
-x,+y,+z
. . . . . . . . . . . . . . . . . . . .
```

```
Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{m \times y0 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,-z
                                  -x, +y, +z
  \{m_0yz \mid (0.0,0.0,0.0)\}
  {2_0y0|(0.0,0.0,0.0)}
                                  -x,+y,-z
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                              +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.0, 0.5, 0.5)\}
                              -x, +y+1/2, +z+1/2
  \{2_0y0|(0.0,0.5,0.5)\}
                              -x, +y+1/2, -z+1/2
*******
space group: 39 {'Hall': 'A 2 -2c', 'HM': 'A b m 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                  -x,-y,+z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                +x,-y,+z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
  \{2\ 00z|(0.0,0.5,0.5)\}
                              -x,-y+1/2,+z+1/2
  \{m_0yz \mid (0.0, 0.5, 0.0)\}
                                -x,+y+1/2,+z
  \{m \times 0z \mid (0.0, 0.5, 0.0)\}
                                +x,-y+1/2,+z
*******
space group: 39:ba-c {'Hall': 'B 2 -2c', 'HM': ' B m a 2'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z
-x,+y,+z+1/2
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                  -x,-y,+z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                +x,-y,+z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                              +x+1/2, +y, +z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                              -x+1/2, -y, +z+1/2
  \{m_0yz \mid (0.5,0.0,0.0)\}
                                -x+1/2,+y,+z
  \{m_x0z \mid (0.5,0.0,0.0)\}
                                +x+1/2,-y,+z
```

```
. . . . . . . . . . . . . . . . . . .
******
space group: 39:cab {'Hall': 'B -2c 2', 'HM': 'B 2 c m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y,-z+1/2
+x,-y,-z
          Seitz | Jones
   \{1 \mid (0.0, 0.0, 0.0)\} + x, +y, +z
| {m_xy0|(0.0,0.0,0.5)} |
                          +x,+y,-z+1/2
| {2_x00|(0.0,0.0,0.0)} |
                             +x,-y,-z
| {m_x0z|(0.0,0.0,0.5)} |
                           +x,-y,+z+1/2
                       | +x+1/2, +y, +z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
  \{m_xy0|(0.5,0.0,0.0)\} \mid +x+1/2,+y,-z
| \{2_{x00} | (0.5,0.0,0.5)\} | +x+1/2,-y,-z+1/2
| \{m_x0z|(0.5,0.0,0.0)\} | +x+1/2,-y,+z
. . . . . . . . . . . . . . . . . . .
******
space group: 39:-cba {'Hall': 'C -2b 2', 'HM': ' C 2 m b'}
Crystal system: Orthorhombic
Setting: -cba
+X,+Y,+Z
+x,+y+1/2,-z
+x,-y,-z
```

+	·
Seitz	Jones
{1 (0.0,0.0,0.0)} {m_xy0 (0.0,0.5,0.0)} {2_x00 (0.0,0.0,0.0)} {m_x0z (0.0,0.5,0.0)} {1 (0.5,0.5,0.0)} {m_xy0 (0.5,0.0,0.0)} {2_x00 (0.5,0.5,0.0)} {m_x0z (0.5,0.0,0.0)}	+x,+y,+z +x,+y+1/2,-z +x,-y,-z +x,-y+1/2,+z +x+1/2,+y+1/2,+z +x+1/2,+y,-z +x+1/2,-y+1/2,-z +x+1/2,-y,+z

.

```
*******
```

```
space group: 39:bca {'Hall': 'C -2b -2b', 'HM': 'C m 2 a'}
```

Crystal system: Orthorhombic

Setting: bca +x,+y,+z +x,+y+1/2,-z -x,+y+1/2,+z

```
Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{m_xy0 | (0.0, 0.5, 0.0)\}
                               +x,+y+1/2,-z
  \{m_0yz \mid (0.0, 0.5, 0.0)\}
                               -x,+y+1/2,+z
  {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
    \{1 \mid (0.5, 0.5, 0.0)\}
                             +x+1/2, +y+1/2, +z
  \{m_xy0 | (0.5,0.0,0.0)\}
                               +x+1/2,+y,-z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                               -x+1/2,+y,+z
  {2_0y0|(0.5,0.5,0.0)}
                             -x+1/2,+y+1/2,-z
******
space group: 39:a-cb {'Hall': 'A -2c -2c', 'HM': ' A c 2 m'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x,+y,-z+1/2
-x,+y,+z+1/2
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{m_xy0|(0.0,0.0,0.5)\}
                               +x,+y,-z+1/2
 \{m_0yz \mid (0.0,0.0,0.5)\}
                               -x,+y,+z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                 -X,+y,-z
    \{1 \mid (0.0, 0.5, 0.5)\}
                             +x, +y+1/2, +z+1/2
                               +x,+y+1/2,-z
  \{m_xy0|(0.0,0.5,0.0)\}
  \{m_0yz \mid (0.0, 0.5, 0.0)\}
                               -x,+y+1/2,+z
  {2_0y0|(0.0,0.5,0.5)} |
                             -x, +y+1/2, -z+1/2
*******
space group: 40 {'Hall': 'A 2 -2a', 'HM': 'A m a 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x+1/2,+y,+z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                    -x,-y,+z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                                 -x+1/2,+y,+z
  \{m_x0z \mid (0.5,0.0,0.0)\}
                                 +x+1/2,-y,+z
    \{1|(0.0,0.5,0.5)\}
                               +x, +y+1/2, +z+1/2
  \{2\_00z \mid (0.0,0.5,0.5)\}
                               -x,-y+1/2,+z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,+y+1/2,+z+1/2
```

 $\{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2$

```
*******
space group: 40:ba-c {'Hall': 'B 2 -2b', 'HM': ' B b m 2'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z
-x,+y+1/2,+z
                                 Jones
          Seitz
   {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 {2_00z|(0.0,0.0,0.0)} |
                                -x,-y,+z
| {m_0yz|(0.0,0.5,0.0)} |
                              -x,+y+1/2,+z
  \{m_x0z|(0.0,0.5,0.0)\}
                             +x,-y+1/2,+z
    {1|(0.5,0.0,0.5)} |
                            +x+1/2,+y,+z+1/2
                           -x+1/2,-y,+z+1/2
  {2_00z|(0.5,0.0,0.5)} |
| \{m_0yz | (0.5,0.5,0.5)\} | -x+1/2,+y+1/2,+z+1/2
| \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2 |
*******
space group: 40:cab {'Hall': 'B -2b 2', 'HM': 'B 2 m b'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y+1/2,-z
+x,-y,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  {m_xy0|(0.0,0.5,0.0)} |
                              +x,+y+1/2,-z
 {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
 \{m_x0z|(0.0,0.5,0.0)\}
                              +x,-y+1/2,+z
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2,+y,+z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
                          +x+1/2,+y+1/2,-z+1/2
 \{2_x00|(0.5,0.0,0.5)\} \mid +x+1/2,-y,-z+1/2
| \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 40:-cba {'Hall': 'C -2c 2', 'HM': ' C 2 c m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x,+y,-z+1/2
```

+x,-y,-z

```
Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{m_xy0|(0.0,0.0,0.5)\}
                                +x,+y,-z+1/2
  \{2_{x00} | (0.0,0.0,0.0)\}
                                  +x,-y,-z
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                +x,-y,+z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                              +x+1/2, +y+1/2, +z
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2,+y+1/2,-z+1/2
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                              +x+1/2,-y+1/2,-z
  \{m_x0z|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,+z+1/2
*******
space group: 40:bca {'Hall': 'C -2c -2c', 'HM': 'C c 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z+1/2
-x,+y,+z+1/2
          Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
 \{m_xy0|(0.0,0.0,0.5)\}
                                +x,+y,-z+1/2
 \{m \ 0 \ yz \mid (0.0, 0.0, 0.5)\}
                                -x,+y,+z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                  -x,+y,-z
    \{1 \mid (0.5, 0.5, 0.0)\}
                              +x+1/2,+y+1/2,+z
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                            -x+1/2,+y+1/2,+z+1/2
  {2_0y0|(0.5,0.5,0.0)}
                              -x+1/2,+y+1/2,-z
*******
space group: 40:a-cb {'Hall': 'A -2a -2a', 'HM': ' A m 2 a'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x+1/2, +y, -z
-x+1/2,+y,+z
          Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{m_xy0|(0.5,0.0,0.0)\}
                                +x+1/2,+y,-z
 {m_0yz|(0.5,0.0,0.0)} |
                                -x+1/2,+y,+z
  {2_0y0|(0.0,0.0,0.0)}
                                  -x,+y,-z
```

+x,+y+1/2,+z+1/2

 $\{m_xy0|(0.5,0.5,0.5)\} \mid +x+1/2,+y+1/2,-z+1/2 \mid$

 $\{1 \mid (0.0, 0.5, 0.5)\}$

```
\{m_0yz \mid (0.5,0.5,0.5)\} \mid -x+1/2,+y+1/2,+z+1/2 \mid
  {2_0y0|(0.0,0.5,0.5)} |
                             -x, +y+1/2, -z+1/2
*******
space group: 41 {'Hall': 'A 2 -2ac', 'HM': 'A b a 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x+1/2,+y,+z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
  {2_00z|(0.0,0.0,0.0)} |
                               -x,-y,+z
 \{m_0yz|(0.5,0.0,0.5)\}
                           -x+1/2,+y,+z+1/2
  \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
                           +x,+y+1/2,+z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                         |-x,-y+1/2,+z+1/2|
| \{m_0yz | (0.5, 0.5, 0.0)\} |
                           -x+1/2,+y+1/2,+z
 \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z
******
space group: 41:ba-c {'Hall': 'B 2 -2bc', 'HM': ' B b a 2'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z
-x, +y+1/2, +z+1/2
    . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
 {2_00z|(0.0,0.0,0.0)} |
                               -x,-y,+z
| \{m_0yz | (0.0,0.5,0.5)\} | -x,+y+1/2,+z+1/2
  \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
    {1|(0.5,0.0,0.5)}
                           +x+1/2,+y,+z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\} \mid -x+1/2,-y,+z+1/2
| \{m_0yz | (0.5,0.5,0.0)\} | -x+1/2,+y+1/2,+z
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z |
*******
space group: 41:cab {'Hall': 'B -2bc 2', 'HM': 'B 2 c b'}
Crystal system: Orthorhombic
Setting: cab
+X,+Y,+Z
+x,+y+1/2,-z+1/2
```

```
+x,-y,-z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{m_xy0|(0.0,0.5,0.5)\}
                            +x,+y+1/2,-z+1/2
  \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x,-y,-z
  \{m_x0z \mid (0.0, 0.5, 0.5)\}
                            +x,-y+1/2,+z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2,+y,+z+1/2
  \{m_xy0|(0.5,0.5,0.0)\}
                            +x+1/2,+y+1/2,-z
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                            +x+1/2,-y,-z+1/2
| {m_x0z|(0.5,0.5,0.0)} | +x+1/2,-y+1/2,+z |
*******
space group: 41:-cba {'Hall': 'C -2bc 2', 'HM': ' C 2 c b'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x,+y+1/2,-z+1/2
+x,-y,-z
           Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  \{m \times y0 \mid (0.0, 0.5, 0.5)\}
                            +x,+y+1/2,-z+1/2
  \{2_{x00} | (0.0, 0.0, 0.0)\}
                                 +x,-y,-z
  \{m_x0z|(0.0,0.5,0.5)\}
                            +x,-y+1/2,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                            +x+1/2, +y+1/2, +z
  \{m_xy0|(0.5,0.0,0.5)\}
                            +x+1/2, +y, -z+1/2
                            +x+1/2,-y+1/2,-z
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                          | +x+1/2, -y, +z+1/2
 \{m_x0z|(0.5,0.0,0.5)\}
 . . . . . . . . . . . . . . . . . . .
*******
space group: 41:bca {'Hall': 'C -2bc -2bc', 'HM': 'C c 2 a'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y+1/2,-z+1/2
-x,+y+1/2,+z+1/2
```

+	++
Seitz	Jones
{1 (0.0,0.0,0.0)} {m_xy0 (0.0,0.5,0.5)} {m_0yz (0.0,0.5,0.5)} {2_0y0 (0.0,0.0,0.0)} {1 (0.5,0.5,0.0)}	+x,+y,+z +x,+y+1/2,-z+1/2 -x,+y+1/2,+z+1/2 -x,+y,-z +x+1/2,+y+1/2,+z

```
\{m \times y0 \mid (0.5, 0.0, 0.5)\} \mid
                              +x+1/2,+y,-z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                              -x+1/2,+y,+z+1/2
                              -x+1/2, +y+1/2, -z
  {2_0y0|(0.5,0.5,0.0)} |
*******
space group: 41:a-cb {'Hall': 'A -2ac -2ac', 'HM': ' A c 2 a'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x+1/2,+y,-z+1/2
-x+1/2, +y, +z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +X,+Y,+Z
  \{m_xy0|(0.5,0.0,0.5)\}
                              +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                              -x+1/2,+y,+z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                  -x, +y, -z
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
  \{m_xy0|(0.5,0.5,0.0)\}
                              +x+1/2, +y+1/2, -z
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,+y+1/2,+z
                              -x, +y+1/2, -z+1/2
  {2_0y0|(0.0,0.5,0.5)}
*******
space group: 42 {'Hall': 'F 2 -2', 'HM': 'F m m 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{2_{00z} | (0.0, 0.0, 0.0)\}
                                  -x,-y,+z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                  -x,+y,+z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                  +x,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
  \{2\_00z \mid (0.0,0.5,0.5)\}
                              -x,-y+1/2,+z+1/2
  \{m_0yz \mid (0.0,0.5,0.5)\}
                              -x, +y+1/2, +z+1/2
  \{m_x0z \mid (0.0,0.5,0.5)\}
                              +x,-y+1/2,+z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                              +x+1/2,+y,+z+1/2
  \{2_{00z} | (0.5, 0.0, 0.5)\}
                              -x+1/2,-y,+z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                              -x+1/2, +y, +z+1/2
  \{m_x0z \mid (0.5,0.0,0.5)\}
                              +x+1/2,-y,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                              +x+1/2,+y+1/2,+z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                              -x+1/2, -y+1/2, +z
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,+y+1/2,+z
  \{m_x0z \mid (0.5, 0.5, 0.0)\}
                           | +x+1/2, -y+1/2, +z
```

```
*******
space group: 42:cab {'Hall': 'F -2 2', 'HM': 'F 2 m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y,-z
+x,-y,-z
           Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  \{m_xy0|(0.0,0.0,0.0)\}
                                 +x,+y,-z
  \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x,-y,-z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                 +x,-y,+z
                            +x,+y+1/2,+z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
  \{m_xy0|(0.0,0.5,0.5)\}
                            +x, +y+1/2, -z+1/2
  \{2_{x00}|(0.0,0.5,0.5)\}
                            +x,-y+1/2,-z+1/2
  \{m_x0z \mid (0.0, 0.5, 0.5)\}
                            +x,-y+1/2,+z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2, +y, +z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                            +x+1/2,+y,-z+1/2
                            +x+1/2,-y,-z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
                            +x+1/2,-y,+z+1/2
  \{m_x0z|(0.5,0.0,0.5)\}
    \{1|(0.5,0.5,0.0)\}
                            +x+1/2, +y+1/2, +z
                            +x+1/2, +y+1/2, -z
  \{m_xy0|(0.5,0.5,0.0)\}
  \{2_{x00}|(0.5,0.5,0.0)\}
                            +x+1/2,-y+1/2,-z
  \{m_x0z|(0.5,0.5,0.0)\}
                            +x+1/2,-y+1/2,+z
*******
space group: 42:bca {'Hall': 'F -2 -2', 'HM': 'F m 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z
           Seitz
                                  Jones
    \{1|(0.0,0.0,0.0)\}
                                 +x,+y,+z
  \{m_xy0|(0.0,0.0,0.0)\}
                                 +x,+y,-z
  \{m_0yz | (0.0,0.0,0.0)\}
                                 -x,+y,+z
  \{2_0y0|(0.0,0.0,0.0)\}
                                 -x,+y,-z
    \{1 \mid (0.0, 0.5, 0.5)\}
                            +x,+y+1/2,+z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                            +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.0,0.5,0.5)\}
                            -x, +y+1/2, +z+1/2
  {2_0y0|(0.0,0.5,0.5)}
                            -x, +y+1/2, -z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2, +y, +z+1/2
  \{m_xy0|(0.5,0.0,0.5)\} \mid +x+1/2,+y,-z+1/2 \mid
```

```
\{m_0yz \mid (0.5,0.0,0.5)\}
                              -x+1/2,+y,+z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                              -x+1/2,+y,-z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                              +x+1/2, +y+1/2, +z
  \{m \times y0 \mid (0.5, 0.5, 0.0)\}
                              +x+1/2, +y+1/2, -z
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                              -x+1/2, +y+1/2, +z
 \{2_0y0|(0.5,0.5,0.0)\} \mid -x+1/2,+y+1/2,-z
*******
space group: 43 {'Hall': 'F 2 -2d', 'HM': 'F d d 2'}
Crystal system: Orthorhombic
+x,+y,+z
-X,-Y,+Z
-x+1/4, +y+1/4, +z+1/4
            Seitz
                                          Jones
     {1|(0.0,0.0,0.0)}
                                        +x,+y,+z
   {2_00z|(0.0,0.0,0.0)}
                                        -x,-y,+z
  \{m_0yz \mid (0.25, 0.25, 0.25)\}
                                 -x+1/4, +y+1/4, +z+1/4
  \{m_x0z \mid (0.75, 0.75, 0.25)\}
                                 +x+3/4,-y+3/4,+z+1/4
     \{1 \mid (0.0, 0.5, 0.5)\}
                                    +x,+y+1/2,+z+1/2
                                    -x,-y+1/2,+z+1/2
   \{2\_00z \mid (0.0,0.5,0.5)\}
  \{m_0yz \mid (0.25, 0.75, 0.75)\}
                                 -x+1/4, +y+3/4, +z+3/4
  \{m_x0z|(0.75,0.25,0.75)\}
                                 +x+3/4, -y+1/4, +z+3/4
     \{1 \mid (0.5, 0.0, 0.5)\}
                                    +x+1/2,+y,+z+1/2
   {2 00z|(0.5,0.0,0.5)}
                                    -x+1/2,-y,+z+1/2
  \{m_0yz \mid (0.75, 0.25, 0.75)\}
                                 -x+3/4, +y+1/4, +z+3/4
  \{m \times 0z \mid (0.25, 0.75, 0.75)\}
                                 +x+1/4,-y+3/4,+z+3/4
     \{1 \mid (0.5, 0.5, 0.0)\}
                                    +x+1/2, +y+1/2, +z
   \{2\ 00z\mid (0.5,0.5,0.0)\}
                                    -x+1/2,-y+1/2,+z
  \{m \ 0yz | (0.75, 0.75, 0.25)\}
                                 -x+3/4, +y+3/4, +z+1/4
                                 +x+1/4,-y+1/4,+z+1/4
  \{m \times 0z \mid (0.25, 0.25, 0.25)\} \mid
*******
space group: 43:cab {'Hall': 'F -2d 2', 'HM': 'F 2 d d'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x+1/4, +y+1/4, -z+1/4
+x,-y,-z
            Seitz
                                          Jones
     {1|(0.0,0.0,0.0)}
                                        +x,+y,+z
  \{m_xy0|(0.25,0.25,0.25)\}
                                 +x+1/4, +y+1/4, -z+1/4
   \{2_{x00} | (0.0,0.0,0.0)\}
                                        +x,-y,-z
  \{m \times 0z \mid (0.25, 0.25, 0.25)\} \mid
                                 +x+1/4,-y+1/4,+z+1/4
     \{1 \mid (0.0, 0.5, 0.5)\}
                                    +x,+y+1/2,+z+1/2
```

```
+x+1/4, +y+3/4, -z+3/4
  \{m_xy0|(0.25,0.75,0.75)\}\
   \{2_{x00}|(0.0,0.5,0.5)\}
                                  +x,-y+1/2,-z+1/2
  \{m_x0z \mid (0.25, 0.75, 0.75)\}
                                +x+1/4, -y+3/4, +z+3/4
                                  +x+1/2, +y, +z+1/2
     \{1 \mid (0.5, 0.0, 0.5)\}
  \{m_xy0|(0.75,0.25,0.75)\}
                                +x+3/4, +y+1/4, -z+3/4
   \{2_{x00}|(0.5,0.0,0.5)\}
                                  +x+1/2,-y,-z+1/2
  \{m_x0z|(0.75,0.25,0.75)\}
                                +x+3/4,-y+1/4,+z+3/4
     \{1 \mid (0.5, 0.5, 0.0)\}
                                  +x+1/2, +y+1/2, +z
  \{m_xy0|(0.75,0.75,0.25)\}
                                +x+3/4, +y+3/4, -z+1/4
   \{2_{x00} | (0.5, 0.5, 0.0)\}
                                  +x+1/2,-y+1/2,-z
  \{m_x0z|(0.75,0.75,0.25)\}
                                +x+3/4,-y+3/4,+z+1/4
******
space group: 43:bca {'Hall': 'F -2d -2d', 'HM': 'F d 2 d'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x+1/4, +y+1/4, -z+1/4
-x+1/4, +y+1/4, +z+1/4
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  \{m_xy0|(0.25,0.25,0.25)\}
                                +x+1/4, +y+1/4, -z+1/4
                                -x+1/4, +y+1/4, +z+1/4
  \{m_0yz \mid (0.25, 0.25, 0.25)\}
   {2_0y0|(0.5,0.5,0.0)}
                                  -x+1/2,+y+1/2,-z
                                  +x,+y+1/2,+z+1/2
     \{1|(0.0,0.5,0.5)\}
  {m_xy0|(0.25,0.75,0.75)}
                                +x+1/4, +y+3/4, -z+3/4
  \{m_0yz \mid (0.25, 0.75, 0.75)\}
                                -x+1/4, +y+3/4, +z+3/4
   {2_0y0|(0.5,0.0,0.5)}
                                  -x+1/2,+y,-z+1/2
     \{1 \mid (0.5, 0.0, 0.5)\}
                                  +x+1/2,+y,+z+1/2
                                +x+3/4, +y+1/4, -z+3/4
  {m_xy0|(0.75,0.25,0.75)}
  \{m_0yz \mid (0.75, 0.25, 0.75)\}
                                -x+3/4, +y+1/4, +z+3/4
   {2_0y0|(0.0,0.5,0.5)}
                                  -x, +y+1/2, -z+1/2
                                  +x+1/2, +y+1/2, +z
     \{1 \mid (0.5, 0.5, 0.0)\}
                                +x+3/4,+y+3/4,-z+1/4
  \{m_xy0|(0.75,0.75,0.25)\}
  \{m_0yz \mid (0.75, 0.75, 0.25)\}
                                -x+3/4, +y+3/4, +z+1/4
   {2_0y0|(0.0,0.0,0.0)}
                                       -x,+y,-z
*******
space group: 44 {'Hall': 'I 2 -2', 'HM': 'I m m 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x,+y,+z
           Seitz
                                    Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                    -x,-y,+z
  \{m_0yz \mid (0.0,0.0,0.0)\} \mid
                                    -x,+y,+z
  \{m \times 0z \mid (0.0, 0.0, 0.0)\}
                                    +x,-y,+z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                           | -x+1/2, -y+1/2, +z+1/2 |
 \{m_0yz \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, +y+1/2, +z+1/2
  \{m_x0z | (0.5, 0.5, 0.5)\} | +x+1/2, -y+1/2, +z+1/2
*******
space group: 44:cab {'Hall': 'I -2 2', 'HM': 'I 2 m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y,-z
+x,-y,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{m_xy0|(0.0,0.0,0.0)\}
                                    +x,+y,-z
 {2_x00|(0.0,0.0,0.0)} |
                                    +x,-y,-z
  \{m_x0z|(0.0,0.0,0.0)\}
                                    +x,-y,+z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2, +y+1/2, +z+1/2
                             +x+1/2, +y+1/2, -z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
 \{2 \times 00 \mid (0.5, 0.5, 0.5)\} \mid +x+1/2, -y+1/2, -z+1/2
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
******
space group: 44:bca {'Hall': 'I -2 -2', 'HM': 'I m 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z
-X,+Y,+Z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{m_xy0|(0.0,0.0,0.0)\}
                                    +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                    -x,+y,+z
  {2_0y0|(0.0,0.0,0.0)} |
                                    -x,+y,-z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  {m_xy0|(0.5,0.5,0.5)}
                             +x+1/2,+y+1/2,-z+1/2
 \{m_0yz \mid (0.5,0.5,0.5)\} \mid -x+1/2,+y+1/2,+z+1/2
| {2_0y0|(0.5,0.5,0.5)} | -x+1/2,+y+1/2,-z+1/2 |
```

.

```
*******
space group: 45 {'Hall': 'I 2 -2c', 'HM': 'I b a 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x, +y, +z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +X,+Y,+Z
  {2_00z|(0.0,0.0,0.0)}
                                  -x,-y,+z
 {m_0yz|(0.0,0.0,0.5)} |
                                -x,+y,+z+1/2
  \{m_x0z | (0.0,0.0,0.5)\} \mid
                                +x,-y,+z+1/2
    \{1 \mid (0.5, 0.5, 0.5)\}
                            +x+1/2,+y+1/2,+z+1/2
  \{2_{00z} | (0.5, 0.5, 0.5)\}
                            -x+1/2,-y+1/2,+z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\} \mid
                              -x+1/2,+y+1/2,+z
  \{m_x0z | (0.5, 0.5, 0.0)\} \mid
                              +x+1/2,-y+1/2,+z
*******
space group: 45:cab {'Hall': 'I -2a 2', 'HM': 'I 2 c b'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x+1/2,+y,-z
+x,-y,-z
          Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{m_xy0 | (0.5,0.0,0.0)\}
                                +x+1/2,+y,-z
 \{2_{x00} | (0.0, 0.0, 0.0)\}
                                  +x,-y,-z
  \{m_x0z|(0.5,0.0,0.0)\}
                                +x+1/2,-y,+z
    \{1|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, +z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                              +x, +y+1/2, -z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
  \{m_x0z | (0.0,0.5,0.5)\} \mid
                              +x,-y+1/2,+z+1/2
*******
space group: 45:bca {'Hall': 'I -2b -2b', 'HM': 'I c 2 a'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y+1/2,-z
-x,+y+1/2,+z
                                    Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{m_xy0|(0.0,0.5,0.0)\}
                                 +x,+y+1/2,-z
  \{m_0yz \mid (0.0, 0.5, 0.0)\}
                                 -x, +y+1/2, +z
                                   -x, +y, -z
  {2_0y0|(0.0,0.0,0.0)}
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2, +y+1/2, +z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                               +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                               -x+1/2,+y,+z+1/2
  \{2_0y0 \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, +y+1/2, -z+1/2
*******
space group: 46 {'Hall': 'I 2 -2a', 'HM': 'I m a 2'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
-x+1/2,+y,+z
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                                 -x+1/2,+y,+z
  \{m_x0z \mid (0.5,0.0,0.0)\}
                                 +x+1/2,-y,+z
    \{1|(0.5,0.5,0.5)\}
                             +x+1/2, +y+1/2, +z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, +z+1/2
 \{m \ 0yz | (0.0, 0.5, 0.5)\}
                               -x, +y+1/2, +z+1/2
  \{m_x0z|(0.0,0.5,0.5)\}
                               +x,-y+1/2,+z+1/2
*******
space group: 46:ba-c {'Hall': 'I 2 -2b', 'HM': ' I b m 2'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z
-x,+y+1/2,+z
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
  \{m_0yz \mid (0.0,0.5,0.0)\}
                                 -x,+y+1/2,+z
  \{m_x0z|(0.0,0.5,0.0)\}
                                 +x,-y+1/2,+z
    \{1|(0.5,0.5,0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, +z+1/2
 \{m_0yz \mid (0.5,0.0,0.5)\}
                               -x+1/2,+y,+z+1/2
  \{m_x0z|(0.5,0.0,0.5)\}
                               +x+1/2,-y,+z+1/2
```

```
space group: 46:cab {'Hall': 'I -2b 2', 'HM': 'I 2 m b'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
+x,+y+1/2,-z
+x,-y,-z
          Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 {m_xy0|(0.0,0.5,0.0)} |
                               +x,+y+1/2,-z
| {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
  \{m_x0z | (0.0,0.5,0.0)\} \mid
                               +x,-y+1/2,+z
    \{1 \mid (0.5, 0.5, 0.5)\}
                          +x+1/2,+y+1/2,+z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                           +x+1/2,+y,-z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                          +x+1/2,-y+1/2,-z+1/2
| \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
*******
space group: 46:-cba {'Hall': 'I -2c 2', 'HM': ' I 2 c m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
+x,+y,-z+1/2
+x,-y,-z
          Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  \{m_xy0|(0.0,0.0,0.5)\}
                               +x,+y,-z+1/2
  {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
  \{m_x0z | (0.0,0.0,0.5)\} \mid
                              +x,-y,+z+1/2
    \{1|(0.5,0.5,0.5)\}
                          +x+1/2,+y+1/2,+z+1/2
 \{m_xy0|(0.5,0.5,0.0)\} +x+1/2,+y+1/2,-z
\{2_{x00}, (0.5, 0.5, 0.5)\} + x+1/2, -y+1/2, -z+1/2
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z
. . . . . . . . . . . . . . . . . . .
*******
space group: 46:bca {'Hall': 'I -2c -2c', 'HM': 'I c 2 m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
+x,+y,-z+1/2
-x,+y,+z+1/2
```

```
Seitz
                                     Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
  \{m \times y0 \mid (0.0, 0.0, 0.5)\}
                                 +x,+y,-z+1/2
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                 -x,+y,+z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                   -x,+y,-z
    \{1|(0.5,0.5,0.5)\}
                             +x+1/2, +y+1/2, +z+1/2
  \{m_xy0 | (0.5, 0.5, 0.0)\}
                               +x+1/2, +y+1/2, -z
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                               -x+1/2,+y+1/2,+z
  \{2_0y0|(0.5,0.5,0.5)\}
                            -x+1/2,+y+1/2,-z+1/2
*******
space group: 46:a-cb {'Hall': 'I -2a -2a', 'HM': ' I m 2 a'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
+x+1/2, +y, -z
-x+1/2,+y,+z
           Seitz
                                     Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
  \{m_xy0|(0.5,0.0,0.0)\}
                                 +x+1/2, +y, -z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                                 -x+1/2,+y,+z
  {2_0y0|(0.0,0.0,0.0)}
                                   -x,+y,-z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                               +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.0, 0.5, 0.5)\}
                               -x, +y+1/2, +z+1/2
  {2_0y0|(0.5,0.5,0.5)}
                             -x+1/2,+y+1/2,-z+1/2
*******
space group: 47 {'Hall': ' -P 2 2', 'HM': 'P m m m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z
           Seitz
                              Jones
    {1|(0.0,0.0,0.0)}
                             +x,+y,+z
  \{2_{00z} | (0.0,0.0,0.0)\}
                             -x,-y,+z
  \{2_{x00}|(0.0,0.0,0.0)\}
                             +x,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                             -x, +y, -z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                             -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                             +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                             -x,+y,+z
  \{m \times 0z \mid (0.0, 0.0, 0.0)\}
                             +x,-y,+z
```

```
*******
space group: 48:1 {'Hall': 'P 2 2 -1n', 'HM': 'P n n n:1'}
Crystal system: Orthorhombic
Setting: 1
+x,+y,+z
-x,-y,+z
+x,-y,-z
-x+1/2,-y+1/2,-z+1/2
          Seitz
                                 Jones
   {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 {2_00z|(0.0,0.0,0.0)} |
                                -x,-y,+z
 {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
    \{-1 \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, -y+1/2, -z+1/2
******
space group: 48:2 {'Hall': ' -P 2ab 2bc', 'HM': 'P n n n:2'}
Crystal system: Orthorhombic
Setting: 2
+x,+y,+z
-x+1/2, -y+1/2, +z
+x,-y+1/2,-z+1/2
          Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                             +x,+y,+z
                         -x+1/2, -y+1/2, +z
 {2_00z|(0.5,0.5,0.0)} |
 \{2_x00|(0.0,0.5,0.5)\} \mid +x,-y+1/2,-z+1/2
 \{2_0y0|(0.5,0.0,0.5)\} \mid -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                             -x,-y,-z
  \{m_xy0|(0.5,0.5,0.0)\}
                          +x+1/2, +y+1/2, -z
 {m_0yz|(0.0,0.5,0.5)} |
                          -x, +y+1/2, +z+1/2
| \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
*******
space group: 49 {'Hall': ' -P 2 2c', 'HM': 'P c c m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z+1/2
   Seitz
                             Jones
   {1|(0.0,0.0,0.0)}
                            +x,+y,+z
```

```
{2_00z|(0.0,0.0,0.0)} |
                               -x,-y,+z
  {2_x00|(0.0,0.0,0.5)}
                            +x,-y,-z+1/2
  {2_0y0|(0.0,0.0,0.5)}
                            -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
                               +x,+y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
 \{m_0yz \mid (0.0,0.0,0.5)\}
                            -x,+y,+z+1/2
  \{m_x0z|(0.0,0.0,0.5)\}
                            +x,-y,+z+1/2
******
space group: 49:cab {'Hall': ' -P 2a 2', 'HM': 'P m a a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2, -y, +z
+x,-y,-z
           Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                            -x+1/2,-y,+z
  \{2_{x00}|(0.0,0.0,0.0)\}
                               +x,-y,-z
  \{2\_0y0|(0.5,0.0,0.0)\}
                            -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                            +x+1/2,+y,-z
 \{m_0yz \mid (0.0,0.0,0.0)\}
                               -x,+y,+z
 \{m \times 0z \mid (0.5, 0.0, 0.0)\}
                            +x+1/2,-y,+z
*******
space group: 49:bca {'Hall': ' -P 2b 2b', 'HM': 'P b m b'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y+1/2,+z
+x,-y+1/2,-z
           Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +X,+Y,+Z
  {2_00z|(0.0,0.5,0.0)}
                            -x,-y+1/2,+z
  \{2_{\times}00 \mid (0.0, 0.5, 0.0)\}
                            +x,-y+1/2,-z
  {2_0y0|(0.0,0.0,0.0)}
                               -x,+y,-z
                               -x,-y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                            +x, +y+1/2, -z
  \{m_xy0|(0.0,0.5,0.0)\}
  \{m_0yz \mid (0.0,0.5,0.0)\}
                            -x,+y+1/2,+z
| {m_x0z|(0.0,0.0,0.0)} |
                               +x,-y,+z
```

```
*******
space group: 50:1 {'Hall': 'P 2 2 -1ab', 'HM': 'P b a n:1'}
Crystal system: Orthorhombic
Setting: 1
+x,+y,+z
-x,-y,+z
+x,-y,-z
-x+1/2,-y+1/2,-z
          Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 {2_00z|(0.0,0.0,0.0)} |
                              -x,-y,+z
| {2_x00|(0.0,0.0,0.0)} |
                              +x,-y,-z
    \{-1 \mid (0.5, 0.5, 0.0)\} \mid -x+1/2, -y+1/2, -z \mid
*******
space group: 50:2 {'Hall': ' -P 2ab 2b', 'HM': 'P b a n:2'}
Crystal system: Orthorhombic
Setting: 2
+x,+y,+z
-x+1/2, -y+1/2, +z
+x,-y+1/2,-z
          Seitz
                               Jones
  {1|(0.0,0.0,0.0)}
                             +x,+y,+z
| \{2_{00z} | (0.5, 0.5, 0.0)\} | -x+1/2, -y+1/2, +z
| \{2_x00|(0.0,0.5,0.0)\} | +x,-y+1/2,-z
  {2 0y0|(0.5,0.0,0.0)} |
                            -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid
                             -x,-y,-z
  \{m_xy0 \mid (0.5, 0.5, 0.0)\} \mid +x+1/2, +y+1/2, -z
| {m_0yz|(0.0,0.5,0.0)} |
                           -x, +y+1/2, +z
                            +x+1/2,-y,+z
| {m_x0z|(0.5,0.0,0.0)} |
*******
space group: 50:1cab {'Hall': 'P 2 2 -1bc', 'HM': ' P n c b:1'}
Crystal system: Orthorhombic
Setting: 1cab
+x,+y,+z
-x,-y,+z
+x,-y,-z
-x,-y+1/2,-z+1/2
. . . . . . . . . . . . . . . . . . . .
          Seitz
                               Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
```

```
{2_00z|(0.0,0.0,0.0)} |
                                -x,-y,+z
  {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
    \{-1 \mid (0.0, 0.5, 0.5)\} \mid -x, -y+1/2, -z+1/2 \mid
*******
space group: 50:2cab {'Hall': ' -P 2b 2bc', 'HM': ' P n c b:2'}
Crystal system: Orthorhombic
Setting: 2cab
+x,+y,+z
-x,-y+1/2,+z
+x,-y+1/2,-z+1/2
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
                              -x, -y+1/2, +z
  {2_00z|(0.0,0.5,0.0)} |
  \{2_{x00}|(0.0,0.5,0.5)\}
                           +x,-y+1/2,-z+1/2
 {2_0y0|(0.0,0.0,0.5)} |
                              -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                              +x,+y+1/2,-z
  \{m_0yz \mid (0.0, 0.5, 0.5)\}
                           -x, +y+1/2, +z+1/2
 {m_x0z|(0.0,0.0,0.5)} |
                             +x,-y,+z+1/2
*******
space group: 50:1bca {'Hall': 'P 2 2 -1ac', 'HM': ' P c n a:1'}
Crystal system: Orthorhombic
Setting: 1bca
+x,+y,+z
-x,-y,+z
+x,-y,-z
-x+1/2, -y, -z+1/2
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  {2_00z|(0.0,0.0,0.0)} |
                                -x,-y,+z
| {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
    \{-1 \mid (0.5, 0.0, 0.5)\} \mid -x+1/2, -y, -z+1/2
. . . . . . . . . . . . . . . . . . .
*******
space group: 50:2bca {'Hall': ' -P 2a 2c', 'HM': ' P c n a:2'}
Crystal system: Orthorhombic
Setting: 2bca
+x,+y,+z
-x+1/2,-y,+z
+x,-y,-z+1/2
```

```
Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                                -x+1/2,-y,+z
  \{2_{x00}|(0.0,0.0,0.5)\}
                                +x,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                             -x+1/2, +y, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                                +x+1/2,+y,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y,+z+1/2
  \{m_x0z \mid (0.5,0.0,0.5)\}
                             +x+1/2,-y,+z+1/2
*******
space group: 51 {'Hall': ' -P 2a 2a', 'HM': 'P m m a'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2, -y, +z
+x+1/2,-y,-z
           Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                             -x+1/2, -y, +z
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                             +x+1/2,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                -X,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_xy0 | (0.5,0.0,0.0)\}
                             +x+1/2,+y,-z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                             -x+1/2, +y, +z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                +x,-y,+z
*******
space group: 51:ba-c {'Hall': ' -P 2b 2', 'HM': ' P m m b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z
           Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +X,+Y,+Z
  \{2_{00z} | (0.0, 0.5, 0.0)\}
                             -x,-y+1/2,+z
  \{2_{\times}00 \mid (0.0,0.0,0.0)\}
                                +x,-y,-z
  {2_0y0|(0.0,0.5,0.0)}
                             -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_xy0 | (0.0, 0.5, 0.0)\}
                             +x,+y+1/2,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                -x,+y,+z
```

```
| \{m_x0z|(0.0,0.5,0.0)\} | +x,-y+1/2,+z |
. . . . . . . . . . . . . . . . . . .
*******
space group: 51:cab {'Hall': ' -P 2 2b', 'HM': 'P b m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x,-y,+z
+x,-y+1/2,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                              Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
| {2_00z|(0.0,0.0,0.0)} |
                            -X,-Y,+Z
\{2_{x00}, (0.0, 0.5, 0.0)\} + x, -y+1/2, -z \}
  \{2_0y0|(0.0,0.5,0.0)\} \mid -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid
                             -x,-y,-z
 {m_xy0|(0.0,0.0,0.0)} |
                            +x,+y,-z
| \{m_0yz | (0.0,0.5,0.0)\} | -x,+y+1/2,+z
| \{m_x0z|(0.0,0.5,0.0)\} | +x,-y+1/2,+z
******
space group: 51:-cba {'Hall': ' -P 2c 2c', 'HM': ' P c m m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x,-y,+z+1/2
+x,-y,-z+1/2
          Seitz
                              Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
| \{2_{00z} | (0.0,0.0,0.5)\} | -x,-y,+z+1/2
\{2_x00|(0.0,0.0,0.5)\}\ |\ +x,-y,-z+1/2
| {2_0y0|(0.0,0.0,0.0)} |
                             -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\} \mid
                            -x,-y,-z
 \{m_xy0 | (0.0,0.0,0.5)\} | +x,+y,-z+1/2
\{ m_0yz | (0.0,0.0,0.5) \} | -x,+y,+z+1/2 
| \{m_x0z|(0.0,0.0,0.0)\} | +x,-y,+z
*******
space group: 51:bca {'Hall': ' -P 2c 2', 'HM': 'P m c m'}
Crystal system: Orthorhombic
Setting: bca
+X,+Y,+Z
-x,-y,+z+1/2
```

```
+x,-y,-z
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.5)\}
                            -x,-y,+z+1/2
  \{2_{x00} | (0.0,0.0,0.0)\}
                              +x,-y,-z
  {2_0y0|(0.0,0.0,0.5)}
                            -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{m_xy0|(0.0,0.0,0.5)\}
                            +x,+y,-z+1/2
  \{m_0yz \mid (0.0,0.0,0.0)\}
                              -x,+y,+z
 {m_x0z|(0.0,0.0,0.5)} |
                            +x,-y,+z+1/2
******
space group: 51:a-cb {'Hall': ' -P 2 2a', 'HM': ' P m a m'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x,-y,+z
+x+1/2,-y,-z
          Seitz
                               Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
 {2 00z|(0.0,0.0,0.0)}
                              -X,-Y,+Z
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                            +x+1/2,-y,-z
  {2_0y0|(0.5,0.0,0.0)}
                            -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                              +x,+y,-z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                            -x+1/2,+y,+z
 \{m_x0z|(0.5,0.0,0.0)\}
                            +x+1/2,-y,+z
*******
space group: 52 {'Hall': ' -P 2a 2bc', 'HM': 'P n n a'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2, -y, +z
+x,-y+1/2,-z+1/2
          Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                                -x+1/2,-y,+z
                              +x,-y+1/2,-z+1/2
 {2_x00|(0.0,0.5,0.5)} |
  {2_0y0|(0.5,0.5,0.5)}
                            -x+1/2, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
```

+x+1/2,+y,-z

 $\{m_xy0|(0.5,0.0,0.0)\}$

```
{m_0yz|(0.0,0.5,0.5)} |
                           -x,+y+1/2,+z+1/2
  \{m_x0z|(0.5,0.5,0.5)\} \mid +x+1/2,-y+1/2,+z+1/2 \mid
*******
space group: 52:ba-c {'Hall': ' -P 2b 2n', 'HM': ' P n n b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y+1/2,+z
+x+1/2,-y+1/2,-z+1/2
      . . . . . . . . . . . . .
          Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.0, 0.5, 0.0)\}
                               -x,-y+1/2,+z
  \{2_{x00}|(0.5,0.5,0.5)\}
                           +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                             -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                               +x,+y+1/2,-z
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                           -x+1/2, +y+1/2, +z+1/2
 \{m_x0z|(0.5,0.0,0.5)\}
                             +x+1/2,-y,+z+1/2
*******
space group: 52:cab {'Hall': ' -P 2n 2b', 'HM': 'P b n n'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2,-y+1/2,+z+1/2
+x,-y+1/2,-z
          Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
 \{2_{00z}|(0.5,0.5,0.5)\}
                           -x+1/2,-y+1/2,+z+1/2
  \{2_{x00}|(0.0,0.5,0.0)\}
                               +x,-y+1/2,-z
  {2_0y0|(0.5,0.0,0.5)}
                             -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.5,0.5,0.5)\}
                           +x+1/2,+y+1/2,-z+1/2
 \{m_0yz \mid (0.0,0.5,0.0)\}
                               -x,+y+1/2,+z
  \{m_x0z \mid (0.5,0.0,0.5)\}
                             +x+1/2,-y,+z+1/2
*******
space group: 52:-cba {'Hall': ' -P 2ab 2c', 'HM': ' P c n n'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
```

```
-x+1/2,-y+1/2,+z
+x,-y,-z+1/2
 . . . . . . . . . . . . . . . . . . .
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                -x+1/2, -y+1/2, +z
  \{2_{x00} | (0.0, 0.0, 0.5)\}
                                  +x,-y,-z+1/2
  \{2_0y0|(0.5,0.5,0.5)\}
                             -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.5,0.5,0.0)\}
                                +x+1/2,+y+1/2,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                  -x,+y,+z+1/2
 \{m_x0z|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,+z+1/2
*******
space group: 52:bca {'Hall': ' -P 2ab 2n', 'HM': 'P n c n'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x+1/2,-y+1/2,+z
+x+1/2,-y+1/2,-z+1/2
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +X,+Y,+Z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                -x+1/2,-y+1/2,+z
  \{2_{x00} | (0.5, 0.5, 0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.0,0.5)} |
                                  -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m \times y0 \mid (0.5, 0.5, 0.0)\}
                                +x+1/2,+y+1/2,-z
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,+y+1/2,+z+1/2
 \{m_x0z | (0.0,0.0,0.5)\}
                                  +x,-y,+z+1/2
******
space group: 52:a-cb {'Hall': ' -P 2n 2bc', 'HM': ' P n a n'}
Crystal system: Orthorhombic
Setting: a-cb
+X,+Y,+Z
-x+1/2, -y+1/2, +z+1/2
+x,-y+1/2,-z+1/2
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,+z+1/2
  \{2_{x00} | (0.0, 0.5, 0.5)\}
                                +x,-y+1/2,-z+1/2
```

-x+1/2,+y,-z

{2_0y0|(0.5,0.0,0.0)} |

```
\{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
 \{m_xy0 | (0.5,0.5,0.5)\} \mid +x+1/2,+y+1/2,-z+1/2 \mid
                            -x,+y+1/2,+z+1/2
| {m_0yz|(0.0,0.5,0.5)} |
  \{m_x0z | (0.5,0.0,0.0)\} \mid
                                +x+1/2,-y,+z
*******
space group: 53 {'Hall': ' -P 2ac 2', 'HM': 'P m n a'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2,-y,+z+1/2
+x,-y,-z
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +X,+Y,+Z
  {2_00z|(0.5,0.0,0.5)} |
                            -x+1/2, -y, +z+1/2
  {2_x00|(0.0,0.0,0.0)} |
                                +x,-y,-z
 {2_0y0|(0.5,0.0,0.5)} |
                           -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                            +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.0,0.0,0.0)\} \mid
                               -x,+y,+z
 \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
*******
space group: 53:ba-c {'Hall': ' -P 2bc 2bc', 'HM': ' P n m b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y+1/2,-z+1/2
 . . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
| \{2_{00z} | (0.0,0.5,0.5)\} | -x,-y+1/2,+z+1/2
  \{2_{x00} | (0.0, 0.5, 0.5)\} \mid
                            +x,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.0,0.0)} |
                                -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
| \{m_xy0|(0.0,0.5,0.5)\} | +x,+y+1/2,-z+1/2
| \{m_0yz | (0.0, 0.5, 0.5)\}
                            -x, +y+1/2, +z+1/2
| {m_x0z|(0.0,0.0,0.0)} |
                                +x,-y,+z
. . . . . . . . . . . . . . . . . . .
*******
space group: 53:cab {'Hall': ' -P 2ab 2ab', 'HM': 'P b m n'}
Crystal system: Orthorhombic
```

Setting: cab

```
+x,+y,+z
-x+1/2,-y+1/2,+z
+x+1/2,-y+1/2,-z
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 {2_00z|(0.5,0.5,0.0)}
                           -x+1/2, -y+1/2, +z
 {2_x00|(0.5,0.5,0.0)}
                           +x+1/2,-y+1/2,-z
  {2_0y0|(0.0,0.0,0.0)}
                                -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_xy0|(0.5,0.5,0.0)\}
                           +x+1/2, +y+1/2, -z
| {m_0yz|(0.5,0.5,0.0)}
                           -x+1/2,+y+1/2,+z
| \{m_x0z|(0.0,0.0,0.0)\}
                                +x,-y,+z
*******
space group: 53:-cba {'Hall': ' -P 2 2ac', 'HM': ' P c n m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x,-y,+z
+x+1/2,-y,-z+1/2
. . . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                -x,-y,+z
 {2_x00|(0.5,0.0,0.5)}
                           +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                            -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                +x,+y,-z
 \{m_0yz \mid (0.5,0.0,0.5)\}\
                           -x+1/2, +y, +z+1/2
 {m_x0z|(0.5,0.0,0.5)} |
                           +x+1/2,-y,+z+1/2
******
space group: 53:bca {'Hall': ' -P 2 2bc', 'HM': 'P n c m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y,+z
+x,-y+1/2,-z+1/2
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                -x,-y,+z
 \{2_x00|(0.0,0.5,0.5)\} \mid +x,-y+1/2,-z+1/2 \mid
```

```
\{2_0y0|(0.0,0.5,0.5)\} \mid -x,+y+1/2,-z+1/2 \mid
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                               +x,+y,-z
| \{m_0yz | (0.0,0.5,0.5)\} | -x,+y+1/2,+z+1/2
| \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
*******
space group: 53:a-cb {'Hall': ' -P 2ab 2', 'HM': ' P m a n'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x+1/2, -y+1/2, +z
+x,-y,-z
          Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
 {2_00z|(0.5,0.5,0.0)}
                          -x+1/2, -y+1/2, +z
 {2_x00|(0.0,0.0,0.0)}
                               +x,-y,-z
  {2_0y0|(0.5,0.5,0.0)}
                          -x+1/2,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
 \{m_xy0|(0.5,0.5,0.0)\}
                          +x+1/2, +y+1/2, -z
 {m_0yz|(0.0,0.0,0.0)} |
                              -x,+y,+z
  \{m_x0z|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,+z \mid
*******
space group: 54 {'Hall': ' -P 2a 2ac', 'HM': 'P c c a'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2, -y, +z
+x+1/2,-y,-z+1/2
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
  {2_00z|(0.5,0.0,0.0)} |
                             -x+1/2,-y,+z
 {2_x00|(0.5,0.0,0.5)}
                          +x+1/2,-y,-z+1/2
 {2_0y0|(0.0,0.0,0.5)} |
                             -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                            +x+1/2,+y,-z
 \{m_0yz \mid (0.5,0.0,0.5)\}
                          -x+1/2,+y,+z+1/2
  \{m_x0z|(0.0,0.0,0.5)\}
                             +x,-y,+z+1/2
*******
```

space group: 54:ba-c {'Hall': ' -P 2b 2c', 'HM': ' P c c b'}

Crystal system: Orthorhombic

```
Setting: ba-c
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
   \{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
| {2_00z|(0.0,0.5,0.0)} |
                             -x,-y+1/2,+z
                             +x,-y,-z+1/2
| {2_x00|(0.0,0.0,0.5)} |
  {2_0y0|(0.0,0.5,0.5)}
                           -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                             +x,+y+1/2,-z
| \{m_0yz | (0.0,0.0,0.5)\}
                             -x, +y, +z+1/2
 \{m_x0z|(0.0,0.5,0.5)\}
                           +x,-y+1/2,+z+1/2
*******
space group: 54:cab {'Hall': ' -P 2a 2b', 'HM': 'P b a a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2,-y,+z
+x,-y+1/2,-z
          Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
| {2_00z|(0.5,0.0,0.0)} |
                             -x+1/2,-y,+z
| {2_x00|(0.0,0.5,0.0)} |
                            +x,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\}
                           -x+1/2, +y+1/2, -z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                             -x,-y,-z
  {m_xy0|(0.5,0.0,0.0)} |
                             +x+1/2,+y,-z
                           -x, +y+1/2, +z
 {m_0yz|(0.0,0.5,0.0)} |
 \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z
*******
space group: 54:-cba {'Hall': ' -P 2ac 2c', 'HM': ' P c a a'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x+1/2, -y, +z+1/2
+x,-y,-z+1/2
          Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                             +x,+y,+z
\{2\_00z|(0.5,0.0,0.5)\} \mid -x+1/2,-y,+z+1/2 \mid
```

```
\{2_{x00} | (0.0,0.0,0.5)\} \mid
                             +x,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.0)} |
                             -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                           +x+1/2, +y, -z+1/2
 \{m_0yz \mid (0.0,0.0,0.5)\}\
                             -x, +y, +z+1/2
| {m_x0z|(0.5,0.0,0.0)} |
                              +x+1/2,-y,+z
******
space group: 54:bca {'Hall': ' -P 2bc 2b', 'HM': 'P b c b'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y+1/2,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 \{2_{00z}|(0.0,0.5,0.5)\} \mid -x,-y+1/2,+z+1/2
  \{2_{x00} | (0.0, 0.5, 0.0)\}
                             +x,-y+1/2,-z
  {2_0y0|(0.0,0.0,0.5)} |
                              -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
| {m_xy0|(0.0,0.5,0.5)} |
                           +x,+y+1/2,-z+1/2
 \{m_0yz \mid (0.0,0.5,0.0)\} \mid
                             -x, +y+1/2, +z
| \{m_x0z|(0.0,0.0,0.5)\} |
                              +x,-y,+z+1/2
******
space group: 54:a-cb {'Hall': ' -P 2b 2ab', 'HM': ' P b a b'}
```

Crystal system: Orthorhombic

Setting: a-cb +x,+y,+z-x,-y+1/2,+z+x+1/2,-y+1/2,-z

+	·
Seitz	Jones
{1 (0.0,0.0,0.0)} {2_00z (0.0,0.5,0.0)} {2_x00 (0.5,0.5,0.0)} {2_0y0 (0.5,0.0,0.0)} {-1 (0.0,0.0,0.0)} {m_xy0 (0.0,0.5,0.0)} {m_0yz (0.5,0.5,0.0)} {m_x0z (0.5,0.0,0.0)}	+x,+y,+z -x,-y+1/2,+z +x+1/2,-y+1/2,-z -x+1/2,+y,-z -x,-y,-z +x,+y+1/2,-z -x+1/2,+y+1/2,+z +x+1/2,-y,+z

```
space group: 55 {'Hall': ' -P 2 2ab', 'HM': 'P b a m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x+1/2,-y+1/2,-z
  . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
   {1|(0.0,0.0,0.0)}
                                +x,+y,+z
| {2_00z|(0.0,0.0,0.0)} |
                              -X,-Y,+Z
  \{2_x00|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\} \mid -x+1/2,+y+1/2,-z
    \{-1 \mid (0.0,0.0,0.0)\}
                               -X,-Y,-Z
  {m_xy0|(0.0,0.0,0.0)} |
                                +x,+y,-z
| \{m_0yz | (0.5, 0.5, 0.0)\} |
                           -x+1/2,+y+1/2,+z
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z |
*******
space group: 55:cab {'Hall': ' -P 2bc 2', 'HM': 'P m c b'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y,-z
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
| {2_00z|(0.0,0.5,0.5)} |
                           -x,-y+1/2,+z+1/2
  {2 x00|(0.0,0.0,0.0)} |
                              +x,-y,-z
  {2_0y0|(0.0,0.5,0.5)} |
                            -x,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
  {m_xy0|(0.0,0.5,0.5)}
                           +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.0,0.0,0.0)\}
                               -x,+y,+z
 \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
*******
space group: 55:bca {'Hall': ' -P 2ac 2ac', 'HM': 'P c m a'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x+1/2,-y,+z+1/2
+x+1/2,-y,-z+1/2
  . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
```

```
\{2\_00z \mid (0.5,0.0,0.5)\}
                             -x+1/2,-y,+z+1/2
                             +x+1/2,-y,-z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
  {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                             +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                             -x+1/2, +y, +z+1/2
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                 +x,-y,+z
******
space group: 56 {'Hall': ' -P 2ab 2ac', 'HM': 'P c c n'}
Crystal system: Orthorhombic
+X,+Y,+Z
-x+1/2, -y+1/2, +z
+x+1/2,-y,-z+1/2
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                             -x+1/2,-y+1/2,+z
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                             +x+1/2,-y,-z+1/2
  {2_0y0|(0.0,0.5,0.5)}
                             -x,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.5,0.5,0.0)\}
                             +x+1/2,+y+1/2,-z
  \{m_0yz \mid (0.5,0.0,0.5)\}
                             -x+1/2, +y, +z+1/2
 \{m \times 0z \mid (0.0, 0.5, 0.5)\}
                             +x,-y+1/2,+z+1/2
*******
space group: 56:cab {'Hall': ' -P 2ac 2bc', 'HM': 'P n a a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2,-y,+z+1/2
+x,-y+1/2,-z+1/2
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{2_{00z}|(0.5,0.0,0.5)\}
                             -x+1/2,-y,+z+1/2
  \{2_{x00}|(0.0,0.5,0.5)\}
                             +x,-y+1/2,-z+1/2
  \{2_0y0|(0.5,0.5,0.0)\}
                             -x+1/2, +y+1/2, -z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                             +x+1/2,+y,-z+1/2
                             -x,+y+1/2,+z+1/2
  \{m_0yz \mid (0.0,0.5,0.5)\}
                             +x+1/2,-y+1/2,+z
  \{m_x0z|(0.5,0.5,0.0)\}
```

```
space group: 56:bca {'Hall': ' -P 2bc 2ab', 'HM': 'P b n b'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y+1/2,+z+1/2
+x+1/2,-y+1/2,-z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{2_{00z} | (0.0, 0.5, 0.5)\} \mid
                            -x,-y+1/2,+z+1/2
 \{2_{x00} | (0.5, 0.5, 0.0)\} \mid
                            +x+1/2,-y+1/2,-z
 {2_0y0|(0.5,0.0,0.5)}
                            -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
                            +x,+y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                            -x+1/2,+y+1/2,+z
  \{m_x0z|(0.5,0.0,0.5)\}
                            +x+1/2,-y,+z+1/2
******
space group: 57 {'Hall': ' -P 2c 2b', 'HM': 'P b c m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z+1/2
+x,-y+1/2,-z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
 {2_00z|(0.0,0.0,0.5)} |
                              -x,-y,+z+1/2
  \{2_{x00} | (0.0, 0.5, 0.0)\}
                              +x,-y+1/2,-z
  {2_0y0|(0.0,0.5,0.5)}
                            -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_xy0|(0.0,0.0,0.5)\}
                              +x,+y,-z+1/2
  \{m_0yz \mid (0.0, 0.5, 0.0)\}
                              -x,+y+1/2,+z
  \{m_x0z|(0.0,0.5,0.5)\}
                            +x,-y+1/2,+z+1/2
*******
space group: 57:ba-c {'Hall': ' -P 2c 2ac', 'HM': ' P c a m'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y,+z+1/2
+x+1/2,-y,-z+1/2
  . . . . . . . . . . . . . . . . . .
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
```

```
{2_00z|(0.0,0.0,0.5)} |
                              -x,-y,+z+1/2
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                            +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.0)}
                              -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.0,0.0,0.5)\}
                               +x,+y,-z+1/2
 \{m_0yz \mid (0.5,0.0,0.5)\}
                            -x+1/2,+y,+z+1/2
  \{m_x0z|(0.5,0.0,0.0)\}
                               +x+1/2,-y,+z
******
space group: 57:cab {'Hall': ' -P 2ac 2a', 'HM': 'P m c a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2,-y,+z+1/2
+x+1/2,-y,-z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.5)\}
                            -x+1/2,-y,+z+1/2
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                              +x+1/2,-y,-z
  {2_0y0|(0.0,0.0,0.5)}
                              -x,+y,-z+1/2
    \{-1 \mid (0.0,0.0,0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                            +x+1/2, +y, -z+1/2
 \{m_0yz \mid (0.5,0.0,0.0)\}
                              -x+1/2,+y,+z
 \{m \times 0z \mid (0.0, 0.0, 0.5)\}
                              +x,-y,+z+1/2
*******
space group: 57:-cba {'Hall': ' -P 2b 2a', 'HM': ' P m a b'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x,-y+1/2,+z
+x+1/2,-y,-z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +X,+Y,+Z
  {2_00z|(0.0,0.5,0.0)}
                              -x,-y+1/2,+z
  \{2_{\times}00 \mid (0.5, 0.0, 0.0)\}
                              +x+1/2,-y,-z
  {2_0y0|(0.5,0.5,0.0)}
                            -x+1/2,+y+1/2,-z
    \{-1 \mid (0.0,0.0,0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                               +x,+y+1/2,-z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                              -x+1/2,+y,+z
| {m_x0z|(0.5,0.5,0.0)} | +x+1/2,-y+1/2,+z
```

```
*******
space group: 57:bca {'Hall': ' -P 2a 2ab', 'HM': 'P b m a'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x+1/2,-y,+z
+x+1/2,-y+1/2,-z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
 {2_00z|(0.5,0.0,0.0)} |
                             -x+1/2,-y,+z
\{2_x00|(0.5,0.5,0.0)\} +x+1/2,-y+1/2,-z
 {2_0y0|(0.0,0.5,0.0)} |
                            -x, +y+1/2, -z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
 \{m_xy0|(0.5,0.0,0.0)\}
                            +x+1/2,+y,-z
| \{m_0yz | (0.5, 0.5, 0.0)\} |
                          -x+1/2,+y+1/2,+z
 \{m_x0z|(0.0,0.5,0.0)\} +x,-y+1/2,+z
*******
space group: 57:a-cb {'Hall': ' -P 2bc 2c', 'HM': ' P c m b'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y,-z+1/2
          Seitz
                                Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                             +x,+y,+z
  \{2\_00z | (0.0,0.5,0.5)\} \mid
                          -x,-y+1/2,+z+1/2
 {2_x00|(0.0,0.0,0.5)} |
                            +x,-y,-z+1/2
  {2_0y0|(0.0,0.5,0.0)} |
                             -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{m_xy0 | (0.0, 0.5, 0.5)\}
                          +x, +y+1/2, -z+1/2
 \{m_0yz | (0.0,0.0,0.5)\}
                            -x,+y,+z+1/2
                             +x,-y+1/2,+z
 \{m_x0z|(0.0,0.5,0.0)\}
*******
space group: 58 {'Hall': ' -P 2 2n', 'HM': 'P n n m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x+1/2,-y+1/2,-z+1/2
          Seitz
                                  Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                  -x,-y,+z
  \{2_x00|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
  \{2 \text{ 0y0} | (0.5, 0.5, 0.5)\}
                            -x+1/2, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                  +x,+y,-z
 \{m_0yz|(0.5,0.5,0.5)\}
                            -x+1/2,+y+1/2,+z+1/2
  \{m_x0z | (0.5, 0.5, 0.5)\} | +x+1/2, -y+1/2, +z+1/2
*******
space group: 58:cab {'Hall': ' -P 2n 2', 'HM': 'P m n n'}
Crystal system: Orthorhombic
Setting: cab
+X,+V,+Z
-x+1/2, -y+1/2, +z+1/2
+x,-y,-z
          Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +X,+Y,+Z
  \{2\_00z \mid (0.5, 0.5, 0.5)\}\ \mid
                            -x+1/2,-y+1/2,+z+1/2
 {2_x00|(0.0,0.0,0.0)}
                                  +x,-y,-z
                            -x+1/2,+y+1/2,-z+1/2
  {2_0y0|(0.5,0.5,0.5)}
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
 \{m \ 0 \ yz \mid (0.0, 0.0, 0.0)\}
                                  -X,+Y,+Z
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
******
space group: 58:bca {'Hall': ' -P 2n 2n', 'HM': 'P n m n'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x+1/2, -y+1/2, +z+1/2
+x+1/2,-y+1/2,-z+1/2
          Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  {2_00z|(0.5,0.5,0.5)}
                            -x+1/2,-y+1/2,+z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.0,0.0)} |
                                  -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
 \{m_0yz | (0.5,0.5,0.5)\}
                            -x+1/2,+y+1/2,+z+1/2
 {m_x0z|(0.0,0.0,0.0)}
                                  +x,-y,+z
```

```
space group: 59:1 {'Hall': 'P 2 2ab -1ab', 'HM': 'P m m n:1'}
Crystal system: Orthorhombic
Setting: 1
+x,+y,+z
-x,-y,+z
+x+1/2,-y+1/2,-z
-x+1/2, -y+1/2, -z
. . . . . . . . . . . . . . . . . . .
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
| {2_00z|(0.0,0.0,0.0)} |
                              -x,-y,+z
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                           +x+1/2,-y+1/2,-z
    \{-1 \mid (0.5, 0.5, 0.0)\} \mid -x+1/2, -y+1/2, -z \mid
*******
space group: 59:2 {'Hall': ' -P 2ab 2a', 'HM': 'P m m n:2'}
Crystal system: Orthorhombic
Setting: 2
+x,+y,+z
-x+1/2,-y+1/2,+z
+x+1/2,-y,-z
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                               +x,+y,+z
| {2_00z|(0.5,0.5,0.0)} |
                           -x+1/2, -y+1/2, +z
  \{2_{x00} | (0.5, 0.0, 0.0)\} \mid
                              +x+1/2,-y,-z
                              -x,+y+1/2,-z
  {2_0y0|(0.0,0.5,0.0)} |
    \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
  {m_xy0|(0.5,0.5,0.0)}
                           +x+1/2,+y+1/2,-z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                             -x+1/2,+y,+z
 {m_x0z|(0.0,0.5,0.0)} |
                              +x,-y+1/2,+z
*******
space group: 59:1cab {'Hall': 'P 2bc 2 -1bc', 'HM': ' P n m m:1'}
Crystal system: Orthorhombic
Setting: 1cab
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y,-z
-x,-y+1/2,-z+1/2
          Seitz
                                 Jones
```

```
{1|(0.0,0.0,0.0)}
                              +x,+y,+z
 \{2\_00z \mid (0.0,0.5,0.5)\} \mid -x,-y+1/2,+z+1/2 \mid
  \{2_x00|(0.0,0.0,0.0)\} | +x,-y,-z
    \{-1 \mid (0.0, 0.5, 0.5)\} \mid -x, -y+1/2, -z+1/2 \mid
*******
space group: 59:2cab {'Hall': ' -P 2c 2bc', 'HM': ' P n m m:2'}
Crystal system: Orthorhombic
Setting: 2cab
+x,+y,+z
-x,-y,+z+1/2
+x,-y+1/2,-z+1/2
. . . . . . . . . . . . . . . . . . .
          Seitz
                                Jones
   {1|(0.0,0.0,0.0)}
                              +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.5)\}\ \mid
                             -x,-y,+z+1/2
| {2_x00|(0.0,0.5,0.5)} | +x,-y+1/2,-z+1/2
| {2_0y0|(0.0,0.5,0.0)} |
                            -x,+y+1/2,-z
                              -x,-y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
 \{m_xy0|(0.0,0.0,0.5)\}
                            +x,+y,-z+1/2
| \{m_0yz | (0.0,0.5,0.5)\} | -x,+y+1/2,+z+1/2
| \{m_x 0z | (0.0, 0.5, 0.0)\} | +x,-y+1/2,+z
*******
space group: 59:1bca {'Hall': 'P 2ac 2ac -1ac', 'HM': ' P m n m:1'}
Crystal system: Orthorhombic
Setting: 1bca
+x,+y,+z
-x+1/2, -y, +z+1/2
+x+1/2,-y,-z+1/2
-x+1/2, -y, -z+1/2
. . . . . . . . . . . . . . . . . . . .
          Seitz
                         Jones
   {1|(0.0,0.0,0.0)}
                           +x,+y,+z
 \{2\_00z | (0.5,0.0,0.5)\} | -x+1/2,-y,+z+1/2
\{2_x00|(0.5,0.0,0.5)\} \mid +x+1/2,-y,-z+1/2 \mid
   \{-1|(0.5,0.0,0.5)\} \mid -x+1/2,-y,-z+1/2 \mid
*******
space group: 59:2bca {'Hall': ' -P 2c 2a', 'HM': ' P m n m:2'}
Crystal system: Orthorhombic
Setting: 2bca
+X,+Y,+Z
-x,-y,+z+1/2
```

```
+x+1/2,-y,-z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.5)\}
                               -x,-y,+z+1/2
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                               +x+1/2,-y,-z
  {2_0y0|(0.5,0.0,0.5)}
                            -x+1/2, +y, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.0,0.0,0.5)\}
                               +x,+y,-z+1/2
  \{m_0yz \mid (0.5,0.0,0.0)\}
                               -x+1/2,+y,+z
 \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2 |
******
space group: 60 {'Hall': ' -P 2n 2ab', 'HM': 'P b c n'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2, -y+1/2, +z+1/2
+x+1/2,-y+1/2,-z
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
 \{2\_00z \mid (0.5, 0.5, 0.5)\} \mid
                            -x+1/2, -y+1/2, +z+1/2
 \{2 \times 00 \mid (0.5, 0.5, 0.0)\}
                               +x+1/2,-y+1/2,-z
  {2_0y0|(0.0,0.0,0.5)}
                                 -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                               -x+1/2,+y+1/2,+z
  \{m \times 0z \mid (0.0, 0.0, 0.5)\}
                                 +x,-y,+z+1/2
******
space group: 60:ba-c {'Hall': ' -P 2n 2c', 'HM': ' P c a n'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x+1/2, -y+1/2, +z+1/2
+x,-y,-z+1/2
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                            -x+1/2,-y+1/2,+z+1/2
 {2_x00|(0.0,0.0,0.5)} |
                                 +x,-y,-z+1/2
  {2_0y0|(0.5,0.5,0.0)} |
                               -x+1/2,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
```

 $\{m_xy0|(0.5,0.5,0.5)\} \mid +x+1/2,+y+1/2,-z+1/2 \mid$

```
\{m_0yz \mid (0.0,0.0,0.5)\} \mid
                                -x,+y,+z+1/2
 \{m_x0z|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,+z
*******
space group: 60:cab {'Hall': ' -P 2a 2n', 'HM': 'P n c a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2, -y, +z
+x+1/2,-y+1/2,-z+1/2
        . . . . . . . . . . . .
          Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
 \{2\_00z \mid (0.5,0.0,0.0)\}
                                -x+1/2,-y,+z
  \{2_{x00} | (0.5, 0.5, 0.5)\}
                           +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.5,0.5)}
                              -x,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
                                +x+1/2, +y, -z
  \{m_xy0 | (0.5,0.0,0.0)\}
 \{m_0yz \mid (0.5, 0.5, 0.5)\}
                           -x+1/2, +y+1/2, +z+1/2
 \{m_x0z|(0.0,0.5,0.5)\}
                              +x,-y+1/2,+z+1/2
*******
space group: 60:-cba {'Hall': ' -P 2bc 2n', 'HM': ' P n a b'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x,-y+1/2,+z+1/2
+x+1/2, -y+1/2, -z+1/2
          Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
 {2_00z|(0.0,0.5,0.5)}
                              -x,-y+1/2,+z+1/2
 \{2_{x00} | (0.5, 0.5, 0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.5,0.0,0.0)}
                                -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
 \{m_xy0|(0.0,0.5,0.5)\}
                              +x,+y+1/2,-z+1/2
 \{m_0yz \mid (0.5, 0.5, 0.5)\}
                           -x+1/2,+y+1/2,+z+1/2
 \{m_x0z \mid (0.5,0.0,0.0)\}
                                +x+1/2,-y,+z
*******
space group: 60:bca {'Hall': ' -P 2ac 2b', 'HM': 'P b n a'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
```

```
-x+1/2,-y,+z+1/2
+x,-y+1/2,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.5)\}
                               -x+1/2,-y,+z+1/2
                                 +x,-y+1/2,-z
  \{2_{x00} | (0.0, 0.5, 0.0)\}
  \{2_0y0|(0.5,0.5,0.5)\}
                             -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0 | (0.5,0.0,0.5)\}
                               +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.0, 0.5, 0.0)\} \mid
                                 -x,+y+1/2,+z
 \{m_x0z|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,+z+1/2
*******
space group: 60:a-cb {'Hall': ' -P 2b 2ac', 'HM': ' P c n b'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x,-y+1/2,+z
+x+1/2,-y,-z+1/2
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +X,+Y,+Z
  \{2\_00z \mid (0.0, 0.5, 0.0)\}
                                 -x,-y+1/2,+z
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                               +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.5,0.5)} |
                             -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m \times y0 \mid (0.0, 0.5, 0.0)\}
                                 +x,+y+1/2,-z
  \{m_0yz \mid (0.5,0.0,0.5)\}
                               -x+1/2,+y,+z+1/2
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
******
space group: 61 {'Hall': ' -P 2ac 2ab', 'HM': 'P b c a'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2,-y,+z+1/2
+x+1/2,-y+1/2,-z
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
 \{2\_00z \mid (0.5,0.0,0.5)\}
                             -x+1/2, -y, +z+1/2
| {2_x00|(0.5,0.5,0.0)}
                             +x+1/2,-y+1/2,-z
  {2_0y0|(0.0,0.5,0.5)}
                             -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
```

```
\{m_xy0|(0.5,0.0,0.5)\} \mid +x+1/2,+y,-z+1/2 \mid
 \{m_0yz \mid (0.5, 0.5, 0.0)\} \mid
                           -x+1/2,+y+1/2,+z
  \{m_x0z|(0.0,0.5,0.5)\} \mid +x,-y+1/2,+z+1/2 \mid
*******
space group: 61:ba-c {'Hall': ' -P 2bc 2ac', 'HM': ' P c a b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y+1/2,+z+1/2
+x+1/2,-y,-z+1/2
          Seitz
                                 Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                +X,+Y,+Z
  \{2_{00z}|(0.0,0.5,0.5)\}
                           -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
                           +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.5,0.0)}
                           -x+1/2, +y+1/2, -z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                -x,-y,-z
  \{m_xy0|(0.0,0.5,0.5)\}
                           +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                           -x+1/2, +y, +z+1/2
  \{m_x0z|(0.5,0.5,0.0)\}
                           +x+1/2,-y+1/2,+z
*******
space group: 62 {'Hall': ' -P 2ac 2n', 'HM': 'P n m a'}
Crystal system: Orthorhombic
+x,+y,+z
-x+1/2, -y, +z+1/2
+x+1/2, -y+1/2, -z+1/2
          Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
 {2_00z|(0.5,0.0,0.5)}
                              -x+1/2,-y,+z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.5,0.0)}
                                -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                              +x+1/2,+y,-z+1/2
 \{m_0yz \mid (0.5, 0.5, 0.5)\}
                           -x+1/2,+y+1/2,+z+1/2
  \{m_x0z \mid (0.0, 0.5, 0.0)\}
                                +x,-y+1/2,+z
*******
space group: 62:ba-c {'Hall': ' -P 2bc 2a', 'HM': ' P m n b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
```

```
-x,-y+1/2,+z+1/2
+x+1/2,-y,-z
. . . . . . . . . . . . . . . . . . .
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                                -x,-y+1/2,+z+1/2
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                                  +x+1/2,-y,-z
  \{2 \text{ 0y0} | (0.5, 0.5, 0.5)\}
                              -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
                                +x,+y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
  \{m_0yz \mid (0.5,0.0,0.0)\} \mid
                                  -x+1/2,+y,+z
 {m_x0z|(0.5,0.5,0.5)} |
                             +x+1/2,-y+1/2,+z+1/2
*******
space group: 62:cab {'Hall': ' -P 2c 2ab', 'HM': 'P b n m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x,-y,+z+1/2
+x+1/2,-y+1/2,-z
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +X,+Y,+Z
  \{2\_00z \mid (0.0,0.0,0.5)\}
                                  -x,-y,+z+1/2
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                                +x+1/2,-y+1/2,-z
  {2_0y0|(0.5,0.5,0.5)} |
                             -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m \times y0 \mid (0.0, 0.0, 0.5)\}
                                  +x,+y,-z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\} \mid
                                -x+1/2,+y+1/2,+z
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
******
space group: 62:-cba {'Hall': ' -P 2n 2ac', 'HM': ' P c m n'}
Crystal system: Orthorhombic
Setting: -cba
+X,+Y,+Z
-x+1/2,-y+1/2,+z+1/2
+x+1/2,-y,-z+1/2
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
 \{2\_00z \mid (0.5, 0.5, 0.5)\} \mid
                             -x+1/2, -y+1/2, +z+1/2
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                                +x+1/2,-y,-z+1/2
  {2_0y0|(0.0,0.5,0.0)} |
                                  -x,+y+1/2,-z
```

```
\{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}\ \mid
                              -x+1/2,+y,+z+1/2
  \{m_x0z | (0.0, 0.5, 0.0)\} |
                                +x,-y+1/2,+z
*******
space group: 62:bca {'Hall': ' -P 2n 2a', 'HM': 'P m c n'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x+1/2, -y+1/2, +z+1/2
+x+1/2,-y,-z
. . . . . . . . . . . . . . . . . . . .
          Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                            -x+1/2,-y+1/2,+z+1/2
                                +x+1/2,-y,-z
 {2_x00|(0.5,0.0,0.0)}
  \{2_0y0|(0.0,0.5,0.5)\}
                              -x,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
 {m_0yz|(0.5,0.0,0.0)}
                                -x+1/2,+y,+z
  \{m_x0z|(0.0,0.5,0.5)\}
                              +x,-y+1/2,+z+1/2
*******
space group: 62:a-cb {'Hall': ' -P 2c 2n', 'HM': ' P n a m'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x,-y,+z+1/2
+x+1/2, -y+1/2, -z+1/2
          Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.5)\}
                                -x,-y,+z+1/2
 \{2_{x00}|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
 {2_0y0|(0.5,0.5,0.0)}
                              -x+1/2,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.0,0.0,0.5)\}
                                +x,+y,-z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, +y+1/2, +z+1/2
  \{m_x0z|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,+z
*******
space group: 63 {'Hall': ' -C 2c 2', 'HM': 'C m c m'}
```

Crystal system: Orthorhombic

```
+x,+y,+z
-x,-y,+z+1/2
+x,-y,-z
```

```
Seitz
                                    Jones
  {1|(0.0,0.0,0.0)}
                                   +x,+y,+z
{2_00z|(0.0,0.0,0.5)}
                                 -x,-y,+z+1/2
{2_x00|(0.0,0.0,0.0)}
                                   +x,-y,-z
{2_0y0|(0.0,0.0,0.5)}
                                 -x,+y,-z+1/2
   \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
\{m_xy0|(0.0,0.0,0.5)\}
                                 +x,+y,-z+1/2
\{m_0yz \mid (0.0,0.0,0.0)\}
                                   -x,+y,+z
\{m_x0z \mid (0.0,0.0,0.5)\}
                                 +x,-y,+z+1/2
   \{1 \mid (0.5, 0.5, 0.0)\}
                              +x+1/2,+y+1/2,+z
\{2\_00z \mid (0.5, 0.5, 0.5)\}
                            -x+1/2, -y+1/2, +z+1/2
\{2_{x00}|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,-z
{2_0y0|(0.5,0.5,0.5)}
                            -x+1/2, +y+1/2, -z+1/2
   \{-1 \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,-y+1/2,-z
\{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
\{m_0yz \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,+y+1/2,+z
\{m_x0z \mid (0.5, 0.5, 0.5)\}
                            +x+1/2,-y+1/2,+z+1/2
```

space group: 63:ba-c {'Hall': ' -C 2c 2c', 'HM': ' C c m m'}

Crystal system: Orthorhombic

Setting: ba-c +x,+y,+z

-x,-y,+z+1/2

+x,-y,-z+1/2

.

+	+
Seitz	Jones
	+x,+y,+z -x,-y,+z+1/2 +x,-y,-z+1/2 -x,+y,-z -x,-y,-z +x,+y,-z+1/2 -x,+y,+z+1/2 +x,-y,+z +x+1/2,+y+1/2,+z -x+1/2,-y+1/2,-z+1/2 +x+1/2,-y+1/2,-z+1/2 -x+1/2,-y+1/2,-z -x+1/2,-y+1/2,-z
{m_xy0 (0.5,0.5,0.5)} {m_0yz (0.5,0.5,0.5)} {m_x0z (0.5,0.5,0.0)}	+x+1/2,+y+1/2,-z+1/2 -x+1/2,+y+1/2,+z+1/2 +x+1/2,-y+1/2,+z

 $\{m_x0z \mid (0.5,0.0,0.0)\}$

 $\{1 \mid (0.0, 0.5, 0.5)\}$

 $\{2_00z \mid (0.0, 0.5, 0.5)\}$

 $\{2_x00|(0.5,0.5,0.5)\} \mid +x+1/2,-y+1/2,-z+1/2$

```
*******
space group: 63:cab {'Hall': ' -A 2a 2a', 'HM': 'A m m a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2, -y, +z
+x+1/2,-y,-z
. . . . . . . . . . . . . .
           Seitz
                                     Jones
    \{1 \mid (0.0,0.0,0.0)\}
                                    +X,+Y,+Z
  {2_00z|(0.5,0.0,0.0)}
                                 -x+1/2, -y, +z
  \{2_{x00}|(0.5,0.0,0.0)\}
                                 +x+1/2,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                    -x,+y,-z
                                    -x,-y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
  \{m_xy0|(0.5,0.0,0.0)\}
                                  +x+1/2, +y, -z
                                 -x+1/2,+y,+z
  \{m_0yz \mid (0.5,0.0,0.0)\}
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                    +x,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                               +x,+y+1/2,+z+1/2
                             -x+1/2,-y+1/2,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
  \{2_{x00}|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.5,0.5)}
                               -x, +y+1/2, -z+1/2
    \{-1|(0.0,0.5,0.5)\}
                               -x,-y+1/2,-z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
                             +x+1/2, +y+1/2, -z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, +y+1/2, +z+1/2
 \{m \times 0z \mid (0.0, 0.5, 0.5)\}
                               +x,-y+1/2,+z+1/2
*******
space group: 63:-cba {'Hall': ' -A 2 2a', 'HM': ' A m a m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x,-y,+z
+x+1/2,-y,-z
           Seitz
                                     Jones
    \{1 \mid (0.0,0.0,0.0)\}
                                    +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                    -x,-y,+z
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                                 +x+1/2,-y,-z
  {2_0y0|(0.5,0.0,0.0)}
                                 -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                    +x,+y,-z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                                 -x+1/2,+y,+z
```

+x+1/2,-y,+z

+x, +y+1/2, +z+1/2

-x,-y+1/2,+z+1/2

```
-x+1/2, +y+1/2, -z+1/2
  {2_0y0|(0.5,0.5,0.5)} |
    \{-1 \mid (0.0, 0.5, 0.5)\}
                               -x,-y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                               +x, +y+1/2, -z+1/2
  \{m \ 0yz | (0.5, 0.5, 0.5)\}
                             -x+1/2,+y+1/2,+z+1/2
 \{m \times 0z \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,-y+1/2,+z+1/2
*******
space group: 63:bca {'Hall': ' -B 2 2b', 'HM': 'B b m m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-X,-Y,+Z
+x,-y+1/2,-z
           Seitz
                                     Jones
    {1|(0.0,0.0,0.0)}
                                    +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                    -x,-y,+z
  \{2_{x00}|(0.0,0.5,0.0)\}
                                  +x,-y+1/2,-z
  \{2_0y0 \mid (0.0,0.5,0.0)\}
                                  -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                    +x,+y,-z
  \{m_0yz \mid (0.0,0.5,0.0)\}
                                  -x,+y+1/2,+z
  \{m_x0z \mid (0.0, 0.5, 0.0)\}
                                 +x,-y+1/2,+z
    \{1 \mid (0.5, 0.0, 0.5)\}
                               +x+1/2,+y,+z+1/2
  \{2\ 00z|(0.5,0.0,0.5)\}
                               -x+1/2,-y,+z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
  \{2_0y0|(0.5,0.5,0.5)\}
                             -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.5, 0.0, 0.5)\}
                               -x+1/2, -y, -z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                               +x+1/2,+y,-z+1/2
  \{m \ 0yz | (0.5, 0.5, 0.5)\}
                             -x+1/2,+y+1/2,+z+1/2
 \{m \times 0z \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,-y+1/2,+z+1/2
*******
space group: 63:a-cb {'Hall': ' -B 2b 2', 'HM': ' B m m b'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
 {2_00z|(0.0,0.5,0.0)}
                                  -x,-y+1/2,+z
| {2_x00|(0.0,0.0,0.0)}
                                    +x,-y,-z
  \{2 \text{ 0y0} | (0.0, 0.5, 0.0)\}
                                  -x,+y+1/2,-z
```

-x,-y,-z

 $\{-1 \mid (0.0, 0.0, 0.0)\}$

```
\{m \times y0 \mid (0.0, 0.5, 0.0)\} \mid
                                 +x,+y+1/2,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                   -x,+y,+z
  \{m_x0z \mid (0.0,0.5,0.0)\}
                                 +x,-y+1/2,+z
                               +x+1/2, +y, +z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,+z+1/2
 \{2_{x00} | (0.5, 0.0, 0.5)\}
                               +x+1/2,-y,-z+1/2
  \{2_0y0|(0.5,0.5,0.5)\}
                             -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.5, 0.0, 0.5)\}
                               -x+1/2,-y,-z+1/2
                             +x+1/2, +y+1/2, -z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
  \{m_0yz \mid (0.5,0.0,0.5)\}
                               -x+1/2,+y,+z+1/2
  {m_x0z|(0.5,0.5,0.5)}
                             +x+1/2,-y+1/2,+z+1/2
*******
space group: 64 {'Hall': ' -C 2bc 2', 'HM': 'C m c a'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y,-z
                                  Jones
           Seitz
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                             -x,-y+1/2,+z+1/2
  \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x,-y,-z
  {2_0y0|(0.0,0.5,0.5)}
                             -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0,0.0,0.0)\}
                                 -X,-Y,-Z
  \{m_xy0|(0.0,0.5,0.5)\}
                             +x, +y+1/2, -z+1/2
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                 -x,+y,+z
  \{m_x0z \mid (0.0,0.5,0.5)\}
                             +x,-y+1/2,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                             +x+1/2,+y+1/2,+z
  \{2\ 00z|(0.5,0.0,0.5)\}
                             -x+1/2,-y,+z+1/2
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                             +x+1/2,-y+1/2,-z
  {2_0y0|(0.5,0.0,0.5)}
                            -x+1/2, +y, -z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                             -x+1/2,-y+1/2,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                             +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                             -x+1/2,+y+1/2,+z
  \{m_x0z|(0.5,0.0,0.5)\} | +x+1/2,-y,+z+1/2
*******
space group: 64:ba-c {'Hall': ' -C 2bc 2bc', 'HM': ' C c m b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y+1/2,-z+1/2
           Seitz
                                  Jones
```

```
{1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  \{2\_00z \mid (0.0,0.5,0.5)\}
                            -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.0,0.5,0.5)\}
                             +x,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.0,0.5,0.5)\}
                             +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.0,0.5,0.5)\}
                             -x, +y+1/2, +z+1/2
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                 +x,-y,+z
    \{1|(0.5,0.5,0.0)\}
                             +x+1/2, +y+1/2, +z
                            -x+1/2,-y,+z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                             +x+1/2,-y,-z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
  \{2_0y0|(0.5,0.5,0.0)\}
                             -x+1/2,+y+1/2,-z
    \{-1 \mid (0.5, 0.5, 0.0)\}
                            -x+1/2,-y+1/2,-z
                            +x+1/2,+y,-z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
  \{m_0yz \mid (0.5,0.0,0.5)\}
                            -x+1/2, +y, +z+1/2
                            +x+1/2,-y+1/2,+z
  \{m_x0z|(0.5,0.5,0.0)\}
*******
space group: 64:cab {'Hall': ' -A 2ac 2ac', 'HM': 'A b m a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2,-y,+z+1/2
+x+1/2,-y,-z+1/2
           Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
 {2_00z|(0.5,0.0,0.5)}
                            -x+1/2,-y,+z+1/2
 \{2_{x00}|(0.5,0.0,0.5)\}
                             +x+1/2,-y,-z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.5,0.0,0.5)\}
                            +x+1/2,+y,-z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                             -x+1/2,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                 +x,-y,+z
    \{1|(0.0,0.5,0.5)\}
                            +x,+y+1/2,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                            -x+1/2,-y+1/2,+z
  \{2_{x00}|(0.5,0.5,0.0)\}
                             +x+1/2,-y+1/2,-z
                             -x,+y+1/2,-z+1/2
  {2_0y0|(0.0,0.5,0.5)}
    \{-1 \mid (0.0, 0.5, 0.5)\}
                            -x,-y+1/2,-z+1/2
  \{m_xy0|(0.5,0.5,0.0)\}
                             +x+1/2,+y+1/2,-z
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                             -x+1/2,+y+1/2,+z
                            +x,-y+1/2,+z+1/2
  \{m_x0z|(0.0,0.5,0.5)\}
 . . . . . . . . . . . . . . . . . . .
*******
space group: 64:-cba {'Hall': ' -A 2 2ac', 'HM': ' A c a m'}
Crystal system: Orthorhombic
Setting: -cba
```

+x,+y,+z

```
-x,-y,+z
+x+1/2,-y,-z+1/2
  . . . . . . . . . . . . . . . . . .
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                              +x+1/2,-y,-z+1/2
  \{2_0y0|(0.5,0.0,0.5)\}
                              -x+1/2,+y,-z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_xy0 | (0.0,0.0,0.0)\}
                                   +x,+y,-z
  \{m_0yz \mid (0.5,0.0,0.5)\}
                              -x+1/2,+y,+z+1/2
  \{m_x0z | (0.5,0.0,0.5)\}
                              +x+1/2,-y,+z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x,+y+1/2,+z+1/2
  \{2_{00z} | (0.0, 0.5, 0.5)\}
                              -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\}
                              -x+1/2,+y+1/2,-z
                              -x,-y+1/2,-z+1/2
     \{-1 \mid (0.0, 0.5, 0.5)\}
  \{m_xy0|(0.0,0.5,0.5)\}
                              +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,+y+1/2,+z
  \{m_x0z \mid (0.5, 0.5, 0.0)\}
                              +x+1/2,-y+1/2,+z
*******
space group: 64:bca {'Hall': ' -B 2 2bc', 'HM': 'B b c m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y,+z
+x,-y+1/2,-z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
  \{2_{x00}|(0.0,0.5,0.5)\}
                              +x,-y+1/2,-z+1/2
  \{2_0y0|(0.0,0.5,0.5)\}
                              -x,+y+1/2,-z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_xy0 | (0.0,0.0,0.0)\}
                                   +x,+y,-z
  \{m_0yz \mid (0.0,0.5,0.5)\}
                              -x, +y+1/2, +z+1/2
  \{m_x0z|(0.0,0.5,0.5)\}
                              +x,-y+1/2,+z+1/2
    \{1|(0.5,0.0,0.5)\}
                              +x+1/2,+y,+z+1/2
                              -x+1/2, -y, +z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
  \{2_{x00}|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\}
                              -x+1/2,+y+1/2,-z
     \{-1 \mid (0.5, 0.0, 0.5)\}
                              -x+1/2,-y,-z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                              +x+1/2, +y, -z+1/2
```

-x+1/2, +y+1/2, +z

+x+1/2,-y+1/2,+z

.

 $\{m_0yz \mid (0.5, 0.5, 0.0)\}$

 $\{m_x0z \mid (0.5, 0.5, 0.0)\}$

```
*******
space group: 64:a-cb {'Hall': ' -B 2bc 2', 'HM': ' B m a b'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y,-z
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.5,0.5)\}
                             -x,-y+1/2,+z+1/2
  \{2_{x00} | (0.0,0.0,0.0)\}
                                  +x,-y,-z
  \{2_0y0|(0.0,0.5,0.5)\}
                             -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{m_xy0|(0.0,0.5,0.5)\}
                             +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                  -x,+y,+z
  \{m_x0z|(0.0,0.5,0.5)\}
                             +x,-y+1/2,+z+1/2
    \{1|(0.5,0.0,0.5)\}
                             +x+1/2, +y, +z+1/2
  \{2_{00z} | (0.5, 0.5, 0.0)\}
                             -x+1/2,-y+1/2,+z
  \{2_{\times}00 \mid (0.5, 0.0, 0.5)\}
                             +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.5,0.0)}
                             -x+1/2,+y+1/2,-z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                             -x+1/2, -y, -z+1/2
  \{m_xy0|(0.5,0.5,0.0)\}
                             +x+1/2, +y+1/2, -z
  \{m_0yz \mid (0.5,0.0,0.5)\}
                             -x+1/2, +y, +z+1/2
| \{m_x0z|(0.5,0.5,0.0)\} | +x+1/2,-y+1/2,+z |
*******
space group: 65 {'Hall': ' -C 2 2', 'HM': 'C m m m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +X,+Y,+Z
  {2_00z|(0.0,0.0,0.0)}
                                  -x,-y,+z
 {2_x00|(0.0,0.0,0.0)}
                                  +x,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                  -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                  +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                  -x,+y,+z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                  +x,-y,+z
    \{1|(0.5,0.5,0.0)\}
                             +x+1/2,+y+1/2,+z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                             -x+1/2, -y+1/2, +z
  \{2_{x00}|(0.5,0.5,0.0)\}
                             +x+1/2,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\}
                             -x+1/2, +y+1/2, -z
    \{-1 \mid (0.5, 0.5, 0.0)\}
                           | -x+1/2, -y+1/2, -z |
```

```
\{m \times y0 \mid (0.5, 0.5, 0.0)\} \mid +x+1/2, +y+1/2, -z \mid
  \{m_0yz \mid (0.5, 0.5, 0.0)\}\
                              -x+1/2,+y+1/2,+z
  \{m_x0z|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,+z \mid
*******
space group: 65:cab {'Hall': ' -A 2 2', 'HM': 'A m m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x,-y,+z
+x,-y,-z
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +X,+Y,+Z
  {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
  \{2_{x00}|(0.0,0.0,0.0)\}
                                   +x,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                   -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                   +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                   -x,+y,+z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                   +x,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                              -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.0,0.5,0.5)\}
                              +x,-y+1/2,-z+1/2
  \{2 \ 0 \ | \ (0.0, 0.5, 0.5)\}
                              -x,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.5, 0.5)\}
                              -x,-y+1/2,-z+1/2
  \{m \times y0 \mid (0.0, 0.5, 0.5)\}
                              +x,+y+1/2,-z+1/2
  \{m_0yz \mid (0.0,0.5,0.5)\}
                              -x, +y+1/2, +z+1/2
  \{m_x0z|(0.0,0.5,0.5)\}
                              +x,-y+1/2,+z+1/2
. . . . . . . . . . . . . . . . . . . .
*******
space group: 65:bca {'Hall': ' -B 2 2', 'HM': 'B m m m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y,+z
+x,-y,-z
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
  \{2_{x00} | (0.0, 0.0, 0.0)\}
                                   +x,-y,-z
 {2_0y0|(0.0,0.0,0.0)}
                                   -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{m \times y0 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                   -x,+y,+z
```

```
\{m_x0z|(0.0,0.0,0.0)\}
                                 +x,-y,+z
    \{1|(0.5,0.0,0.5)\}
                            +x+1/2,+y,+z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                            -x+1/2, -y, +z+1/2
  \{2 \times 00 \mid (0.5, 0.0, 0.5)\}
                            +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                            -x+1/2,+y,-z+1/2
    \{-1 \mid (0.5, 0.0, 0.5)\}
                            -x+1/2,-y,-z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                            +x+1/2,+y,-z+1/2
                            -x+1/2, +y, +z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
  \{m_x0z|(0.5,0.0,0.5)\}
                            +x+1/2,-y,+z+1/2
*******
space group: 66 {'Hall': ' -C 2 2c', 'HM': 'C c c m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
 {2_x00|(0.0,0.0,0.5)}
                                 +x,-y,-z+1/2
  {2_0y0|(0.0,0.0,0.5)}
                                 -x,+y,-z+1/2
    \{-1 \mid (0.0,0.0,0.0)\}
                                   -x,-y,-z
  \{m_xy0 | (0.0,0.0,0.0)\}
                                   +x,+y,-z
 \{m \ 0yz | (0.0,0.0,0.5)\}
                                 -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                 +x,-y,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                               +x+1/2,+y+1/2,+z
 \{2\_00z \mid (0.5, 0.5, 0.0)\}
                               -x+1/2, -y+1/2, +z
 \{2_{x00}|(0.5,0.5,0.5)\}
                            +x+1/2,-y+1/2,-z+1/2
  \{2 \text{ 0y0} | (0.5, 0.5, 0.5)\}
                            -x+1/2, +y+1/2, -z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                               -x+1/2, -y+1/2, -z
  \{m_xy0 | (0.5, 0.5, 0.0)\}
                               +x+1/2, +y+1/2, -z
  \{m_0yz \mid (0.5, 0.5, 0.5)\}
                            -x+1/2,+y+1/2,+z+1/2
  \{m_x0z | (0.5, 0.5, 0.5)\}
                            +x+1/2,-y+1/2,+z+1/2
*******
space group: 66:cab {'Hall': ' -A 2a 2', 'HM': 'A m a a'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x+1/2,-y,+z
+x,-y,-z
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
 {2_00z|(0.5,0.0,0.0)} |
                                 -x+1/2,-y,+z
```

```
\{2_{\times}00 \mid (0.0, 0.0, 0.0)\}
                                     +x,-y,-z
{2_0y0|(0.5,0.0,0.0)}
                                   -x+1/2,+y,-z
   \{-1 \mid (0.0, 0.0, 0.0)\}
                                     -x,-y,-z
\{m \times y0 \mid (0.5, 0.0, 0.0)\}
                                   +x+1/2, +y, -z
\{m_0yz \mid (0.0,0.0,0.0)\}
                                     -x,+y,+z
\{m_x0z \mid (0.5,0.0,0.0)\}
                                   +x+1/2,-y,+z
   \{1 \mid (0.0, 0.5, 0.5)\}
                                 +x, +y+1/2, +z+1/2
\{2\_00z \mid (0.5, 0.5, 0.5)\}
                              -x+1/2, -y+1/2, +z+1/2
                                +x,-y+1/2,-z+1/2
\{2_{x00} | (0.0, 0.5, 0.5)\}
\{2_0y0|(0.5,0.5,0.5)\}
                              -x+1/2,+y+1/2,-z+1/2
   \{-1 \mid (0.0, 0.5, 0.5)\}
                                 -x,-y+1/2,-z+1/2
\{m_xy0|(0.5,0.5,0.5)\}
                              +x+1/2, +y+1/2, -z+1/2
\{m_0yz \mid (0.0,0.5,0.5)\}
                                 -x, +y+1/2, +z+1/2
\{m_x0z|(0.5,0.5,0.5)\}
                              +x+1/2,-y+1/2,+z+1/2
```

space group: 66:bca {'Hall': ' -B 2b 2b', 'HM': 'B b m b'}

Crystal system: Orthorhombic

Setting: bca +x,+y,+z -x,-y+1/2,+z +x,-y+1/2,-z

```
Seitz
                                     Jones
   \{1 \mid (0.0, 0.0, 0.0)\}
                                    +X,+Y,+Z
{2_00z|(0.0,0.5,0.0)}
                                  -x,-y+1/2,+z
\{2_{x00} | (0.0, 0.5, 0.0)\}
                                  +x,-y+1/2,-z
{2_0y0|(0.0,0.0,0.0)}
                                    -x,+y,-z
   \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
\{m \times y0 \mid (0.0, 0.5, 0.0)\}
                                  +x,+y+1/2,-z
\{m_0yz \mid (0.0,0.5,0.0)\}
                                  -x,+y+1/2,+z
\{m_x0z \mid (0.0,0.0,0.0)\}
                                    +x,-y,+z
   \{1|(0.5,0.0,0.5)\}
                               +x+1/2,+y,+z+1/2
\{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,+z+1/2
\{2_{x00}|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
\{2_0y0|(0.5,0.0,0.5)\}
                               -x+1/2,+y,-z+1/2
   \{-1 \mid (0.5, 0.0, 0.5)\}
                               -x+1/2,-y,-z+1/2
                             +x+1/2,+y+1/2,-z+1/2
\{m_xy0|(0.5,0.5,0.5)\}
\{m_0yz \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, +y+1/2, +z+1/2
{m_x0z|(0.5,0.0,0.5)}
                               +x+1/2,-y,+z+1/2
```

.

```
******
```

```
space group: 67 {'Hall': ' -C 2b 2', 'HM': 'C m m a'}
Crystal system: Orthorhombic
```

+x,+y,+z -x,-y+1/2,+z

+x,-y,-z

.

```
Seitz
                                  Jones
  \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
{2_00z|(0.0,0.5,0.0)}
                               -x,-y+1/2,+z
\{2_{x00}|(0.0,0.0,0.0)\}
                                 +x,-y,-z
{2_0y0|(0.0,0.5,0.0)}
                               -x,+y+1/2,-z
  \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
{m_xy0|(0.0,0.5,0.0)}
                               +x,+y+1/2,-z
\{m_0yz \mid (0.0,0.0,0.0)\}
                                 -X,+Y,+Z
\{m_x0z \mid (0.0,0.5,0.0)\}
                               +x,-y+1/2,+z
  \{1 \mid (0.5, 0.5, 0.0)\}
                            +x+1/2,+y+1/2,+z
\{2\_00z \mid (0.5,0.0,0.0)\}
                               -x+1/2,-y,+z
\{2_{x00}|(0.5,0.5,0.0)\}
                            +x+1/2,-y+1/2,-z
{2_0y0|(0.5,0.0,0.0)}
                               -x+1/2,+y,-z
  \{-1 \mid (0.5, 0.5, 0.0)\}
                            -x+1/2,-y+1/2,-z
\{m_xy0|(0.5,0.0,0.0)\}
                               +x+1/2,+y,-z
\{m_0yz \mid (0.5, 0.5, 0.0)\}
                            -x+1/2,+y+1/2,+z
\{m_x0z | (0.5,0.0,0.0)\}
                               +x+1/2,-y,+z
```

space group: 67:ba-c {'Hall': ' -C 2b 2b', 'HM': ' C m m b'}

Crystal system: Orthorhombic

Setting: ba-c

+x,+y,+z

-x,-y+1/2,+z

+x,-y+1/2,-z

```
Seitz
                                   Jones
  \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
\{2\_00z \mid (0.0, 0.5, 0.0)\}
                                -x,-y+1/2,+z
\{2_{x00} | (0.0, 0.5, 0.0)\}
                                +x,-y+1/2,-z
{2_0y0|(0.0,0.0,0.0)}
                                  -x,+y,-z
  \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
\{m_xy0|(0.0,0.5,0.0)\}
                                +x,+y+1/2,-z
\{m_0yz \mid (0.0,0.5,0.0)\}
                                -x,+y+1/2,+z
\{m_x0z \mid (0.0,0.0,0.0)\}
                                  +x,-y,+z
  \{1 \mid (0.5, 0.5, 0.0)\}
                             +x+1/2, +y+1/2, +z
\{2\_00z \mid (0.5,0.0,0.0)\}
                                -x+1/2,-y,+z
\{2_{x00}|(0.5,0.0,0.0)\}
                                +x+1/2,-y,-z
{2_0y0|(0.5,0.5,0.0)}
                             -x+1/2,+y+1/2,-z
  \{-1 \mid (0.5, 0.5, 0.0)\}
                             -x+1/2, -y+1/2, -z
\{m_xy0|(0.5,0.0,0.0)\}
                                +x+1/2,+y,-z
\{m_0yz \mid (0.5,0.0,0.0)\}
                                -x+1/2,+y,+z
\{m_x0z \mid (0.5, 0.5, 0.0)\}
                             +x+1/2,-y+1/2,+z
```

.

```
******
```

space group: 67:cab {'Hall': ' -A 2c 2c', 'HM': 'A b m m'}

```
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x,-y,+z+1/2
+x,-y,-z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +X,+Y,+Z
  {2_00z|(0.0,0.0,0.5)} |
                                -x,-y,+z+1/2
  \{2_{x00}|(0.0,0.0,0.5)\}
                                +x,-y,-z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                   -x,+y,-z
    \{-1 \mid (0.0,0.0,0.0)\}
                                   -x,-y,-z
  \{m_xy0|(0.0,0.0,0.5)\}
                                +x,+y,-z+1/2
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                   +x,-y,+z
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
                                -x,-y+1/2,+z
  \{2_{00z} | (0.0, 0.5, 0.0)\}
                                +x,-y+1/2,-z
  \{2_{x00} | (0.0, 0.5, 0.0)\}
  {2_0y0|(0.0,0.5,0.5)}
                              -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.5, 0.5)\}
                              -x,-y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.0)\}
                                +x,+y+1/2,-z
  \{m_0yz \mid (0.0, 0.5, 0.0)\}
                                -x,+y+1/2,+z
  \{m_x0z|(0.0,0.5,0.5)\} | +x,-y+1/2,+z+1/2
*******
space group: 67:-cba {'Hall': ' -A 2 2c', 'HM': ' A c m m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x,-y,+z
+x,-y,-z+1/2
                                    Jones
           Seitz
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +X,+Y,+Z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                  -x,-y,+z
  \{2_{x00}|(0.0,0.0,0.5)\}
                                +x,-y,-z+1/2
  {2_0y0|(0.0,0.0,0.5)}
                                -x,+y,-z+1/2
    \{-1 \mid (0.0,0.0,0.0)\}
                                   -x,-y,-z
  \{m_xy0 | (0.0,0.0,0.0)\}
                                   +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                +x,-y,+z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, +z+1/2
  \{2_{00z} | (0.0, 0.5, 0.5)\}
                              -x,-y+1/2,+z+1/2
  \{2_{\times}00 \mid (0.0, 0.5, 0.0)\}
                                +x,-y+1/2,-z
  {2_0y0|(0.0,0.5,0.0)}
                                -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.5, 0.5)\}
                              -x,-y+1/2,-z+1/2
  \{m \times y0 \mid (0.0, 0.5, 0.5)\}
                              +x, +y+1/2, -z+1/2
```

-x,+y+1/2,+z

 $\{m_0yz \mid (0.0, 0.5, 0.0)\} \mid$

```
\{ m_x 0z | (0.0, 0.5, 0.0) \} + x, -y+1/2, +z 
*******
space group: 67:bca {'Hall': ' -B 2 2c', 'HM': 'B m c m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y,+z
+x,-y,-z+1/2
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                  -x,-y,+z
  \{2_{x00}|(0.0,0.0,0.5)\}
                                +x,-y,-z+1/2
  {2_0y0|(0.0,0.0,0.5)}
                                -x, +y, -z+1/2
    \{-1 \mid (0.0,0.0,0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                  +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                +x,-y,+z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                              +x+1/2, +y, +z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                             -x+1/2, -y, +z+1/2
  \{2_{x00} | (0.5, 0.0, 0.0)\}
                                +x+1/2,-y,-z
  {2_0y0|(0.5,0.0,0.0)}
                                -x+1/2,+y,-z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                             -x+1/2, -y, -z+1/2
  \{m \times y0 \mid (0.5, 0.0, 0.5)\}
                             +x+1/2,+y,-z+1/2
  \{m_0yz \mid (0.5,0.0,0.0)\}
                                -x+1/2,+y,+z
  \{m \times 0z \mid (0.5, 0.0, 0.0)\}
                                +x+1/2,-y,+z
 . . . . . . . . . . . . . . . . . . .
*******
space group: 67:a-cb {'Hall': ' -B 2c 2', 'HM': ' B m a m'}
Crystal system: Orthorhombic
Setting: a-cb
+x,+y,+z
-x,-y,+z+1/2
+x,-y,-z
           Seitz
                                    Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.5)\}
                                -x,-y,+z+1/2
  \{2_{x00}|(0.0,0.0,0.0)\}
                                  +x,-y,-z
  {2_0y0|(0.0,0.0,0.5)}
                                -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  {m_xy0|(0.0,0.0,0.5)}
                                +x,+y,-z+1/2
 \{m_0yz \mid (0.0,0.0,0.0)\}
                                  -x,+y,+z
  \{m \times 0z \mid (0.0, 0.0, 0.5)\}
                                +x,-y,+z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                             +x+1/2,+y,+z+1/2
```

```
\{2\_00z \mid (0.5,0.0,0.0)\}
                               -x+1/2, -y, +z
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                             +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.0)}
                               -x+1/2,+y,-z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                             -x+1/2, -y, -z+1/2
  \{m_xy0|(0.5,0.0,0.0)\}
                               +x+1/2,+y,-z
  \{m_0yz \mid (0.5,0.0,0.5)\}
                             -x+1/2, +y, +z+1/2
  \{m_x0z \mid (0.5,0.0,0.0)\}
                               +x+1/2,-y,+z
*******
space group: 68:1 {'Hall': 'C 2 2 -1bc', 'HM': 'C c c a:1'}
Crystal system: Orthorhombic
Setting: 1
+x,+y,+z
-x,-y,+z
+x,-y,-z
-x,-y+1/2,-z+1/2
           Seitz
                                   Jones
    {1|(0.0,0.0,0.0)}
                                  +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                  -x,-y,+z
  {2_x00|(0.0,0.0,0.0)}
                                  +x,-y,-z
    \{-1 \mid (0.0, 0.5, 0.5)\}
                             -x,-y+1/2,-z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                             +x+1/2,+y+1/2,+z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                             -x+1/2, -y+1/2, +z
  \{2 \times 00 \mid (0.5, 0.5, 0.0)\}
                             +x+1/2,-y+1/2,-z
                             -x+1/2, -y, -z+1/2
    \{-1|(0.5,0.0,0.5)\}
*******
space group: 68:2 {'Hall': ' -C 2b 2bc', 'HM': 'C c c a:2'}
Crystal system: Orthorhombic
Setting: 2
+x,+y,+z
-x,-y+1/2,+z
+x,-y+1/2,-z+1/2
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.0, 0.5, 0.0)\}
                                  -x,-y+1/2,+z
  \{2_{x00} | (0.0, 0.5, 0.5)\}
                               +x,-y+1/2,-z+1/2
  \{2_0y0|(0.0,0.0,0.5)\}
                                  -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                                  +x,+y+1/2,-z
                               -x,+y+1/2,+z+1/2
 \{m_0yz \mid (0.0,0.5,0.5)\}
  \{m_x0z | (0.0,0.0,0.5)\}
                                  +x,-y,+z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                               +x+1/2,+y+1/2,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                                  -x+1/2, -y, +z
```

```
{2_x00|(0.5,0.0,0.5)} |
                               +x+1/2,-y,-z+1/2
  \{2_0y0|(0.5,0.5,0.5)\}
                            -x+1/2, +y+1/2, -z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,-y+1/2,-z
  \{m_xy0 | (0.5,0.0,0.0)\}
                                +x+1/2,+y,-z
  \{m_0yz \mid (0.5,0.0,0.5)\}\ \mid
                               -x+1/2,+y,+z+1/2
 \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 68:1ba-c {'Hall': 'C 2 2 -1bc', 'HM': 'C c c b:1'}
Crystal system: Orthorhombic
Setting: 1ba-c
+X,+Y,+Z
-x,-y,+z
+x,-y,-z
-x,-y+1/2,-z+1/2
           Seitz
                                  Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
  {2_x00|(0.0,0.0,0.0)} |
                                 +x,-y,-z
    \{-1 \mid (0.0, 0.5, 0.5)\}
                            -x,-y+1/2,-z+1/2
    \{1 \mid (0.5, 0.5, 0.0)\}
                            +x+1/2,+y+1/2,+z
  \{2\_00z \mid (0.5, 0.5, 0.0)\} \mid
                            -x+1/2, -y+1/2, +z
  \{2_x00|(0.5,0.5,0.0)\} \mid +x+1/2,-y+1/2,-z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                          | -x+1/2, -y, -z+1/2
*******
space group: 68:2ba-c {'Hall': ' -C 2b 2c', 'HM': 'C c c b:2'}
Crystal system: Orthorhombic
Setting: 2ba-c
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +X,+Y,+Z
  {2_00z|(0.0,0.5,0.0)}
                                 -x,-y+1/2,+z
  \{2_{\times}00 \mid (0.0, 0.0, 0.5)\}
                                 +x,-y,-z+1/2
  \{2_0y0|(0.0,0.5,0.5)\}
                               -x, +y+1/2, -z+1/2
                                   -x,-y,-z
    \{-1 \mid (0.0,0.0,0.0)\}
  \{m_xy0|(0.0,0.5,0.0)\}
                                 +x,+y+1/2,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                 -x,+y,+z+1/2
  \{m_x0z|(0.0,0.5,0.5)\}\ |
                               +x,-y+1/2,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                               +x+1/2,+y+1/2,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                                 -x+1/2,-y,+z
  \{2_x00|(0.5,0.5,0.5)\} \mid +x+1/2,-y+1/2,-z+1/2
```

```
-x+1/2,+y,-z+1/2
  {2_0y0|(0.5,0.0,0.5)} |
    \{-1 \mid (0.5, 0.5, 0.0)\}
                                -x+1/2,-y+1/2,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                                  +x+1/2,+y,-z
  \{m \ 0yz | (0.5, 0.5, 0.5)\}
                             -x+1/2, +y+1/2, +z+1/2
 \{m \times 0z \mid (0.5, 0.0, 0.5)\}
                                +x+1/2,-y,+z+1/2
*******
space group: 68:1cab {'Hall': 'A 2 2 -1ac', 'HM': ' A b a a:1'}
Crystal system: Orthorhombic
Setting: 1cab
+x,+y,+z
-X,-Y,+Z
+x,-y,-z
-x+1/2, -y, -z+1/2
. . . . . . . . . . . . . . . . . . . .
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2_{00z}|(0.0,0.0,0.0)\}
                                  -x,-y,+z
  \{2_{x00} | (0.0,0.0,0.0)\}
                                  +x,-y,-z
    \{-1|(0.5,0.0,0.5)\}
                             -x+1/2, -y, -z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
                             +x, +y+1/2, +z+1/2
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                             -x,-y+1/2,+z+1/2
  \{2_{x00} | (0.0, 0.5, 0.5)\}
                             +x,-y+1/2,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                            | -x+1/2, -y+1/2, -z
******
space group: 68:2cab {'Hall': ' -A 2a 2c', 'HM': ' A b a a:2'}
Crystal system: Orthorhombic
Setting: 2cab
+x,+y,+z
-x+1/2,-y,+z
+x,-y,-z+1/2
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2_{00z} | (0.5, 0.0, 0.0)\}
                                  -x+1/2,-y,+z
  \{2_{x00}|(0.0,0.0,0.5)\}
                                  +x,-y,-z+1/2
  \{2_0y0|(0.5,0.0,0.5)\}
                                -x+1/2,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                                  +x+1/2,+y,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                  -x,+y,+z+1/2
  \{m_x0z \mid (0.5,0.0,0.5)\}
                                +x+1/2,-y,+z+1/2
                                +x,+y+1/2,+z+1/2
    \{1|(0.0,0.5,0.5)\}
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, +z+1/2
  \{2_{x00} | (0.0, 0.5, 0.0)\}
                                  +x,-y+1/2,-z
  {2_0y0|(0.5,0.5,0.0)} |
                                -x+1/2,+y+1/2,-z
```

```
\{-1 \mid (0.0, 0.5, 0.5)\}
                               -x,-y+1/2,-z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
 {m_0yz|(0.0,0.5,0.0)} |
                                -x, +y+1/2, +z
  \{m_x0z | (0.5, 0.5, 0.0)\} \mid
                               +x+1/2, -y+1/2, +z
*******
space group: 68:1-cba {'Hall': 'A 2 2 -1ac', 'HM': 'A c a a:1'}
Crystal system: Orthorhombic
Setting: 1-cba
+x,+y,+z
-x,-y,+z
+x,-y,-z
-x+1/2,-y,-z+1/2
           Seitz
                                  Jones
    {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
  {2_x00|(0.0,0.0,0.0)} |
                                 +x,-y,-z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                            -x+1/2,-y,-z+1/2
                            +x, +y+1/2, +z+1/2
    \{1|(0.0,0.5,0.5)\}
  \{2\_00z \mid (0.0, 0.5, 0.5)\}
                           |-x,-y+1/2,+z+1/2|
  \{2_x00|(0.0,0.5,0.5)\} \mid +x,-y+1/2,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                           | -x+1/2, -y+1/2, -z |
*******
space group: 68:2-cba {'Hall': ' -A 2ac 2c', 'HM': 'A c a a:2'}
Crystal system: Orthorhombic
Setting: 2-cba
+x,+y,+z
-x+1/2, -y, +z+1/2
+x,-y,-z+1/2
           Seitz
                                    Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.5)\}
                               -x+1/2,-y,+z+1/2
 {2_x00|(0.0,0.0,0.5)}
                                 +x,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.0)}
                                 -x+1/2,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
                               +x+1/2, +y, -z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                 -x,+y,+z+1/2
                                 +x+1/2,-y,+z
  \{m_x0z \mid (0.5,0.0,0.0)\}
    \{1 \mid (0.0, 0.5, 0.5)\}
                               +x,+y+1/2,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                               -x+1/2, -y+1/2, +z
 \{2_{x00} | (0.0, 0.5, 0.0)\}
                                 +x,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.5)\}
                            -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.0, 0.5, 0.5)\}
                               -x,-y+1/2,-z+1/2
```

```
\{m_xy0|(0.5,0.5,0.0)\}
                               +x+1/2,+y+1/2,-z
  \{m_0yz \mid (0.0,0.5,0.0)\}
                                 -x,+y+1/2,+z
  \{m_x0z|(0.5,0.5,0.5)\} | +x+1/2,-y+1/2,+z+1/2
*******
space group: 68:1bca {'Hall': 'B 2 2 -1bc', 'HM': ' B b c b:1'}
Crystal system: Orthorhombic
Setting: 1bca
+x,+y,+z
-x,-y,+z
+x,-y,-z
-x,-y+1/2,-z+1/2
 . . . . . . . . . . . . . . . . . .
                                   Jones
           Seitz
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                 -x,-y,+z
  \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x,-y,-z
    \{-1 \mid (0.0, 0.5, 0.5)\}
                             -x,-y+1/2,-z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                             +x+1/2,+y,+z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                             -x+1/2, -y, +z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
                             +x+1/2,-y,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                             -x+1/2, -y+1/2, -z
*******
space group: 68:2bca {'Hall': ' -B 2bc 2b', 'HM': ' B b c b:2'}
Crystal system: Orthorhombic
Setting: 2bca
+x,+y,+z
-x,-y+1/2,+z+1/2
+x,-y+1/2,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2_{00z} | (0.0, 0.5, 0.5)\}
                               -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.0,0.5,0.0)\}
                                 +x,-y+1/2,-z
 \{2_0y0|(0.0,0.0,0.5)\}
                                 -x,+y,-z+1/2
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
                               +x,+y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
  \{m_0yz \mid (0.0,0.5,0.0)\}
                                 -x,+y+1/2,+z
  \{m_x0z|(0.0,0.0,0.5)\}
                                 +x,-y,+z+1/2
    {1|(0.5,0.0,0.5)}
                               +x+1/2,+y,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                               -x+1/2,-y+1/2,+z
 \{2_{x00}|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
  {2_0y0|(0.5,0.0,0.0)}
                                 -x+1/2,+y,-z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                               -x+1/2,-y,-z+1/2
  \{m_xy0|(0.5,0.5,0.0)\}
                               +x+1/2, +y+1/2, -z
```

```
\{m_0yz \mid (0.5, 0.5, 0.5)\} \mid -x+1/2, +y+1/2, +z+1/2 \mid
  \{m_x0z|(0.5,0.0,0.0)\}\ |
                                  +x+1/2,-y,+z
*******
space group: 68:1a-cb {'Hall': 'B 2 2 -1bc', 'HM': 'B b a b:1'}
Crystal system: Orthorhombic
Setting: 1a-cb
+X,+Y,+Z
-x,-y,+z
+x,-y,-z
-x,-y+1/2,-z+1/2
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                  -x,-y,+z
  \{2_{x00}|(0.0,0.0,0.0)\}
                                  +x,-y,-z
    \{-1 \mid (0.0, 0.5, 0.5)\}
                             -x,-y+1/2,-z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                             +x+1/2,+y,+z+1/2
  \{2_{00z} | (0.5, 0.0, 0.5)\}
                             -x+1/2,-y,+z+1/2
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                             +x+1/2,-y,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.0)\}
                             -x+1/2, -y+1/2, -z
*******
space group: 68:2a-cb {'Hall': ' -B 2b 2bc', 'HM': 'B b a b:2'}
Crystal system: Orthorhombic
Setting: 2a-cb
+x,+y,+z
-x,-y+1/2,+z
+x,-y+1/2,-z+1/2
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  {2_00z|(0.0,0.5,0.0)}
                                  -x,-y+1/2,+z
  \{2_{x00}|(0.0,0.5,0.5)\}
                               +x,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.0,0.5)}
                                  -x,+y,-z+1/2
    \{-1 \mid (0.0,0.0,0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                                  +x,+y+1/2,-z
  \{m_0yz \mid (0.0, 0.5, 0.5)\}
                               -x, +y+1/2, +z+1/2
  \{m_x0z \mid (0.0,0.0,0.5)\}
                                  +x,-y,+z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                               +x+1/2,+y,+z+1/2
  \{2_{00z} | (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,+z+1/2
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                               +x+1/2,-y+1/2,-z
  {2_0y0|(0.5,0.0,0.0)}
                                 -x+1/2,+y,-z
    \{-1 \mid (0.5, 0.0, 0.5)\}
                               -x+1/2,-y,-z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
                             +x+1/2, +y+1/2, -z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                               -x+1/2,+y+1/2,+z
```

```
| \{m_x0z|(0.5,0.0,0.0)\} |
                                  +x+1/2,-y,+z
*******
space group: 69 {'Hall': ' -F 2 2', 'HM': 'F m m m'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y,+z
+x,-y,-z
           Seitz
                                   Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                  -x,-y,+z
  \{2_{x00}|(0.0,0.0,0.0)\}
                                  +x,-y,-z
  \{2_0y0|(0.0,0.0,0.0)\}
                                  -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{m_xy0|(0.0,0.0,0.0)\}
                                  +x,+y,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                  -x,+y,+z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                  +x,-y,+z
                              +x,+y+1/2,+z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
  \{2\_00z \mid (0.0,0.5,0.5)\}
                              -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.0,0.5,0.5)\}
                             +x,-y+1/2,-z+1/2
  {2_0y0|(0.0,0.5,0.5)}
                              -x, +y+1/2, -z+1/2
    \{-1 \mid (0.0, 0.5, 0.5)\}
                              -x,-y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                             +x,+y+1/2,-z+1/2
  \{m \ 0yz | (0.0, 0.5, 0.5)\}
                              -x, +y+1/2, +z+1/2
  \{m_x0z \mid (0.0, 0.5, 0.5)\}
                              +x,-y+1/2,+z+1/2
    \{1|(0.5,0.0,0.5)\}
                              +x+1/2,+y,+z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                             -x+1/2, -y, +z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
                              +x+1/2,-y,-z+1/2
  \{2 \text{ 0y0} | (0.5, 0.0, 0.5)\}
                              -x+1/2, +y, -z+1/2
    \{-1|(0.5,0.0,0.5)\}
                              -x+1/2, -y, -z+1/2
  \{m_xy0 | (0.5,0.0,0.5)\}
                             +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                              -x+1/2,+y,+z+1/2
  {m_x0z|(0.5,0.0,0.5)}
                              +x+1/2,-y,+z+1/2
    \{1|(0.5,0.5,0.0)\}
                             +x+1/2,+y+1/2,+z
  \{2_{00z}|(0.5,0.5,0.0)\}
                             -x+1/2,-y+1/2,+z
  \{2_{x00}|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,-z
                              -x+1/2,+y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\}
    \{-1 \mid (0.5, 0.5, 0.0)\}
                             -x+1/2, -y+1/2, -z
  \{m_xy0|(0.5,0.5,0.0)\}
                             +x+1/2,+y+1/2,-z
                             -x+1/2, +y+1/2, +z
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                             +x+1/2,-y+1/2,+z
  \{m_x0z \mid (0.5, 0.5, 0.0)\}
  . . . . . . . . . . . . . . . . . . .
*******
space group: 70:1 {'Hall': 'F 2 2 -1d', 'HM': 'F d d d:1'}
Crystal system: Orthorhombic
Setting: 1
+x,+y,+z
```

Jones {1|(0.0,0.0,0.0)} +x,+y,+z{2_00z|(0.0,0.0,0.0)} -x,-y,+z $\{2_{x00} | (0.0, 0.0, 0.0)\}$ +x,-y,-z $\{-1 \mid (0.25, 0.25, 0.25)\}$ -x+1/4, -y+1/4, -z+1/4 $\{1 \mid (0.0, 0.5, 0.5)\}$ +x,+y+1/2,+z+1/2 $\{2_00z \mid (0.0, 0.5, 0.5)\}$ -x,-y+1/2,+z+1/2 $\{2_{x00}|(0.0,0.5,0.5)\}$ +x,-y+1/2,-z+1/2 $\{-1 \mid (0.25, 0.75, 0.75)\}$ -x+1/4, -y+3/4, -z+3/4 $\{1|(0.5,0.0,0.5)\}$ +x+1/2,+y,+z+1/2 $\{2_00z \mid (0.5,0.0,0.5)\}$ -x+1/2,-y,+z+1/2 $\{2_{x00}|(0.5,0.0,0.5)\}$ +x+1/2,-y,-z+1/2-x+3/4, -y+1/4, -z+3/4 $\{-1 \mid (0.75, 0.25, 0.75)\}$ $\{1 \mid (0.5, 0.5, 0.0)\}$ +x+1/2, +y+1/2, +z $\{2_00z \mid (0.5, 0.5, 0.0)\}$ -x+1/2,-y+1/2,+z $\{2_{x00} | (0.5, 0.5, 0.0)\}$ +x+1/2,-y+1/2,-z $\{-1 \mid (0.75, 0.75, 0.25)\}$ -x+3/4, -y+3/4, -z+1/4

.

```
*******
```

space group: 70:2 {'Hall': ' -F 2uv 2vw', 'HM': 'F d d d:2'}

Crystal system: Orthorhombic

Setting: 2 +x,+y,+z -x+1/4,-y+1/4,+z +x,-y+1/4,-z+1/4

```
\{2_{00z}|(0.75,0.25,0.5)\} | -x+3/4,-y+1/4,+z+1/2
  \{2_{x00}|(0.5,0.25,0.75)\}
                            +x+1/2,-y+1/4,-z+3/4
                                -x+3/4,+y,-z+3/4
  {2_0y0|(0.75,0.0,0.75)}
                                -x+1/2, -y, -z+1/2
     \{-1 \mid (0.5, 0.0, 0.5)\}
  {m_xy0|(0.75,0.25,0.5)}
                              +x+3/4,+y+1/4,-z+1/2
 \{m_0yz \mid (0.5, 0.25, 0.75)\}
                              -x+1/2, +y+1/4, +z+3/4
  \{m_x0z|(0.75,0.0,0.75)\}
                                +x+3/4,-y,+z+3/4
     \{1 \mid (0.5, 0.5, 0.0)\}
                                +x+1/2,+y+1/2,+z
  \{2_{00z}|(0.75,0.75,0.0)\}
                                -x+3/4, -y+3/4, +z
                             +x+1/2,-y+3/4,-z+1/4
 {2_x00|(0.5,0.75,0.25)}
  \{2_0y0|(0.75,0.5,0.25)\}
                              -x+3/4,+y+1/2,-z+1/4
     \{-1 \mid (0.5, 0.5, 0.0)\}
                                -x+1/2,-y+1/2,-z
  \{m_xy0|(0.75,0.75,0.0)\}
                                +x+3/4, +y+3/4, -z
| \{m_0yz | (0.5,0.75,0.25)\} | -x+1/2,+y+3/4,+z+1/4
\{m_x0z|(0.75,0.5,0.25)\}\ |\ +x+3/4,-y+1/2,+z+1/4\ |
*******
space group: 71 {'Hall': ' -I 2 2', 'HM': 'I m m m'}
Crystal system: Orthorhombic
+x,+y,+z
```

-x,-y,+z

+x,-y,-z

Seitz	Jones
	+x,+y,+z -x,-y,+z +x,-y,-z -x,+y,-z -x,-y,-z +x,+y,-z -x,+y,+z +x,-y,+z +x+1/2,+y+1/2,+z+1/2 -x+1/2,-y+1/2,-z+1/2 -x+1/2,-y+1/2,-z+1/2 -x+1/2,-y+1/2,-z+1/2 -x+1/2,-y+1/2,-z+1/2 +x+1/2,-y+1/2,-z+1/2 +x+1/2,-y+1/2,-z+1/2
{m_0yz (0.5,0.5,0.5)} {m_x0z (0.5,0.5,0.5)}	-x+1/2,+y+1/2,+z+1/2 +x+1/2,-y+1/2,+z+1/2

.

```
*******
```

```
space group: 72 {'Hall': ' -I 2 2c', 'HM': 'I b a m'}
Crystal system: Orthorhombic
```

+x,+y,+z

-x,-y,+z

+x,-y,-z+1/2

```
Seitz
                                    Jones
  \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
{2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
\{2_{x00}|(0.0,0.0,0.5)\}
                                 +x,-y,-z+1/2
{2_0y0|(0.0,0.0,0.5)}
                                 -x,+y,-z+1/2
  \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
\{m_xy0 | (0.0,0.0,0.0)\}
                                   +x,+y,-z
\{m_0yz \mid (0.0,0.0,0.5)\}
                                 -x,+y,+z+1/2
\{m_x0z \mid (0.0,0.0,0.5)\}
                                 +x,-y,+z+1/2
  \{1|(0.5,0.5,0.5)\}
                            +x+1/2,+y+1/2,+z+1/2
                            -x+1/2, -y+1/2, +z+1/2
\{2\_00z \mid (0.5, 0.5, 0.5)\}
\{2_{x00}|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,-z
{2_0y0|(0.5,0.5,0.0)}
                              -x+1/2,+y+1/2,-z
  \{-1 \mid (0.5, 0.5, 0.5)\}
                            -x+1/2,-y+1/2,-z+1/2
\{m_xy0|(0.5,0.5,0.5)\}
                            +x+1/2, +y+1/2, -z+1/2
                              -x+1/2,+y+1/2,+z
\{m_0yz \mid (0.5, 0.5, 0.0)\}
\{m_x0z|(0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,+z
```

space group: 72:cab {'Hall': ' -I 2a 2', 'HM': 'I m c b'}

Crystal system: Orthorhombic

Setting: cab +x,+y,+z -x+1/2,-y,+z +x,-y,-z

.

+	
Seitz	Jones
 {1 (0.0,0.0,0.0)} {2_00z (0.5,0.0,0.0)} {2_x00 (0.0,0.0,0.0)} {2_y00 (0.5,0.0,0.0)} {-1 (0.0,0.0,0.0)} {m_xy0 (0.5,0.0,0.0)} {m_0yz (0.0,0.0,0.0)} {m_x0z (0.5,0.0,0.0)} {1 (0.5,0.5,0.5)} {2_y0z (0.0,0.5,0.5)} {2_x00 (0.0,0.5,0.5)} {2_y00 (0.0,0.5,0.5)} {2_ny0 (0.0,0.5,0.5)} {m_xy0 (0.0,0.5,0.5)}	+x,+y,+z -x+1/2,-y,+z +x,-y,-z -x+1/2,+y,-z -x,-y,-z +x+1/2,+y,-z -x,+y,+z +x+1/2,-y,+z +x+1/2,-y+1/2,+z+1/2 -x,-y+1/2,+z+1/2 +x+1/2,-y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 +x,+y+1/2,-z+1/2
{m_0yz (0.5,0.5,0.5)}	-x+1/2,+y+1/2,+z+1/2
{m_x0z (0.0,0.5,0.5)}	+x,-y+1/2,+z+1/2

.

```
******
```

space group: 72:bca {'Hall': ' -I 2b 2b', 'HM': 'I c m a'}

```
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y+1/2,+z
+x,-y+1/2,-z
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +X,+Y,+Z
  \{2_{00z} | (0.0, 0.5, 0.0)\}
                                  -x,-y+1/2,+z
  \{2_{x00}|(0.0,0.5,0.0)\}
                                  +x,-y+1/2,-z
  {2_0y0|(0.0,0.0,0.0)}
                                    -x,+y,-z
    \{-1 \mid (0.0,0.0,0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                                  +x,+y+1/2,-z
  \{m_0yz \mid (0.0,0.5,0.0)\}
                                  -x,+y+1/2,+z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                    +x,-y,+z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  {2_00z|(0.5,0.0,0.5)}
                                -x+1/2, -y, +z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
                                +x+1/2,-y,-z+1/2
                             -x+1/2, +y+1/2, -z+1/2
  {2_0y0|(0.5,0.5,0.5)}
    \{-1|(0.5,0.5,0.5)\}
                             -x+1/2,-y+1/2,-z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                                +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                                -x+1/2,+y,+z+1/2
  \{m_x0z|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,+z+1/2
*******
space group: 73 {'Hall': ' -I 2b 2c', 'HM': 'I b c a'}
Crystal system: Orthorhombic
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z+1/2
           Seitz
                                      Jones
    {1|(0.0,0.0,0.0)}
                                    +x,+y,+z
  \{2\_00z \mid (0.0, 0.5, 0.0)\}
                                  -x,-y+1/2,+z
  \{2_{x00} | (0.0,0.0,0.5)\}
                                  +x,-y,-z+1/2
                                -x,+y+1/2,-z+1/2
  {2_0y0|(0.0,0.5,0.5)}
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                                  +x,+y+1/2,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                  -x,+y,+z+1/2
  \{m_x0z \mid (0.0,0.5,0.5)\}
                                +x,-y+1/2,+z+1/2
    \{1 \mid (0.5, 0.5, 0.5)\}
                              +x+1/2,+y+1/2,+z+1/2
  \{2_{00z} | (0.5, 0.0, 0.5)\}
                                -x+1/2,-y,+z+1/2
  \{2_{x00}|(0.5,0.5,0.0)\}
                                +x+1/2,-y+1/2,-z
                                  -x+1/2, +y, -z
  {2_0y0|(0.5,0.0,0.0)}
    \{-1 \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,-z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                                +x+1/2, +y, -z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                -x+1/2,+y+1/2,+z
```

+x+1/2,-y,+z

 $\{m_x0z \mid (0.5,0.0,0.0)\}$

```
*******
space group: 73:ba-c {'Hall': ' -I 2a 2b', 'HM': ' I c a b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x+1/2, -y, +z
+x,-y+1/2,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                                 -x+1/2, -y, +z
  \{2_{x00} | (0.0, 0.5, 0.0)\}
                                 +x,-y+1/2,-z
  \{2_0y0|(0.5,0.5,0.0)\}
                               -x+1/2,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                                 +x+1/2,+y,-z
  \{m_0yz \mid (0.0,0.5,0.0)\}
                                 -x, +y+1/2, +z
  \{m_x0z \mid (0.5, 0.5, 0.0)\}
                               +x+1/2,-y+1/2,+z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  \{2\_00z \mid (0.0,0.5,0.5)\}
                               -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.5,0.0,0.5)\}
                               +x+1/2,-y,-z+1/2
  {2_0y0|(0.0,0.0,0.5)}
                                 -x,+y,-z+1/2
    \{-1|(0.5,0.5,0.5)\}
                             -x+1/2, -y+1/2, -z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                               +x, +y+1/2, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                               -x+1/2,+y,+z+1/2
  \{m_x0z|(0.0,0.0,0.5)\}
                                 +x,-y,+z+1/2
******
space group: 74 {'Hall': ' -I 2b 2', 'HM': 'I m m a'}
Crystal system: Orthorhombic
+X,+Y,+Z
-x,-y+1/2,+z
+x,-y,-z
           Seitz
                                     Jones
    \{1 \mid (0.0,0.0,0.0)\}
                                    +X,+Y,+Z
  {2_00z|(0.0,0.5,0.0)}
                                 -x,-y+1/2,+z
  \{2_{x00} | (0.0,0.0,0.0)\}
                                    +x,-y,-z
  {2_0y0|(0.0,0.5,0.0)}
                                  -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.0,0.5,0.0)\}
                                  +x,+y+1/2,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                    -x,+y,+z
  \{m_x0z | (0.0,0.5,0.0)\}
                                  +x,-y+1/2,+z
    \{1|(0.5,0.5,0.5)\}
                             +x+1/2, +y+1/2, +z+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                               -x+1/2,-y,+z+1/2
  \{2_x00|(0.5,0.5,0.5)\} \mid +x+1/2,-y+1/2,-z+1/2 \mid
```

```
{2_0y0|(0.5,0.0,0.5)} |
                               -x+1/2,+y,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, -z+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                               +x+1/2,+y,-z+1/2
  \{m \ 0yz | (0.5, 0.5, 0.5)\}
                             -x+1/2,+y+1/2,+z+1/2
                               +x+1/2,-y,+z+1/2
 \{m \times 0z \mid (0.5, 0.0, 0.5)\}
*******
space group: 74:ba-c {'Hall': ' -I 2a 2a', 'HM': ' I m m b'}
Crystal system: Orthorhombic
Setting: ba-c
+x,+y,+z
-x+1/2,-y,+z
+x+1/2,-y,-z
           Seitz
                                     Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.5,0.0,0.0)\}
                                  -x+1/2, -y, +z
  \{2_{x00}|(0.5,0.0,0.0)\}
                                  +x+1/2,-y,-z
  {2_0y0|(0.0,0.0,0.0)}
                                    -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{m_xy0|(0.5,0.0,0.0)\}
                                  +x+1/2, +y, -z
  \{m_0yz \mid (0.5,0.0,0.0)\}
                                  -x+1/2,+y,+z
  \{m_x0z \mid (0.0,0.0,0.0)\}
                                    +x,-y,+z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2, +y+1/2, +z+1/2
  \{2\ 00z|(0.0,0.5,0.5)\}
                               -x,-y+1/2,+z+1/2
  \{2_{x00}|(0.0,0.5,0.5)\}
                               +x,-y+1/2,-z+1/2
                             -x+1/2, +y+1/2, -z+1/2
  \{2_0y0|(0.5,0.5,0.5)\}
    \{-1|(0.5,0.5,0.5)\}
                             -x+1/2, -y+1/2, -z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                               +x,+y+1/2,-z+1/2
  \{m \ 0yz | (0.0, 0.5, 0.5)\}
                               -x,+y+1/2,+z+1/2
                             +x+1/2,-y+1/2,+z+1/2
  \{m \times 0z \mid (0.5, 0.5, 0.5)\}
*******
space group: 74:cab {'Hall': ' -I 2c 2c', 'HM': 'I b m m'}
Crystal system: Orthorhombic
Setting: cab
+x,+y,+z
-x,-y,+z+1/2
+x,-y,-z+1/2
           Seitz
                                     Jones
    {1|(0.0,0.0,0.0)}
                                    +x,+y,+z
 \{2\_00z \mid (0.0,0.0,0.5)\}
                                  -x,-y,+z+1/2
 {2_x00|(0.0,0.0,0.5)}
                                  +x,-y,-z+1/2
  \{2 \ 0 \ | \ (0.0, 0.0, 0.0)\}
                                    -x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
```

```
\{m_xy0|(0.0,0.0,0.5)\}
                                  +x,+y,-z+1/2
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                  -x,+y,+z+1/2
                                    +x,-y,+z
  \{m_x0z|(0.0,0.0,0.0)\}
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                -x+1/2, -y+1/2, +z
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                                +x+1/2,-y+1/2,-z
  {2_0y0|(0.5,0.5,0.5)}
                             -x+1/2,+y+1/2,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, -z+1/2
  \{m_xy0|(0.5,0.5,0.0)\}
                                +x+1/2, +y+1/2, -z
  \{m \ 0yz | (0.5, 0.5, 0.0)\}
                                -x+1/2,+y+1/2,+z
  {m_x0z|(0.5,0.5,0.5)}
                             +x+1/2,-y+1/2,+z+1/2
******
space group: 74:-cba {'Hall': ' -I 2 2b', 'HM': ' I c m m'}
Crystal system: Orthorhombic
Setting: -cba
+x,+y,+z
-x,-y,+z
+x,-y+1/2,-z
           Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{2\_00z \mid (0.0,0.0,0.0)\}
                                    -x,-y,+z
  \{2_{x00} | (0.0, 0.5, 0.0)\}
                                  +x,-y+1/2,-z
  \{2 \ 0 \ | \ (0.0, 0.5, 0.0)\}
                                  -x,+y+1/2,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
                                    +x,+y,-z
  \{m \times y0 \mid (0.0, 0.0, 0.0)\}
  \{m_0yz \mid (0.0,0.5,0.0)\}
                                  -x,+y+1/2,+z
  \{m_x0z \mid (0.0, 0.5, 0.0)\}
                                  +x,-y+1/2,+z
    \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,+z+1/2
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                                +x+1/2,-y,-z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                                -x+1/2,+y,-z+1/2
    \{-1 \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, -z+1/2
  \{m_xy0|(0.5,0.5,0.5)\}
                              +x+1/2, +y+1/2, -z+1/2
  \{m_0yz \mid (0.5,0.0,0.5)\}
                                -x+1/2,+y,+z+1/2
  \{m_x0z|(0.5,0.0,0.5)\}
                                +x+1/2,-y,+z+1/2
*******
space group: 74:bca {'Hall': ' -I 2 2a', 'HM': 'I m c m'}
Crystal system: Orthorhombic
Setting: bca
+x,+y,+z
-x,-y,+z
+x+1/2,-y,-z
                                      Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
{2_00z|(0.0,0.0,0.0)}
                                    -x,-y,+z
\{2_{x00} | (0.5, 0.0, 0.0)\}
                                  +x+1/2,-y,-z
{2_0y0|(0.5,0.0,0.0)}
                                  -x+1/2,+y,-z
   \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
\{m_xy0 | (0.0,0.0,0.0)\}
                                    +x,+y,-z
                                  -x+1/2, +y, +z
\{m_0yz \mid (0.5,0.0,0.0)\}
\{m_x0z \mid (0.5,0.0,0.0)\}
                                  +x+1/2,-y,+z
                             +x+1/2,+y+1/2,+z+1/2
   \{1 \mid (0.5, 0.5, 0.5)\}
\{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2, -y+1/2, +z+1/2
                               +x,-y+1/2,-z+1/2
\{2_{x00} | (0.0, 0.5, 0.5)\}
{2_0y0|(0.0,0.5,0.5)}
                               -x,+y+1/2,-z+1/2
   \{-1 \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,-z+1/2
\{m_xy0|(0.5,0.5,0.5)\}
                             +x+1/2, +y+1/2, -z+1/2
\{m_0yz \mid (0.0,0.5,0.5)\}
                               -x, +y+1/2, +z+1/2
\{m_x0z|(0.0,0.5,0.5)\}
                               +x,-y+1/2,+z+1/2
```

space group: 74:a-cb {'Hall': ' -I 2c 2', 'HM': ' I m a m'}

Crystal system: Orthorhombic

Setting: a-cb

+x,+y,+z

-x,-y,+z+1/2

+x,-y,-z

.

Seitz	Jones
+	+x,+y,+z -x,-y,+z+1/2 +x,-y,-z -x,+y,-z+1/2 -x,-y,-z +x,+y,-z+1/2 -x,+y,+z +x,-y,+z+1/2 +x+1/2,+y+1/2,+z+1/2 -x+1/2,-y+1/2,-z +x+1/2,-y+1/2,-z -x+1/2,-y+1/2,-z -x+1/2,-y+1/2,-z +x+1/2,+y+1/2,-z -x+1/2,+y+1/2,-z -x+1/2,+y+1/2,-z
{m_x0z (0.5,0.5,0.0)}	+x+1/2,-y+1/2,+z

.

space group: 75 {'Hall': 'P 4', 'HM': 'P 4'}

Crystal system: Tetragonal

+x,+y,+z

```
-y,+x,+z
           Seitz
                              Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                           +x,+y,+z
 \{4^+_{00z}|(0.0,0.0,0.0)\} \mid -y,+x,+z
  {2_00z|(0.0,0.0,0.0)}
                            -x,-y,+z
  \{4^-_00z \mid (0.0,0.0,0.0)\} \mid +y,-x,+z
*******
space group: 76 {'Hall': ' P 4w', 'HM': 'P 41'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+1/4
           Seitz
                                 Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
  \{4^+_{00z}|(0.0,0.0,0.25)\}
                             -y, +x, +z+1/4
                             -x,-y,+z+1/2
   {2_00z|(0.0,0.0,0.5)}
  \{4^{-}00z \mid (0.0,0.0,0.75)\} \mid +y,-x,+z+3/4
******
space group: 77 {'Hall': ' P 4c', 'HM': 'P 42'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+1/2
           Seitz
                                Jones
     {1|(0.0,0.0,0.0)}
                              +x,+y,+z
  \{4^+_{00z} | (0.0,0.0,0.5)\} \mid -y,+x,+z+1/2
  {2_00z|(0.0,0.0,0.0)}
                              -x,-y,+z
  \{4^{-}00z \mid (0.0,0.0,0.5)\} \mid +y,-x,+z+1/2
*******
space group: 78 {'Hall': ' P 4cw', 'HM': 'P 43'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+3/4
           Seitz
                                 Jones
     {1|(0.0,0.0,0.0)}
                               +x,+y,+z
```

```
\{4^+_00z \mid (0.0,0.0,0.75)\} \mid -y,+x,+z+3/4 \mid
  {2_00z|(0.0,0.0,0.5)}
                              | -x, -y, +z+1/2 |
  \{4^{-}00z \mid (0.0,0.0,0.25)\} \mid +y,-x,+z+1/4 \mid
*******
space group: 79 {'Hall': 'I 4', 'HM': 'I 4'}
Crystal system: Tetragonal
+X,+Y,+Z
-y,+x,+z
. . . . . . . . . . . . . . . . . . .
            Seitz
                                      Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                     +x,+y,+z
  {4^+_00z|(0.0,0.0,0.0)}
                                     -y,+x,+z
   {2_00z|(0.0,0.0,0.0)}
                                     -x,-y,+z
  \{4^-_00z \mid (0.0,0.0,0.0)\}
                                     +y,-x,+z
     \{1 \mid (0.5, 0.5, 0.5)\}
                             | +x+1/2,+y+1/2,+z+1/2
  \{4^+_{00z}|(0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,+z+1/2
   {2_00z|(0.5,0.5,0.5)}
                             -x+1/2,-y+1/2,+z+1/2
  \{4^-_00z \mid (0.5, 0.5, 0.5)\} \mid +y+1/2, -x+1/2, +z+1/2
******
space group: 80 {'Hall': ' I 4bw', 'HM': 'I 41'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x+1/2,+z+1/4
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
  \{4^+_{00z}|(0.0,0.5,0.25)\}\ |
                                  -y, +x+1/2, +z+1/4
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                -x+1/2, -y+1/2, +z+1/2
  {4^-_00z|(0.5,0.0,0.75)}
                                  +y+1/2,-x,+z+3/4
     \{1 \mid (0.5, 0.5, 0.5)\}
                                +x+1/2,+y+1/2,+z+1/2
  \{4^+_00z|(0.5,0.0,0.75)\}
                                  -y+1/2,+x,+z+3/4
   \{2_{00z} | (0.0,0.0,0.0)\}
                                      -x,-y,+z
  \{4^-_00z|(0.0,0.5,0.25)\}
                                  +y, -x+1/2, +z+1/4
*******
space group: 81 {'Hall': ' P -4', 'HM': 'P -4'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
            Seitz
                                 Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                             +x,+y,+z
  \{-4^+,00z|(0.0,0.0,0.0)\} | +y,-x,-z
  {2 00z|(0.0,0.0,0.0)}
                             -x,-y,+z
  \{-4^{-}00z \mid (0.0,0.0,0.0)\} \mid -y,+x,-z \mid
*******
space group: 82 {'Hall': ' I -4', 'HM': 'I -4'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                     +x,+y,+z
  \{-4^+_00z \mid (0.0,0.0,0.0)\}
                                     +y,-x,-z
   {2_00z|(0.0,0.0,0.0)}
                                     -x,-y,+z
  \{-4^-00z \mid (0.0,0.0,0.0)\} \mid
                                     -y,+x,-z
     \{1 \mid (0.5, 0.5, 0.5)\}
                             +x+1/2,+y+1/2,+z+1/2
  \{-4^+00z|(0.5,0.5,0.5)\} | +y+1/2,-x+1/2,-z+1/2
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,-y+1/2,+z+1/2
  \{-4^-00z \mid (0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,-z+1/2
*******
space group: 83 {'Hall': ' -P 4', 'HM': 'P 4/m'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
            Seitz
                                Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                             +x,+y,+z
  {4^+_00z|(0.0,0.0,0.0)}
                             | -y,+x,+z |
   {2_00z|(0.0,0.0,0.0)}
                             -x,-y,+z
  \{4^-00z \mid (0.0,0.0,0.0)\}
                             +y,-x,+z
     \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
  \{-4^+,00z|(0.0,0.0,0.0)\} \mid +y,-x,-z \mid
   \{m_xy0|(0.0,0.0,0.0)\}
                             | +x,+y,-z |
  \{-4^-00z \mid (0.0,0.0,0.0)\} \mid -y,+x,-z \mid
*******
space group: 84 {'Hall': '-P 4c', 'HM': 'P 42/m'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+1/2
```

```
Seitz
                                     Jones
   \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
\{4^+_00z \mid (0.0,0.0,0.5)\}
                                 -y,+x,+z+1/2
{2_00z|(0.0,0.0,0.0)}
                                    -x,-y,+z
\{4^-_00z \mid (0.0,0.0,0.5)\}
                                 +y,-x,+z+1/2
   \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
\{-4^+_00z \mid (0.0,0.0,0.5)\}
                                 +y,-x,-z+1/2
 \{m \times y0 \mid (0.0, 0.0, 0.0)\}
                                   +X,+Y,-Z
\{-4^-00z \mid (0.0,0.0,0.5)\} \mid -y,+x,-z+1/2
```

space group: 85:1 {'Hall': 'P 4ab -1ab', 'HM': 'P 4/n:1'}

Crystal system: Tetragonal

Setting: 1 +x,+y,+z

-y+1/2,+x+1/2,+z

-x+1/2,-y+1/2,-z

space group: 85:2 {'Hall': ' -P 4a', 'HM': 'P 4/n:2'}

Crystal system: Tetragonal

Setting: 2 +x,+y,+z -y+1/2,+x,+z

Seitz	Jones
{1 (0.0,0.0,0.0)} {4^+_00z (0.5,0.0,0.0)} {2_00z (0.5,0.5,0.0)} {4^00z (0.0,0.5,0.0)} {-1 (0.0,0.0,0.0)} {-4^+_00z (0.5,0.0,0.0)} {m_xy0 (0.5,0.5,0.0)} {-4^00z (0.0,0.5,0.0)}	+x,+y,+z -y+1/2,+x,+z -x+1/2,-y+1/2,+z +y,-x+1/2,+z -x,-y,-z +y+1/2,-x,-z +x+1/2,+y+1/2,-z -y,+x+1/2,-z

.

```
space group: 86:1 {'Hall': ' P 4n -1n', 'HM': 'P 42/n:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
-x+1/2, -y+1/2, -z+1/2
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,+z+1/2
     \{-1|(0.5,0.5,0.5)\}
                             | -x+1/2, -y+1/2, -z+1/2 |
   \{2\_00z \mid (0.0,0.0,0.0)\}
                                      -x,-y,+z
*******
space group: 86:2 {'Hall': '-P 4bc', 'HM': 'P 42/n:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y, +x+1/2, +z+1/2
  . . . . . . . . . . . . . . . . .
            Seitz
                                      Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                     +x,+y,+z
 \{4^+_{00z} | (0.0, 0.5, 0.5)\}
                              |-y,+x+1/2,+z+1/2|
  {2_00z|(0.5,0.5,0.0)}
                                -x+1/2,-y+1/2,+z
  \{4^{-}00z \mid (0.5,0.0,0.5)\}
                                +y+1/2,-x,+z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                     -x,-y,-z
  \{-4^+ 00z \mid (0.0, 0.5, 0.5)\} \mid +y, -x+1/2, -z+1/2
  \{m \times y0 \mid (0.5, 0.5, 0.0)\}
                                +x+1/2, +y+1/2, -z
  \{-4^-00z|(0.5,0.0,0.5)\}
                               -y+1/2,+x,-z+1/2
*******
space group: 87 {'Hall': ' -I 4', 'HM': 'I 4/m'}
Crystal system: Tetragonal
+X,+Y,+Z
-y,+x,+z
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  \{4^+_00z \mid (0.0,0.0,0.0)\}
                                       -y,+x,+z
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
  {4^-_00z|(0.0,0.0,0.0)}
                                       +y,-x,+z
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                       -x,-y,-z
  \{-4^+ 00z \mid (0.0,0.0,0.0)\}
                                       +y,-x,-z
```

+x,+y,-z

 $\{m_xy0|(0.0,0.0,0.0)\}$

```
-y, +x, -z
  \{-4^-00z|(0.0,0.0,0.0)\}
     \{1 \mid (0.5, 0.5, 0.5)\}
                                +x+1/2,+y+1/2,+z+1/2
  \{4^+_{00z}|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,+z+1/2
   \{2\ 00z\mid (0.5,0.5,0.5)\}
                                -x+1/2, -y+1/2, +z+1/2
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,-x+1/2,+z+1/2
     \{-1|(0.5,0.5,0.5)\}
                                -x+1/2,-y+1/2,-z+1/2
  \{-4^+_{00z}|(0.5,0.5,0.5)\} \mid +y+1/2,-x+1/2,-z+1/2
   \{m_xy0|(0.5,0.5,0.5)\}
                                +x+1/2, +y+1/2, -z+1/2
  \{-4^-00z \mid (0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,-z+1/2
********
space group: 88:1 {'Hall': ' I 4bw -1bw', 'HM': 'I 41/a:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y, +x+1/2, +z+1/4
-x,-y+1/2,-z+1/4
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  \{4^+_{00z} | (0.0, 0.5, 0.25)\}
                                  -y, +x+1/2, +z+1/4
    \{-1 \mid (0.0, 0.5, 0.25)\}
                                  -x,-y+1/2,-z+1/4
   {2_00z|(0.5,0.5,0.5)}
                                -x+1/2,-y+1/2,+z+1/2
     \{1 \mid (0.5, 0.5, 0.5)\}
                                +x+1/2, +y+1/2, +z+1/2
  \{4^+_{00z}|(0.5,0.0,0.75)\}
                                  -y+1/2,+x,+z+3/4
    \{-1 \mid (0.5, 0.0, 0.75)\}
                                  -x+1/2,-y,-z+3/4
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
*******
space group: 88:2 {'Hall': '-I 4ad', 'HM': 'I 41/a:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y+3/4, +x+1/4, +z+1/4
              Seitz
                                           Jones
       {1|(0.0,0.0,0.0)}
                                          +x,+y,+z
   \{4^+_{00z}|(0.75,0.25,0.25)\}
                                   -y+3/4, +x+1/4, +z+1/4
     {2_00z|(0.5,0.0,0.5)}
                                      -x+1/2,-y,+z+1/2
   {4^-_00z|(0.75,0.75,0.75)}
                                   +y+3/4,-x+3/4,+z+3/4
       \{-1 \mid (0.0, 0.0, 0.0)\}
                                          -x,-y,-z
  \{-4^+_00z|(0.75,0.25,0.25)\}
                                   +y+3/4,-x+1/4,-z+1/4
     {m_xy0|(0.5,0.0,0.5)}
                                     +x+1/2,+y,-z+1/2
  \{-4^-00z \mid (0.75, 0.75, 0.75)\}
                                   -y+3/4,+x+3/4,-z+3/4
       \{1 \mid (0.5, 0.5, 0.5)\}
                                   +x+1/2,+y+1/2,+z+1/2
   \{4^+ 00z \mid (0.25, 0.75, 0.75)\} \mid -y+1/4, +x+3/4, +z+3/4
```

```
-x,-y+1/2,+z
     {2_00z|(0.0,0.5,0.0)}
   \{4^{-}00z|(0.25,0.25,0.25)\} + y+1/4,-x+1/4,+z+1/4
       \{-1 \mid (0.5, 0.5, 0.5)\}
                                   -x+1/2, -y+1/2, -z+1/2
  \{-4^+ 00z \mid (0.25, 0.75, 0.75)\}
                                   +y+1/4,-x+3/4,-z+3/4
     \{m_xy0 | (0.0, 0.5, 0.0)\}
                                       +x,+y+1/2,-z
  \{-4^{-}00z \mid (0.25, 0.25, 0.25)\} \mid -y+1/4, +x+1/4, -z+1/4
*******
space group: 89 {'Hall': 'P 4 2', 'HM': 'P 4 2 2'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
+x,-y,-z
            Seitz
                                Jones
     {1|(0.0,0.0,0.0)}
                             +x,+y,+z
 \{4^+_{00z} | (0.0,0.0,0.0)\} \mid -y,+x,+z
   \{2_{x00} | (0.0,0.0,0.0)\}
                              +x,-y,-z
   \{2_{00z} | (0.0,0.0,0.0)\}
                              -x,-y,+z
   {2_xx0|(0.0,0.0,0.0)}
                              +y,+x,-z
  \{4^-_00z \mid (0.0,0.0,0.0)\} \mid +y,-x,+z
   {2_0y0|(0.0,0.0,0.0)}
                             -x,+y,-z
   \{2_x-x0\mid (0.0,0.0,0.0)\} \mid -y,-x,-z
*******
space group: 90 {'Hall': ' P 4ab 2ab', 'HM': 'P 42 1 2'}
Crystal system: Tetragonal
+x,+y,+z
-y+1/2,+x+1/2,+z
+x+1/2,-y+1/2,-z
            Seitz
                                    Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{4^+_00z \mid (0.5, 0.5, 0.0)\}
                              -y+1/2,+x+1/2,+z
   \{2_{x00} | (0.5, 0.5, 0.0)\}
                              +x+1/2,-y+1/2,-z
   {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
   \{2_{xx0} | (0.0,0.0,0.0)\}
                                   +y,+x,-z
  \{4^-00z \mid (0.5, 0.5, 0.0)\}
                              +y+1/2,-x+1/2,+z
   {2_0y0|(0.5,0.5,0.0)}
                              -x+1/2,+y+1/2,-z
   \{2_x-x0\mid(0.0,0.0,0.0)\}\ \mid
                                   -y,-x,-z
*******
```

space group: 91 {'Hall': ' P 4w 2c', 'HM': 'P 41 2 2'}

Crystal system: Tetragonal

```
+x,+y,+z
-y, +x, +z+1/4
+x,-y,-z+1/2
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{4^+_{00z}|(0.0,0.0,0.25)\}
                               -y, +x, +z+1/4
   \{2_{x00}|(0.0,0.0,0.5)\}
                               +x,-y,-z+1/2
   {2_00z|(0.0,0.0,0.5)}
                               -x,-y,+z+1/2
   \{2_x \times 0 \mid (0.0, 0.0, 0.75)\}
                               +y,+x,-z+3/4
  \{4^{-}00z \mid (0.0,0.0,0.75)\} \mid +y,-x,+z+3/4
   {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
  \{2_x-x0|(0.0,0.0,0.25)\}
                              | -y, -x, -z+1/4
*******
space group: 92 {'Hall': 'P 4abw 2nw', 'HM': 'P 41 21 2'}
Crystal system: Tetragonal
+x,+y,+z
-y+1/2,+x+1/2,+z+1/4
+x+1/2,-y+1/2,-z+3/4
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +X,+Y,+Z
  \{4^+_{00z}|(0.5,0.5,0.25)\}
                               -y+1/2,+x+1/2,+z+1/4
   \{2_{x00} | (0.5, 0.5, 0.75)\}
                                +x+1/2,-y+1/2,-z+3/4
   {2_00z|(0.0,0.0,0.5)}
                                    -x,-y,+z+1/2
                                      +y,+x,-z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
  \{4^- 00z \mid (0.5, 0.5, 0.75)\} \mid
                               +y+1/2,-x+1/2,+z+3/4
   {2_0y0|(0.5,0.5,0.25)}
                               -x+1/2,+y+1/2,-z+1/4
   \{2_x-x0|(0.0,0.0,0.5)\}
                                    -y, -x, -z+1/2
******
space group: 93 {'Hall': ' P 4c 2', 'HM': 'P 42 2 2'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z+1/2
+x,-y,-z
            Seitz
                                  Jones
     {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  \{4^+_{00z} | (0.0,0.0,0.5)\}
                              -y,+x,+z+1/2
   \{2_{x00} | (0.0,0.0,0.0)\}
                                +x,-y,-z
```

-x,-y,+z

+y,+x,-z+1/2

 $\{2_00z \mid (0.0,0.0,0.0)\}$

 $\{2_x \times 0 \mid (0.0, 0.0, 0.5)\}$

```
\{4^-_00z \mid (0.0,0.0,0.5)\} \mid +y,-x,+z+1/2 \mid
   {2_0y0|(0.0,0.0,0.0)}
                               -x,+y,-z
   \{2_x-x0|(0.0,0.0,0.5)\}\ |\ -y,-x,-z+1/2
*******
space group: 94 {'Hall': 'P 4n 2n', 'HM': 'P 42 21 2'}
Crystal system: Tetragonal
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x+1/2,-y+1/2,-z+1/2
            Seitz
                                     Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,+z+1/2
   \{2_{x00}|(0.5,0.5,0.5)\}
                              +x+1/2,-y+1/2,-z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                    -x,-y,+z
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                                    +y,+x,-z
  \{4^{-}00z|(0.5,0.5,0.5)\} | +y+1/2,-x+1/2,+z+1/2
   \{2_0y0|(0.5,0.5,0.5)\}
                              -x+1/2,+y+1/2,-z+1/2
   \{2_x-x0|(0.0,0.0,0.0)\}
                                    -y,-x,-z
*******
space group: 95 {'Hall': ' P 4cw 2c', 'HM': 'P 43 2 2'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+3/4
+x,-y,-z+1/2
           Seitz
                                  Jones
     {1|(0.0,0.0,0.0)}
                                +x,+y,+z
  \{4^+_{00z}|(0.0,0.0,0.75)\} \mid -y,+x,+z+3/4
   \{2_{x00}|(0.0,0.0,0.5)\}
                             +x,-y,-z+1/2
   \{2\_00z \mid (0.0,0.0,0.5)\}
                             | -x, -y, +z+1/2
   \{2_x \times 0 \mid (0.0, 0.0, 0.25)\}
                             | +y,+x,-z+1/4
  \{4^{-}00z \mid (0.0,0.0,0.25)\} \mid +y,-x,+z+1/4
  {2_0y0|(0.0,0.0,0.0)}
                                -x,+y,-z
  \{2_x-x0\mid(0.0,0.0,0.75)\}\ \mid -y,-x,-z+3/4
*******
space group: 96 {'Hall': 'P 4nw 2abw', 'HM': 'P 43 21 2'}
Crystal system: Tetragonal
+x,+y,+z
-y+1/2,+x+1/2,+z+3/4
+x+1/2,-y+1/2,-z+1/4
```

```
Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.75)\}
                                -y+1/2,+x+1/2,+z+3/4
   \{2_{x00}|(0.5,0.5,0.25)\}
                                +x+1/2,-y+1/2,-z+1/4
   \{2\_00z \mid (0.0,0.0,0.5)\}
                                     -x,-y,+z+1/2
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                                       +y,+x,-z
  \{4^-_00z \mid (0.5, 0.5, 0.25)\}
                                +y+1/2,-x+1/2,+z+1/4
   {2_0y0|(0.5,0.5,0.75)}
                                -x+1/2,+y+1/2,-z+3/4
   \{2_x-x0|(0.0,0.0,0.5)\}
                                     -y,-x,-z+1/2
*******
space group: 97 {'Hall': 'I 4 2', 'HM': 'I 4 2 2'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
+x,-y,-z
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
  {4^+_00z|(0.0,0.0,0.0)}
                                      -y,+x,+z
   \{2_{x00} | (0.0,0.0,0.0)\}
                                      +x,-y,-z
   {2 00z|(0.0,0.0,0.0)}
                                      -X,-Y,+Z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                      +y,+x,-z
  \{4^- 00z \mid (0.0,0.0,0.0)\}
                                      +y,-x,+z
   {2_0y0|(0.0,0.0,0.0)}
                                      -x,+y,-z
   \{2_x-x0\mid(0.0,0.0,0.0)\}
                                      -y,-x,-z
     \{1 \mid (0.5, 0.5, 0.5)\}
                               +x+1/2, +y+1/2, +z+1/2
  \{4^+_{00z} | (0.5, 0.5, 0.5)\}
                               -y+1/2,+x+1/2,+z+1/2
   \{2_{x00} | (0.5, 0.5, 0.5)\}
                               +x+1/2,-y+1/2,-z+1/2
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                               -x+1/2,-y+1/2,+z+1/2
                               +y+1/2,+x+1/2,-z+1/2
   \{2_{xx0}|(0.5,0.5,0.5)\}
  {4^-_00z|(0.5,0.5,0.5)}
                               +y+1/2,-x+1/2,+z+1/2
   \{2_0y0|(0.5,0.5,0.5)\}
                               -x+1/2,+y+1/2,-z+1/2
   \{2_x-x0|(0.5,0.5,0.5)\} \mid -y+1/2,-x+1/2,-z+1/2
*******
space group: 98 {'Hall': ' I 4bw 2bw', 'HM': 'I 41 2 2'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x+1/2, +z+1/4
+x,-y+1/2,-z+1/4
            Seitz
                                        Jones
```

```
\{1|(0.0,0.0,0.0)\}
                                       +x,+y,+z
  \{4^+_{00z}|(0.0,0.5,0.25)\}
                                  -y, +x+1/2, +z+1/4
   \{2_{x00}|(0.0,0.5,0.25)\}
                                  +x,-y+1/2,-z+1/4
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                -x+1/2, -y+1/2, +z+1/2
   \{2_{x} \times 0 \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,+x+1/2,-z+1/2
  \{4^-_00z \mid (0.5, 0.0, 0.75)\}
                                  +y+1/2,-x,+z+3/4
   {2_0y0|(0.5,0.0,0.75)}
                                  -x+1/2,+y,-z+3/4
   \{2_x-x0|(0.0,0.0,0.0)\}
                                       -y,-x,-z
     \{1 \mid (0.5, 0.5, 0.5)\}
                                +x+1/2, +y+1/2, +z+1/2
  \{4^+_{00z}|(0.5,0.0,0.75)\}
                                  -y+1/2,+x,+z+3/4
   {2_x00|(0.5,0.0,0.75)}
                                  +x+1/2,-y,-z+3/4
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
   {2_xx0|(0.0,0.0,0.0)}
                                       +y,+x,-z
  {4^-_00z|(0.0,0.5,0.25)}
                                  +y,-x+1/2,+z+1/4
   {2_0y0|(0.0,0.5,0.25)}
                                  -x, +y+1/2, -z+1/4
   \{2_x-x0\mid(0.5,0.5,0.5)\}
                                -y+1/2, -x+1/2, -z+1/2
*******
space group: 99 {'Hall': 'P 4 -2', 'HM': 'P 4 m m'}
Crystal system: Tetragonal
+X,+Y,+Z
-y,+x,+z
-x,+y,+z
            Seitz
                                Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
  \{4^+_{00z}|(0.0,0.0,0.0)\}
                               -y,+x,+z
   \{m_0yz \mid (0.0,0.0,0.0)\}
                               -x,+y,+z
   {2_00z|(0.0,0.0,0.0)}
                               -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                               -y,-x,+z
  \{4^-_00z \mid (0.0,0.0,0.0)\}
                               +y,-x,+z
   \{m_x0z|(0.0,0.0,0.0)\}
                               +x,-y,+z
   \{m_x \times z \mid (0.0, 0.0, 0.0)\}
                               +y,+x,+z
*******
space group: 100 {'Hall': 'P 4 -2ab', 'HM': 'P 4 b m'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
-x+1/2,+y+1/2,+z
            Seitz
                                     Jones
     {1|(0.0,0.0,0.0)}
                                    +x,+y,+z
  {4^+_00z|(0.0,0.0,0.0)} |
                                   -y,+x,+z
   \{m_0yz \mid (0.5, 0.5, 0.0)\}
                               -x+1/2,+y+1/2,+z
```

-x,-y,+z

{2_00z|(0.0,0.0,0.0)}

```
\{m_x-xz\mid(0.5,0.5,0.0)\}\mid -y+1/2,-x+1/2,+z
  \{4^-_00z \mid (0.0,0.0,0.0)\} \mid
                                   +y,-x,+z
   \{m_x0z \mid (0.5,0.5,0.0)\}
                              +x+1/2,-y+1/2,+z
                            +y+1/2,+x+1/2,+z
   \{m_xxz|(0.5,0.5,0.0)\}
*******
space group: 101 {'Hall': ' P 4c -2c', 'HM': 'P 42 c m'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+1/2
-x,+y,+z+1/2
            Seitz
                                  Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  \{4^+_{00z}|(0.0,0.0,0.5)\}
                              -y, +x, +z+1/2
   \{m_0yz \mid (0.0,0.0,0.5)\}
                              -x,+y,+z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                -y,-x,+z
  \{4^-00z \mid (0.0,0.0,0.5)\}
                              +y,-x,+z+1/2
   \{m_x0z | (0.0,0.0,0.5)\}
                              +x,-y,+z+1/2
   \{m_x \times z \mid (0.0, 0.0, 0.0)\}
                                +y, +x, +z
*******
space group: 102 {'Hall': ' P 4n -2n', 'HM': 'P 42 n m'}
Crystal system: Tetragonal
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
-x+1/2, +y+1/2, +z+1/2
            Seitz
                                      Jones
     {1|(0.0,0.0,0.0)}
                                     +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,+z+1/2
                              -x+1/2,+y+1/2,+z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
   {2_00z|(0.0,0.0,0.0)}
                                     -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                     -y,-x,+z
  {4^-_00z|(0.5,0.5,0.5)} |
                              +y+1/2,-x+1/2,+z+1/2
   \{m_x0z|(0.5,0.5,0.5)\}
                              +x+1/2,-y+1/2,+z+1/2
   \{m_x \times z \mid (0.0, 0.0, 0.0)\}
                                     +y,+x,+z
*******
space group: 103 {'Hall': 'P 4 -2c', 'HM': 'P 4 c c'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
```

```
-x,+y,+z+1/2
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  {4^+_00z|(0.0,0.0,0.0)}
                                 -y,+x,+z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                               -x,+y,+z+1/2
   \{2\_00z \mid (0.0,0.0,0.0)\}
                                 -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                               -y,-x,+z+1/2
  {4^-_00z|(0.0,0.0,0.0)}
                                 +y,-x,+z
   \{m_x0z | (0.0,0.0,0.5)\}
                               +x,-y,+z+1/2
   \{m_x \times z \mid (0.0, 0.0, 0.5)\}
                             +y,+x,+z+1/2
******
space group: 104 {'Hall': 'P 4 -2n', 'HM': 'P 4 n c'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
-x+1/2, +y+1/2, +z+1/2
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
  \{4^+_{00z}|(0.0,0.0,0.0)\}
                                      -y,+x,+z
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
                             -x+1/2,+y+1/2,+z+1/2
   \{2\_00z \mid (0.0,0.0,0.0)\}
                                      -x,-y,+z
   \{m_x-xz \mid (0.5,0.5,0.5)\}
                               -y+1/2,-x+1/2,+z+1/2
  \{4^{-}00z \mid (0.0,0.0,0.0)\} \mid
                                      +y,-x,+z
   \{m_x0z|(0.5,0.5,0.5)\}
                               +x+1/2,-y+1/2,+z+1/2
   \{m \times xz \mid (0.5, 0.5, 0.5)\}
                             +y+1/2,+x+1/2,+z+1/2
*******
space group: 105 {'Hall': ' P 4c -2', 'HM': 'P 42 m c'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+1/2
-x,+y,+z
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{4^+_{00z}|(0.0,0.0,0.5)\}
                               -y, +x, +z+1/2
   \{m_0yz \mid (0.0,0.0,0.0)\}
                                 -x,+y,+z
   {2_00z|(0.0,0.0,0.0)}
```

-x,-y,+z -y,-x,+z+1/2

+y,-x,+z+1/2

+x,-y,+z

{m_x-xz|(0.0,0.0,0.5)} {4^-_00z|(0.0,0.0,0.5)}

 $\{m \times 0z \mid (0.0,0.0,0.0)\}$

```
\{m_xxz | (0.0,0.0,0.5)\} | +y,+x,+z+1/2 |
*******
space group: 106 {'Hall': ' P 4c -2ab', 'HM': 'P 42 b c'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z+1/2
-x+1/2,+y+1/2,+z
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
  \{4^+ 00z \mid (0.0,0.0,0.5)\} \mid
                                    -y, +x, +z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                  -x+1/2,+y+1/2,+z
   \{2\_00z \mid (0.0,0.0,0.0)\}
                                      -x,-y,+z
   \{m_x-xz\mid(0.5,0.5,0.5)\}
                               -y+1/2, -x+1/2, +z+1/2
  \{4^{-}00z \mid (0.0,0.0,0.5)\}
                                    +y,-x,+z+1/2
   \{m_x0z|(0.5,0.5,0.0)\}
                                  +x+1/2,-y+1/2,+z
   \{m_xxz | (0.5, 0.5, 0.5)\}
                              +y+1/2,+x+1/2,+z+1/2
*******
space group: 107 {'Hall': 'I 4 -2', 'HM': 'I 4 m m'}
Crystal system: Tetragonal
+X,+Y,+Z
-y,+x,+z
-x,+y,+z
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
  \{4^+_{00z} | (0.0,0.0,0.0)\}
                                      -y,+x,+z
   \{m_0yz \mid (0.0,0.0,0.0)\}
                                       -x,+y,+z
   {2_00z|(0.0,0.0,0.0)}
                                      -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                      -y,-x,+z
  \{4^-00z \mid (0.0,0.0,0.0)\}
                                      +y,-x,+z
   \{m_x0z \mid (0.0,0.0,0.0)\}
                                      +x,-y,+z
   \{m_xxz | (0.0,0.0,0.0)\}
                                      +y,+x,+z
     \{1 \mid (0.5, 0.5, 0.5)\}
                              +x+1/2,+y+1/2,+z+1/2
  \{4^+_{00z}|(0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,+z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
                               -x+1/2,+y+1/2,+z+1/2
   \{2_{00z} | (0.5, 0.5, 0.5)\}
                               -x+1/2,-y+1/2,+z+1/2
   \{m \times -xz \mid (0.5, 0.5, 0.5)\}
                               -y+1/2,-x+1/2,+z+1/2
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                               +y+1/2,-x+1/2,+z+1/2
   \{m_x0z|(0.5,0.5,0.5)\}
                              | +x+1/2,-y+1/2,+z+1/2
   \{m_xxz | (0.5, 0.5, 0.5)\}
                              +y+1/2,+x+1/2,+z+1/2
```

```
*******
space group: 108 {'Hall': 'I 4 -2c', 'HM': 'I 4 c m'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
-x,+y,+z+1/2
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  \{4^+_00z \mid (0.0,0.0,0.0)\}
                                       -y,+x,+z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                     -x,+y,+z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                                     -y,-x,+z+1/2
  \{4^-00z \mid (0.0,0.0,0.0)\}
                                       +y,-x,+z
   \{m_x0z \mid (0.0,0.0,0.5)\}
                                     +x,-y,+z+1/2
   \{m_xxz|(0.0,0.0,0.5)\}
                                     +y,+x,+z+1/2
      \{1 \mid (0.5, 0.5, 0.5)\}
                                +x+1/2,+y+1/2,+z+1/2
  \{4^+_00z|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,+z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                  -x+1/2,+y+1/2,+z
   \{2_{00z} | (0.5, 0.5, 0.5)\}
                                -x+1/2,-y+1/2,+z+1/2
   \{m_x-xz \mid (0.5,0.5,0.0)\}
                                  -y+1/2,-x+1/2,+z
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,-x+1/2,+z+1/2
   \{m_x0z \mid (0.5, 0.5, 0.0)\}
                                  +x+1/2,-y+1/2,+z
   \{m_x \times z \mid (0.5, 0.5, 0.0)\}
                                  +y+1/2,+x+1/2,+z
*******
space group: 109 {'Hall': ' I 4bw -2', 'HM': 'I 41 m d'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x+1/2, +z+1/4
-x,+y,+z
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +X,+Y,+Z
  \{4^+_{00z}|(0.0,0.5,0.25)\}
                                    -y, +x+1/2, +z+1/4
   \{m_0yz \mid (0.0,0.0,0.0)\}
                                        -X,+y,+z
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2,-y+1/2,+z+1/2
  \{m_x-xz\mid (0.0,0.5,0.25)\}
                                    -y, -x+1/2, +z+1/4
  \{4^-_00z \mid (0.5, 0.0, 0.75)\}
                                    +y+1/2,-x,+z+3/4
   \{m_x0z|(0.5,0.5,0.5)\}
                                 +x+1/2,-y+1/2,+z+1/2
   \{m_xz|(0.5,0.0,0.75)\}
                                    +y+1/2,+x,+z+3/4
     \{1 \mid (0.5, 0.5, 0.5)\}
                                 +x+1/2, +y+1/2, +z+1/2
                                    -y+1/2,+x,+z+3/4
  \{4^+_{00z}|(0.5,0.0,0.75)\}
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2,+y+1/2,+z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                        -x,-y,+z
  \{m_x-xz|(0.5,0.0,0.75)\}
                                    -y+1/2,-x,+z+3/4
  \{4^- 00z \mid (0.0, 0.5, 0.25)\}
                                    +y,-x+1/2,+z+1/4
```

+x,-y,+z

 $\{m \times 0z \mid (0.0, 0.0, 0.0)\}$

```
\{m_xxz \mid (0.0,0.5,0.25)\} \mid +y,+x+1/2,+z+1/4
*******
space group: 110 {'Hall': ' I 4bw -2c', 'HM': 'I 41 c d'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x+1/2, +z+1/4
-x,+y,+z+1/2
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  {4^+ 00z|(0.0,0.5,0.25)}
                                   -y, +x+1/2, +z+1/4
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                     -x,+y,+z+1/2
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2, -y+1/2, +z+1/2
  \{m_x-xz \mid (0.0,0.5,0.75)\}
                                   -y, -x+1/2, +z+3/4
  {4^-_00z|(0.5,0.0,0.75)}
                                   +y+1/2,-x,+z+3/4
   \{m_x0z \mid (0.5, 0.5, 0.0)\}
                                   +x+1/2, -y+1/2, +z
   \{m_xz|(0.5,0.0,0.25)\}
                                   +y+1/2,+x,+z+1/4
     \{1 \mid (0.5, 0.5, 0.5)\}
                                +x+1/2,+y+1/2,+z+1/2
  \{4^+_{00z}|(0.5,0.0,0.75)\}
                                   -y+1/2,+x,+z+3/4
   \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                   -x+1/2,+y+1/2,+z
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
  \{m_x-xz\mid(0.5,0.0,0.25)\}
                                   -y+1/2,-x,+z+1/4
  \{4^-_00z \mid (0.0, 0.5, 0.25)\}
                                   +y, -x+1/2, +z+1/4
   \{m \times 0z \mid (0.0, 0.0, 0.5)\}
                                     +x,-y,+z+1/2
   \{m_xxz | (0.0,0.5,0.75)\}
                                   +y, +x+1/2, +z+3/4
******
space group: 111 {'Hall': ' P -4 2', 'HM': 'P -4 2 m'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
+x,-y,-z
            Seitz
                                  Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  \{-4^+_00z \mid (0.0,0.0,0.0)\} \mid
                                +y,-x,-z
   \{2_{x00} | (0.0,0.0,0.0)\}
                                +x,-y,-z
   {2_00z|(0.0,0.0,0.0)}
                                -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                -y,-x,+z
  \{-4^-00z \mid (0.0,0.0,0.0)\}
                                -y,+x,-z
   {2_0y0|(0.0,0.0,0.0)}
                                -x,+y,-z
   \{m_xxz | (0.0,0.0,0.0)\}
                                +y,+x,+z
```

```
*******
space group: 112 {'Hall': ' P -4 2c', 'HM': 'P -4 2 c'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
+x,-y,-z+1/2
            Seitz
                                  Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                +y,-x,-z
                              +x,-y,-z+1/2
  \{2_{x00}|(0.0,0.0,0.5)\}
   {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                               -y,-x,+z+1/2
  \{-4^-00z \mid (0.0,0.0,0.0)\}
                                 -y, +x, -z
   {2_0y0|(0.0,0.0,0.5)}
                               -x,+y,-z+1/2
   \{m_xxz|(0.0,0.0,0.5)\}
                              +y,+x,+z+1/2
******
space group: 113 {'Hall': 'P -4 2ab', 'HM': 'P -4 21 m'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
+x+1/2,-y+1/2,-z
           Seitz
                                    Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
 \{-4^+_00z \mid (0.0,0.0,0.0)\}
                                  +y,-x,-z
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                               +x+1/2,-y+1/2,-z
   {2_00z|(0.0,0.0,0.0)}
                                  -x,-y,+z
   \{m_x-xz \mid (0.5,0.5,0.0)\}
                               -y+1/2, -x+1/2, +z
  \{-4^-00z \mid (0.0,0.0,0.0)\} \mid
                                   -y,+x,-z
   {2_0y0|(0.5,0.5,0.0)}
                               -x+1/2, +y+1/2, -z
   \{m_x \times z \mid (0.5, 0.5, 0.0)\}
                              +y+1/2,+x+1/2,+z
*******
space group: 114 {'Hall': 'P -4 2n', 'HM': 'P -4 21 c'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
+x+1/2,-y+1/2,-z+1/2
           Seitz
                                      Jones
     {1|(0.0,0.0,0.0)}
                                     +x,+y,+z
 \{-4^+_00z \mid (0.0,0.0,0.0)\} \mid
                                     +y,-x,-z
```

```
\{2_{x00}|(0.5,0.5,0.5)\}
                             +x+1/2,-y+1/2,-z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                     -x,-y,+z
   \{m_x-xz \mid (0.5,0.5,0.5)\}
                               -y+1/2, -x+1/2, +z+1/2
  \{-4^-_00z \mid (0.0,0.0,0.0)\}
                                     -y,+x,-z
                               -x+1/2,+y+1/2,-z+1/2
   {2_0y0|(0.5,0.5,0.5)}
   \{m_xz|(0.5,0.5,0.5)\}
                              +y+1/2,+x+1/2,+z+1/2
*******
space group: 115 {'Hall': ' P -4 -2', 'HM': 'P -4 m 2'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
-x,+y,+z
            Seitz
                                Jones
     {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 \{-4^+_00z \mid (0.0,0.0,0.0)\}
                             | +y,-x,-z
   \{m_0yz \mid (0.0,0.0,0.0)\}
                               -x,+y,+z
   {2_00z|(0.0,0.0,0.0)}
                               -x,-y,+z
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                               +y,+x,-z
  \{-4^{-}00z \mid (0.0,0.0,0.0)\} \mid -y,+x,-z
   \{m_x0z \mid (0.0,0.0,0.0)\}
                             +x,-y,+z
   \{2_x-x0\mid (0.0,0.0,0.0)\}
                             -y,-x,-z
*******
space group: 116 {'Hall': ' P -4 -2c', 'HM': 'P -4 c 2'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
-x,+y,+z+1/2
            Seitz
                                  Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                 +y,-x,-z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                               -x,+y,+z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
   \{2_{xx0}|(0.0,0.0,0.5)\}
                               +y,+x,-z+1/2
  \{-4^-00z \mid (0.0,0.0,0.0)\}
                                 -y,+x,-z
   \{m_x0z \mid (0.0,0.0,0.5)\}
                               +x,-y,+z+1/2
   \{2_x-x0\mid(0.0,0.0,0.5)\}
                             | -y, -x, -z+1/2
*******
```

space group: 117 {'Hall': ' P -4 -2ab', 'HM': 'P -4 b 2'}

```
+x,+y,+z
+y,-x,-z
-x+1/2,+y+1/2,+z
            Seitz
                                     Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
| {-4^+_00z|(0.0,0.0,0.0)} |
                                    +y,-x,-z
   \{m \ 0yz | (0.5, 0.5, 0.0)\}
                               -x+1/2,+y+1/2,+z
   {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                               +y+1/2,+x+1/2,-z
  \{-4^-00z \mid (0.0,0.0,0.0)\} \mid
                                    -y,+x,-z
   \{m_x0z|(0.5,0.5,0.0)\} +x+1/2,-y+1/2,+z 
   \{2_x-x0|(0.5,0.5,0.0)\} \mid -y+1/2,-x+1/2,-z \mid
*******
space group: 118 {'Hall': ' P -4 -2n', 'HM': 'P -4 n 2'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
-x+1/2,+y+1/2,+z+1/2
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +X,+Y,+Z
 \{-4^+_00z|(0.0,0.0,0.0)\}
                                      +y,-x,-z
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
                               -x+1/2,+y+1/2,+z+1/2
   \{2\_00z \mid (0.0,0.0,0.0)\}
                                      -x,-y,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.5)\}
                                +y+1/2, +x+1/2, -z+1/2
  \{-4^-00z \mid (0.0,0.0,0.0)\} \mid
                                      -y,+x,-z
   \{m_x0z|(0.5,0.5,0.5)\}
                               +x+1/2,-y+1/2,+z+1/2
   \{2_x-x0|(0.5,0.5,0.5)\}
                              -y+1/2,-x+1/2,-z+1/2
*******
space group: 119 {'Hall': ' I -4 -2', 'HM': 'I -4 m 2'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
-x,+y,+z
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
 \{-4^+00z|(0.0,0.0,0.0)\}
                                      +y,-x,-z
   \{m_0yz \mid (0.0,0.0,0.0)\}
                                      -x,+y,+z
```

-x,-y,+z

+y,+x,-z

 $\{2_00z \mid (0.0,0.0,0.0)\}$

 $\{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}$

```
\{-4^-00z \mid (0.0,0.0,0.0)\} \mid
                                        -y,+x,-z
   \{m_x0z | (0.0,0.0,0.0)\}
                                        +x,-y,+z
   \{2_x-x0|(0.0,0.0,0.0)\}
                                        -y,-x,-z
     \{1 \mid (0.5, 0.5, 0.5)\}
                                 +x+1/2, +y+1/2, +z+1/2
  \{-4^+_{00z} | (0.5, 0.5, 0.5)\}
                                 +y+1/2,-x+1/2,-z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2,+y+1/2,+z+1/2
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2, -y+1/2, +z+1/2
   \{2_{xx0}|(0.5,0.5,0.5)\}
                                 +y+1/2, +x+1/2, -z+1/2
  \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                 -y+1/2,+x+1/2,-z+1/2
                                 +x+1/2,-y+1/2,+z+1/2
   \{m_x0z|(0.5,0.5,0.5)\}
   \{2_x-x0\mid(0.5,0.5,0.5)\}
                                 -y+1/2, -x+1/2, -z+1/2
*******
space group: 120 {'Hall': ' I -4 -2c', 'HM': 'I -4 c 2'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
-x,+y,+z+1/2
            Seitz
                                         Jones
     \{1|(0.0,0.0,0.0)\}
                                        +x,+y,+z
  \{-4^+_00z \mid (0.0,0.0,0.0)\}
                                        +y,-x,-z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                      -x,+y,+z+1/2
   \{2\_00z \mid (0.0,0.0,0.0)\}
                                        -x,-y,+z
   \{2 \times \times 0 \mid (0.0, 0.0, 0.5)\}
                                      +y,+x,-z+1/2
  \{-4^-00z \mid (0.0,0.0,0.0)\}
                                        -y,+x,-z
   \{m_x0z \mid (0.0,0.0,0.5)\}
                                      +x,-y,+z+1/2
   \{2_x-x0|(0.0,0.0,0.5)\}
                                      -y,-x,-z+1/2
     \{1|(0.5,0.5,0.5)\}
                                 +x+1/2, +y+1/2, +z+1/2
  \{-4^+_{00z}|(0.5,0.5,0.5)\}
                                 +y+1/2,-x+1/2,-z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                    -x+1/2,+y+1/2,+z
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2, -y+1/2, +z+1/2
   \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                                    +y+1/2,+x+1/2,-z
                                 -y+1/2,+x+1/2,-z+1/2
  \{-4^-00z \mid (0.5, 0.5, 0.5)\}
   \{m_x0z|(0.5,0.5,0.0)\}
                                    +x+1/2,-y+1/2,+z
   \{2_x-x0\mid(0.5,0.5,0.0)\}
                                    -y+1/2,-x+1/2,-z
*******
space group: 121 {'Hall': ' I -4 2', 'HM': 'I -4 2 m'}
Crystal system: Tetragonal
+x,+y,+z
+y,-x,-z
+x,-y,-z
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
```

```
\{-4^+_00z \mid (0.0,0.0,0.0)\} \mid
                                      +y,-x,-z
   \{2_{x00} | (0.0,0.0,0.0)\}
                                      +x,-y,-z
   {2_00z|(0.0,0.0,0.0)}
                                      -x,-y,+z
   \{m \times -xz \mid (0.0,0.0,0.0)\}
                                      -y,-x,+z
  \{-4^-_00z \mid (0.0,0.0,0.0)\}
                                      -y,+x,-z
   {2_0y0|(0.0,0.0,0.0)}
                                      -x,+y,-z
   \{m_xxz | (0.0,0.0,0.0)\}
                                      +y,+x,+z
     \{1|(0.5,0.5,0.5)\}
                                +x+1/2, +y+1/2, +z+1/2
  \{-4^+_{00z}|(0.5,0.5,0.5)\}
                               +y+1/2,-x+1/2,-z+1/2
   \{2_{x00}|(0.5,0.5,0.5)\}
                               +x+1/2,-y+1/2,-z+1/2
   \{2_{00z} | (0.5, 0.5, 0.5)\}
                                -x+1/2,-y+1/2,+z+1/2
   \{m_x-xz \mid (0.5,0.5,0.5)\}
                               -y+1/2, -x+1/2, +z+1/2
  \{-4^-00z|(0.5,0.5,0.5)\}
                               -y+1/2,+x+1/2,-z+1/2
   \{2_0y0|(0.5,0.5,0.5)\}
                              -x+1/2,+y+1/2,-z+1/2
   \{m_xz|(0.5,0.5,0.5)\}
                              +y+1/2,+x+1/2,+z+1/2
*******
space group: 122 {'Hall': ' I -4 2bw', 'HM': 'I -4 2 d'}
Crystal system: Tetragonal
+X,+Y,+Z
+y,-x,-z
+x,-y+1/2,-z+1/4
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +X,+Y,+Z
  \{-4^+00z \mid (0.0,0.0,0.0)\} \mid
                                      +y,-x,-z
   \{2_{x00}|(0.0,0.5,0.25)\}
                                  +x,-y+1/2,-z+1/4
   {2_00z|(0.0,0.0,0.0)}
                                      -x,-y,+z
  \{m_x-xz|(0.5,0.0,0.75)\}
                                  -y+1/2,-x,+z+3/4
  \{-4^-00z|(0.0,0.0,0.0)\}
                                      -y,+x,-z
   {2_0y0|(0.0,0.5,0.25)}
                                  -x,+y+1/2,-z+1/4
   \{m_xz|(0.5,0.0,0.75)\}
                                  +y+1/2,+x,+z+3/4
     \{1|(0.5,0.5,0.5)\}
                                +x+1/2,+y+1/2,+z+1/2
  \{-4^+_00z|(0.5,0.5,0.5)\}
                                +y+1/2,-x+1/2,-z+1/2
                                  +x+1/2,-y,-z+3/4
   \{2_{x00}|(0.5,0.0,0.75)\}
   \{2_{00z} | (0.5, 0.5, 0.5)\}
                                -x+1/2,-y+1/2,+z+1/2
  \{m_x-xz \mid (0.0,0.5,0.25)\}
                                  -y, -x+1/2, +z+1/4
  \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                -y+1/2,+x+1/2,-z+1/2
                                  -x+1/2, +y, -z+3/4
   {2_0y0|(0.5,0.0,0.75)}
   \{m_xxz | (0.0,0.5,0.25)\}
                                  +y, +x+1/2, +z+1/4
*******
space group: 123 {'Hall': ' -P 4 2', 'HM': 'P 4/m m m'}
Crystal system: Tetragonal
```

```
+x,+y,+z
-y,+x,+z
+x,-y,-z
```

```
Seitz
                                  Jones
   \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
\{4^+_{00z} | (0.0,0.0,0.0)\}
                                -y,+x,+z
 \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x,-y,-z
 {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
 \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                 +y,+x,-z
\{4^-_00z \mid (0.0,0.0,0.0)\}
                                 +y,-x,+z
 {2 0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
 \{2_x-x0|(0.0,0.0,0.0)\}
                                 -y,-x,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
\{-4^+_00z \mid (0.0,0.0,0.0)\}
                                +y,-x,-z
 \{m_0yz \mid (0.0,0.0,0.0)\}
                                 -x,+y,+z
 {m_xy0|(0.0,0.0,0.0)}
                                 +x,+y,-z
 \{m_x-xz \mid (0.0,0.0,0.0)\}
                                 -y,-x,+z
\{-4^-_00z \mid (0.0,0.0,0.0)\}
                                -y,+x,-z
 \{m_x0z | (0.0,0.0,0.0)\}
                                 +x,-y,+z
 \{m_x \times z \mid (0.0, 0.0, 0.0)\}
                                 +y,+x,+z
```

space group: 124 {'Hall': ' -P 4 2c', 'HM': 'P 4/m c c'}

Crystal system: Tetragonal

+x,+y,+z -y,+x,+z +x,-y,-z+1/2

.

+	
Seitz	
[\{1 (0.0,0.0,0.0)\}	+x,+y,+z
\ \{4^+_00z\\(0.0,0.0,0.0\)\} \ \{2_\times0\\(0.0,0.0,0.0,0.5\)\}	-y,+x,+z +x,-y,-z+1/2
$ \left\{ \begin{array}{l} \{2_00z \mid (0.0,0.0,0.0,0.0)\} \\ \{2_xx0 \mid (0.0,0.0,0.5)\} \\ \end{array} \right. $	-x,-y,+z +y,+x,-z+1/2
{4^00z (0.0,0.0,0.0)} {2_0y0 (0.0,0.0,0.5)}	+y,-x,+z -x,+y,-z+1/2
{2_x-x0 (0.0,0.0,0.5)} {-1 (0.0,0.0,0.0)}	-y,-x,-z+1/2 -x,-y,-z
{-4^+_00z (0.0,0.0,0.0)} {m_0yz (0.0,0.0,0.5)}	+y,-x,-z -x,+y,+z+1/2
{m_xy0 (0.0,0.0,0.0)} {m_x-xz (0.0,0.0,0.5)}	+x,+y,-z -y,-x,+z+1/2
{-4^00z (0.0,0.0,0.0)} {m_x0z (0.0,0.0,0.5)}	-y,+x,-z +x,-y,+z+1/2
{m_xxz (0.0,0.0,0.5)}	+y,+x,+z+1/2

.

```
*******
```

space group: 125:1 {'Hall': 'P 4 2 -1ab', 'HM': 'P 4/n b m:1'}

```
Setting: 1
+x,+y,+z
-y,+x,+z
+x,-y,-z
-x+1/2,-y+1/2,-z
```

Seitz	Jones
{1 (0.0,0.0,0.0)}	+x,+y,+z
{4^+_00z (0.0,0.0,0.0)}	-y,+x,+z
{2_x00 (0.0,0.0,0.0)}	+x,-y,-z
{-1 (0.5,0.5,0.0)}	-x+1/2,-y+1/2,-z
{2_00z (0.0,0.0,0.0)}	-x,-y,+z
{2_xx0 (0.0,0.0,0.0)}	+y,+x,-z
{-4^+_00z (0.5,0.5,0.0)}	+y+1/2,-x+1/2,-z
{4^00z (0.0,0.0,0.0)}	+y,-x,+z

space group: 125:2 {'Hall': ' -P 4a 2b', 'HM': 'P 4/n b m:2'}

Crystal system: Tetragonal

Setting: 2 +x,+y,+z -y+1/2,+x,+z +x,-y+1/2,-z

Seitz	Jones
	+x,+y,+z -y+1/2,+x,+z +x,-y+1/2,-z -x+1/2,-y+1/2,+z +y,+x,-z +y,-x+1/2,+z -x+1/2,+y,-z -y+1/2,-x+1/2,-z -x,-y,-z +y+1/2,-x,-z -x,+y+1/2,+z +x+1/2,+y+1/2,-z -y,-x,+z
{-4^00z (0.0,0.5,0.0)} {m_x0z (0.5,0.0,0.0)} {m_xxz (0.5,0.5,0.0)}	-y,+x+1/2,-z -y,+x+1/2,-z +x+1/2,-y,+z +y+1/2,+x+1/2,+z

.

```
*******
```

space group: 126:1 {'Hall': 'P 4 2 -1n', 'HM': 'P 4/n n c:1'}

Crystal system: Tetragonal

Setting: 1

```
+x,+y,+z
-y, +x, +z
+x,-y,-z
-x+1/2, -y+1/2, -z+1/2
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
  {4^+_00z|(0.0,0.0,0.0)}
                                        -y, +x, +z
   \{2_{x00} | (0.0,0.0,0.0)\}
                                        +x,-y,-z
      \{-1 \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2, -y+1/2, -z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                        -x,-y,+z
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                                        +y,+x,-z
  \{-4^+_{00z}|(0.5,0.5,0.5)\} \mid +y+1/2,-x+1/2,-z+1/2
  \{4^-00z \mid (0.0,0.0,0.0)\}
                                        +y,-x,+z
*******
space group: 126:2 {'Hall': ' -P 4a 2bc', 'HM': 'P 4/n n c:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y+1/2,+x,+z
+x,-y+1/2,-z+1/2
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
  \{4^+_{00z} | (0.5, 0.0, 0.0)\}
                                     -y+1/2,+x,+z
   \{2_{x00}|(0.0,0.5,0.5)\}
                                   +x,-y+1/2,-z+1/2
   \{2\ 00z|(0.5,0.5,0.0)\}
                                   -x+1/2, -y+1/2, +z
   \{2_x \times 0 \mid (0.0, 0.0, 0.5)\}
                                     +y,+x,-z+1/2
  \{4^-_00z \mid (0.0, 0.5, 0.0)\}
                                     +y,-x+1/2,+z
   {2_0y0|(0.5,0.0,0.5)}
                                   -x+1/2,+y,-z+1/2
   \{2_x-x0|(0.5,0.5,0.5)\}
                                 -y+1/2, -x+1/2, -z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                        -x,-y,-z
  \{-4^+00z \mid (0.5,0.0,0.0)\}
                                     +y+1/2,-x,-z
   \{m_0yz \mid (0.0,0.5,0.5)\}
                                   -x,+y+1/2,+z+1/2
   \{m_xy0|(0.5,0.5,0.0)\}
                                   +x+1/2,+y+1/2,-z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                                     -y,-x,+z+1/2
  \{-4^-00z \mid (0.0,0.5,0.0)\}
                                     -y, +x+1/2, -z
   \{m_x0z|(0.5,0.0,0.5)\}
                                   +x+1/2,-y,+z+1/2
   \{m_{xxz}|(0.5,0.5,0.5)\}
                                 +y+1/2,+x+1/2,+z+1/2
*******
space group: 127 {'Hall': ' -P 4 2ab', 'HM': 'P 4/m b m'}
Crystal system: Tetragonal
+x,+y,+z
```

-y,+x,+z

```
+x+1/2,-y+1/2,-z
```

+	Jones
\[\{1 \ \((0.0, 0.0, 0.0) \) \\ \\ \{4^+ _00z \ \((0.0, 0.0, 0.0) \) \\ \\ \{2 _x00 \ \((0.5, 0.5, 0.0) \) \\ \\ \{2 _00z \ \((0.0, 0.0, 0.0, 0.0) \) \}	+x,+y,+z
{2_xx0 (0.5,0.5,0.0)} {4^00z (0.0,0.0,0.0)} {2_0y0 (0.5,0.5,0.0)} {2_x-x0 (0.5,0.5,0.0)} {-1 (0.0,0.0,0.0)}	+y+1/2,+x+1/2,-z +y,-x,+z -x+1/2,+y+1/2,-z -y+1/2,-x+1/2,-z
\[\{-4^+_00z (0.0,0.0,0.0)\} \] \[\{m_0yz (0.5,0.5,0.0)\} \] \[\{m_xy0 (0.0,0.0,0.0)\} \] \[\{m_x-xz (0.5,0.5,0.0)\} \]	-x,-y,-z +y,-x,-z -x+1/2,+y+1/2,+z +x,+y,-z -y+1/2,-x+1/2,+z
\[\{-4^00z \ (0.0,0.0,0.0) \} \] \[\{m_\times z \ (0.5,0.5,0.0) \} \] \[\{m_\times z \ (0.5,0.5,0.0) \} \] \[\+	-y,+x,-z +x+1/2,-y+1/2,+z +y+1/2,+x+1/2,+z

space group: 128 {'Hall': ' -P 4 2n', 'HM': 'P 4/m n c'}

Crystal system: Tetragonal

+x,+y,+z -y,+x,+z

+x+1/2,-y+1/2,-z+1/2

.......

+	+
Seitz	Jones
{1 (0.0,0.0,0.0)}	+x,+y,+z
{4^+_00z (0.0,0.0,0.0)}	-y,+x,+z
{2_x00 (0.5,0.5,0.5)}	+x+1/2,-y+1/2,-z+1/2
[{2_00z (0.0,0.0,0.0)}	-x,-y,+z
{2_xx0 (0.5,0.5,0.5)}	+y+1/2,+x+1/2,-z+1/2
{4^00z (0.0,0.0,0.0)}	+y,-x,+z
{2_0y0 (0.5,0.5,0.5)}	-x+1/2, +y+1/2, -z+1/2
$\{2_x-x0\}(0.5,0.5,0.5)\}$	-y+1/2,-x+1/2,-z+1/2
$\{-1 \mid (0.0,0.0,0.0)\}$	-x,-y,-z
$\{-4^+_00z (0.0,0.0,0.0)\}$	+y,-x,-z
$\{m_0yz \mid (0.5, 0.5, 0.5)\}$	-x+1/2,+y+1/2,+z+1/2
[\{m_xy0 (0.0,0.0,0.0)\}	+x,+y,-z
$\{m_x-xz\mid(0.5,0.5,0.5)\}$	-y+1/2,-x+1/2,+z+1/2
{-4^00z (0.0,0.0,0.0)}	-y,+x,-z
$\{m_x0z (0.5,0.5,0.5)\}$	+x+1/2,-y+1/2,+z+1/2
{m_xxz (0.5,0.5,0.5)}	+y+1/2,+x+1/2,+z+1/2
+	++

```
space group: 129:1 {'Hall': 'P 4ab 2ab -1ab', 'HM': 'P 4/n m m:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y+1/2,+x+1/2,+z
+x+1/2,-y+1/2,-z
-x+1/2,-y+1/2,-z
  . . . . . . . . . . . . . . . . . .
                                       Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                      +X,+Y,+Z
  \{4^+_{00z}|(0.5,0.5,0.0)\}
                                -y+1/2,+x+1/2,+z
   \{2_{x00}|(0.5,0.5,0.0)\}
                                +x+1/2,-y+1/2,-z
      \{-1 \mid (0.5, 0.5, 0.0)\}
                                 -x+1/2, -y+1/2, -z
   {2 00z|(0.0,0.0,0.0)}
                                      -x,-y,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                      +y, +x, -z
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                      +y,-x,-z
  \{4^-00z|(0.5,0.5,0.0)\}
                               +y+1/2,-x+1/2,+z
*******
space group: 129:2 {'Hall': ' -P 4a 2a', 'HM': 'P 4/n m m:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y+1/2,+x,+z
+x+1/2,-y,-z
            Seitz
                                       Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
  \{4^+ 00z \mid (0.5,0.0,0.0)\}
                                    -y+1/2,+x,+z
   \{2_{x00} | (0.5, 0.0, 0.0)\}
                                    +x+1/2,-y,-z
   {2_00z|(0.5,0.5,0.0)}
                                 -x+1/2,-y+1/2,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                                 +y+1/2,+x+1/2,-z
  \{4^-_00z \mid (0.0, 0.5, 0.0)\}
                                    +y,-x+1/2,+z
   {2_0y0|(0.0,0.5,0.0)}
                                    -x,+y+1/2,-z
   \{2_x-x0\mid(0.0,0.0,0.0)\}
                                      -y,-x,-z
      [-1|(0.0,0.0,0.0)}
                                      -x,-y,-z
  \{-4^+_00z \mid (0.5,0.0,0.0)\}
                                    +y+1/2,-x,-z
   \{m_0yz \mid (0.5,0.0,0.0)\}
                                    -x+1/2,+y,+z
   \{m_xy0|(0.5,0.5,0.0)\}
                                 +x+1/2, +y+1/2, -z
   \{m_x-xz \mid (0.5,0.5,0.0)\}
                                 -y+1/2,-x+1/2,+z
  \{-4^-00z \mid (0.0,0.5,0.0)\}
                                   -y, +x+1/2, -z
   \{m_x0z|(0.0,0.5,0.0)\}
                                    +x,-y+1/2,+z
   \{m_xxz | (0.0,0.0,0.0)\}
                                      +y, +x, +z
```

space group: 130:1 {'Hall': 'P 4ab 2n -1ab', 'HM': 'P 4/n c c:1'}

```
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y+1/2,+x+1/2,+z
+x+1/2,-y+1/2,-z+1/2
-x+1/2, -y+1/2, -z
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.0)\}
                                   -y+1/2,+x+1/2,+z
   \{2_{x00} | (0.5, 0.5, 0.5)\}
                                 +x+1/2,-y+1/2,-z+1/2
     \{-1|(0.5,0.5,0.0)\}
                                   -x+1/2,-y+1/2,-z
   {2_00z|(0.0,0.0,0.0)}
                                        -x,-y,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.5)\}
                                      +y,+x,-z+1/2
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                        +y,-x,-z
  \{4^-00z|(0.5,0.5,0.0)\}
                                   +y+1/2,-x+1/2,+z
******
space group: 130:2 {'Hall': ' -P 4a 2ac', 'HM': 'P 4/n c c:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y+1/2,+x,+z
+x+1/2,-y,-z+1/2
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
  \{4^+ 00z \mid (0.5,0.0,0.0)\}
                                      -y+1/2,+x,+z
   \{2_{\times}00 \mid (0.5, 0.0, 0.5)\}
                                   +x+1/2,-y,-z+1/2
   \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                   -x+1/2, -y+1/2, +z
   \{2_{xx0}|(0.5,0.5,0.5)\}
                                 +y+1/2,+x+1/2,-z+1/2
  \{4^-00z|(0.0,0.5,0.0)\}
                                      +y,-x+1/2,+z
   {2_0y0|(0.0,0.5,0.5)}
                                   -x,+y+1/2,-z+1/2
   \{2_x-x0|(0.0,0.0,0.5)\}
                                     -y,-x,-z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                        -x,-y,-z
  \{-4^+00z|(0.5,0.0,0.0)\}
                                      +y+1/2,-x,-z
                                   -x+1/2, +y, +z+1/2
   \{m_0yz \mid (0.5,0.0,0.5)\}
   \{m_xy0|(0.5,0.5,0.0)\}
                                   +x+1/2,+y+1/2,-z
   \{m_x-xz \mid (0.5,0.5,0.5)\}
                                 -y+1/2, -x+1/2, +z+1/2
  \{-4^-00z \mid (0.0,0.5,0.0)\}
                                      -y, +x+1/2, -z
                                   +x,-y+1/2,+z+1/2
   \{m_x0z \mid (0.0,0.5,0.5)\}
   \{m_xxz|(0.0,0.0,0.5)\}
                                      +y,+x,+z+1/2
```

space group: 131 {'Hall': '-P 4c 2', 'HM': 'P 42/m m c'}

```
+x,+y,+z
-y,+x,+z+1/2
+x,-y,-z
```

Seitz	Jones
	+x,+y,+z -y,+x,+z+1/2 +x,-y,-z -x,-y,+z +y,+x,-z+1/2 +y,-x,+z+1/2 -x,+y,-z -y,-x,-z+1/2 -x,-y,-z +y,-x,-z+1/2 -x,+y,+z +x,+y,-z -y,-x,+z+1/2 -y,+x,-z+1/2
{m_x0z (0.0,0.0,0.0)} {m_xxz (0.0,0.0,0.5)}	+x,-y,+z +y,+x,+z+1/2

.

space group: 132 {'Hall': '-P 4c 2c', 'HM': 'P 42/m c m'}

Crystal system: Tetragonal

+x,+y,+z -y,+x,+z+1/2 +x,-y,-z+1/2

.

+	
Seitz	Jones
Seitz {1 (0.0,0.0,0.0)} {4^+_00z (0.0,0.0,0.5)} {2_x00 (0.0,0.0,0.5)} {2_00z (0.0,0.0,0.0)} {2_xx0 (0.0,0.0,0.0)} {4^00z (0.0,0.0,0.5)} {2_0y0 (0.0,0.0,0.5)} {2_x-x0 (0.0,0.0,0.5)} {2_1(0.0,0.0,0.0)} {-1 (0.0,0.0,0.0)} {-4^+_00z (0.0,0.0,0.5)} {m_0yz (0.0,0.0,0.5)} {m_xy0 (0.0,0.0,0.0)}	Jones +x,+y,+z -y,+x,+z+1/2 +x,-y,-z+1/2 -x,-y,+z +y,+x,-z +y,-x,+z+1/2 -x,+y,-z+1/2 -y,-x,-z -x,-y,-z +y,-x,-z+1/2 -x,+y,-z+1/2 -x,+y,+z+1/2 +x,+y,-z
{m_x-xz (0.0,0.0,0.0)}	-y,-x,+z
{-4^00z (0.0,0.0,0.5)} {m_x0z (0.0,0.0,0.5)} {m_xxz (0.0,0.0,0.0)}	-y,+x,-z+1/2 +x,-y,+z+1/2 +y,+x,+z
+	

.

```
*******
space group: 133:1 {'Hall': ' P 4n 2c -1n', 'HM': 'P 42/n b c:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x,-y,-z+1/2
-x+1/2, -y+1/2, -z+1/2
. . . . . . . . . . . . . . . . . . .
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +X,+Y,+Z
  \{4^+_{00z}|(0.5,0.5,0.5)\}
                                -y+1/2, +x+1/2, +z+1/2
   \{2_{x00} | (0.0,0.0,0.5)\}
                                     +x,-y,-z+1/2
     \{-1 \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2, -y+1/2, -z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                                   +y+1/2,+x+1/2,-z
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                       +y,-x,-z
 {4^-_00z|(0.5,0.5,0.5)}
                             +y+1/2,-x+1/2,+z+1/2
*******
space group: 133:2 {'Hall': '-P 4ac 2b', 'HM': 'P 42/n b c:2'}
Crystal system: Tetragonal
Setting: 2
+X,+Y,+Z
-y+1/2,+x,+z+1/2
+x,-y+1/2,-z
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
  \{4^+_{00z}|(0.5,0.0,0.5)\}
                                   -y+1/2,+x,+z+1/2
   \{2_{x00} | (0.0, 0.5, 0.0)\}
                                     +x,-y+1/2,-z
   {2_00z|(0.5,0.5,0.0)}
                                   -x+1/2, -y+1/2, +z
   \{2_x \times 0 \mid (0.0, 0.0, 0.5)\}
                                     +y,+x,-z+1/2
                                   +y,-x+1/2,+z+1/2
  \{4^-00z|(0.0,0.5,0.5)\}
   {2_0y0|(0.5,0.0,0.0)}
                                     -x+1/2, +y, -z
   \{2_x-x0\mid(0.5,0.5,0.5)\}
                                 -y+1/2, -x+1/2, -z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                       -x,-y,-z
  \{-4^+_{00z} | (0.5,0.0,0.5)\}
                                   +y+1/2,-x,-z+1/2
   \{m_0yz \mid (0.0,0.5,0.0)\}
                                     -x,+y+1/2,+z
   \{m_xy0|(0.5,0.5,0.0)\}
                                   +x+1/2, +y+1/2, -z
   \{m_x-xz\mid (0.0,0.0,0.5)\}
                                     -y,-x,+z+1/2
  \{-4^-00z \mid (0.0,0.5,0.5)\}
                                   -y, +x+1/2, -z+1/2
   \{m_x0z \mid (0.5,0.0,0.0)\}
                                     +x+1/2,-y,+z
   {m_xxz|(0.5,0.5,0.5)}
                                +y+1/2,+x+1/2,+z+1/2
```

```
*******
space group: 134:1 {'Hall': ' P 4n 2 -1n', 'HM': 'P 42/n n m:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x,-y,-z
-x+1/2,-y+1/2,-z+1/2
            Seitz
                                        Jones
     {1|(0.0,0.0,0.0)}
                                       +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,+z+1/2
   \{2_{x00} | (0.0,0.0,0.0)\}
                                       +x,-y,-z
     \{-1 \mid (0.5, 0.5, 0.5)\}
                                -x+1/2,-y+1/2,-z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.5)\}
                                 +y+1/2,+x+1/2,-z+1/2
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                       +y,-x,-z
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                              +y+1/2,-x+1/2,+z+1/2
*******
space group: 134:2 {'Hall': '-P 4ac 2bc', 'HM': 'P 42/n n m:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y+1/2,+x,+z+1/2
+x,-y+1/2,-z+1/2
 . . . . . . . . . . . . . . . . . .
            Seitz
                                      Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                     +x,+y,+z
  \{4^+_{00z} | (0.5, 0.0, 0.5)\}
                                -y+1/2,+x,+z+1/2
   \{2_{x00}|(0.0,0.5,0.5)\}
                                +x,-y+1/2,-z+1/2
   \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                -x+1/2,-y+1/2,+z
   \{2_{xx0}|(0.0,0.0,0.0)\}
                                     +y, +x, -z
  \{4^-00z|(0.0,0.5,0.5)\}
                                +y,-x+1/2,+z+1/2
   \{2_0y0|(0.5,0.0,0.5)\}
                                 -x+1/2,+y,-z+1/2
   \{2_x-x0\mid(0.5,0.5,0.0)\}
                                 -y+1/2,-x+1/2,-z
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                     -x,-y,-z
  \{-4^+00z|(0.5,0.0,0.5)\}
                                +y+1/2,-x,-z+1/2
   \{m_0yz \mid (0.0,0.5,0.5)\}
                                -x, +y+1/2, +z+1/2
   \{m_xy0|(0.5,0.5,0.0)\}
                                +x+1/2, +y+1/2, -z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                     -y,-x,+z
                                -y, +x+1/2, -z+1/2
  \{-4^-00z \mid (0.0,0.5,0.5)\}
                                +x+1/2,-y,+z+1/2
   \{m_x0z \mid (0.5,0.0,0.5)\}
   \{m_{xxz} | (0.5, 0.5, 0.0)\}
                                +y+1/2,+x+1/2,+z
```

```
space group: 135 {'Hall': '-P 4c 2ab', 'HM': 'P 42/m b c'}
Crystal system: Tetragonal
+x,+y,+z
-y, +x, +z+1/2
+x+1/2,-y+1/2,-z
             Seitz
                                          Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                         +X,+Y,+Z
  \{4^+_{00z}|(0.0,0.0,0.5)\}
                                       -y,+x,+z+1/2
   \{2_{x00} | (0.5, 0.5, 0.0)\}
                                    +x+1/2,-y+1/2,-z
   {2_00z|(0.0,0.0,0.0)}
                                         -x,-y,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,+x+1/2,-z+1/2
  \{4^-_00z \mid (0.0,0.0,0.5)\}
                                       +y,-x,+z+1/2
   {2_0y0|(0.5,0.5,0.0)}
                                    -x+1/2,+y+1/2,-z
   \{2_x-x0|(0.5,0.5,0.5)\}
                                  -y+1/2, -x+1/2, -z+1/2
      \{-1 \mid (0.0, 0.0, 0.0)\}
                                         -x,-y,-z
  \{-4^+00z \mid (0.0,0.0,0.5)\}
                                       +y,-x,-z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                    -x+1/2,+y+1/2,+z
   \{m_xy0|(0.0,0.0,0.0)\}
                                         +x,+y,-z
   \{m_x-xz \mid (0.5,0.5,0.5)\}
                                  -y+1/2, -x+1/2, +z+1/2
  \{-4^-00z \mid (0.0,0.0,0.5)\}
                                      -y,+x,-z+1/2
   \{m_x0z \mid (0.5, 0.5, 0.0)\}
                                    +x+1/2,-y+1/2,+z
   \{m_x \times z \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,+x+1/2,+z+1/2
*******
space group: 136 {'Hall': '-P 4n 2n', 'HM': 'P 42/m n m'}
Crystal system: Tetragonal
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x+1/2,-y+1/2,-z+1/2
             Seitz
                                          Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                         +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.5)\}
                                  -y+1/2, +x+1/2, +z+1/2
   \{2_{x00}|(0.5,0.5,0.5)\}
                                  +x+1/2,-y+1/2,-z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                         -x,-y,+z
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                                         +y,+x,-z
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,-x+1/2,+z+1/2
   {2_0y0|(0.5,0.5,0.5)}
                                  -x+1/2,+y+1/2,-z+1/2
   \{2_x-x0 \mid (0.0,0.0,0.0)\}
                                         -y,-x,-z
      \{-1 \mid (0.0, 0.0, 0.0)\}
                                         -x,-y,-z
  \{-4^+_00z|(0.5,0.5,0.5)\}
                                  +y+1/2,-x+1/2,-z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                  -x+1/2,+y+1/2,+z+1/2
   \{m_xy0|(0.0,0.0,0.0)\}
                                         +x,+y,-z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                         -y,-x,+z
  \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                  -y+1/2,+x+1/2,-z+1/2
   \{m_x0z | (0.5, 0.5, 0.5)\}
                                  +x+1/2,-y+1/2,+z+1/2
   \{m \times xz \mid (0.0,0.0,0.0)\}
                                         +y,+x,+z
```

```
*******
space group: 137:1 {'Hall': ' P 4n 2n -1n', 'HM': 'P 42/n m c:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x+1/2,-y+1/2,-z+1/2
-x+1/2, -y+1/2, -z+1/2
. . . . . . . . . . . . . . . . . . .
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.5)\}
                                -y+1/2, +x+1/2, +z+1/2
   {2_x00|(0.5,0.5,0.5)}
                                 +x+1/2,-y+1/2,-z+1/2
     \{-1 \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2, -y+1/2, -z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                        -x,-y,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                        +y,+x,-z
  \{-4^+ 00z \mid (0.0,0.0,0.0)\}
                                       +y,-x,-z
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,-x+1/2,+z+1/2
*******
space group: 137:2 {'Hall': '-P 4ac 2a', 'HM': 'P 42/n m c:2'}
Crystal system: Tetragonal
Setting: 2
+X,+Y,+Z
-y+1/2,+x,+z+1/2
+x+1/2,-y,-z
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
  \{4^+_{00z}|(0.5,0.0,0.5)\}
                                   -y+1/2,+x,+z+1/2
   \{2_{x00} | (0.5, 0.0, 0.0)\}
                                     +x+1/2,-y,-z
   \{2_{00z} | (0.5, 0.5, 0.0)\}
                                   -x+1/2,-y+1/2,+z
   {2_xx0|(0.5,0.5,0.5)}
                                 +y+1/2,+x+1/2,-z+1/2
  \{4^-_00z \mid (0.0, 0.5, 0.5)\}
                                   +y,-x+1/2,+z+1/2
   {2_0y0|(0.0,0.5,0.0)}
                                     -x,+y+1/2,-z
   \{2_x-x0|(0.0,0.0,0.5)\}
                                     -y,-x,-z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                        -x,-y,-z
  \{-4^+00z|(0.5,0.0,0.5)\}
                                   +y+1/2,-x,-z+1/2
   \{m_0yz \mid (0.5,0.0,0.0)\}
                                     -x+1/2,+y,+z
   \{m_xy0|(0.5,0.5,0.0)\}
                                   +x+1/2, +y+1/2, -z
   \{m_x-xz \mid (0.5,0.5,0.5)\}
                                 -y+1/2, -x+1/2, +z+1/2
                                   -y, +x+1/2, -z+1/2
  \{-4^-00z \mid (0.0,0.5,0.5)\}
   \{m_x0z \mid (0.0,0.5,0.0)\}
                                     +x,-y+1/2,+z
   \{m_xxz | (0.0,0.0,0.5)\}
                                     +y,+x,+z+1/2
```

```
*******
space group: 138:1 {'Hall': ' P 4n 2ab -1n', 'HM': 'P 42/n c m:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x+1/2,-y+1/2,-z
-x+1/2,-y+1/2,-z+1/2
            Seitz
                                         Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                        +x,+y,+z
  \{4^+_{00z}|(0.5,0.5,0.5)\}
                                 -y+1/2,+x+1/2,+z+1/2
   \{2_{x00} | (0.5, 0.5, 0.0)\}
                                   +x+1/2,-y+1/2,-z
     \{-1|(0.5,0.5,0.5)\}
                                 -x+1/2,-y+1/2,-z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                        -x,-y,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.5)\}
                                     +y,+x,-z+1/2
  \{-4^+_00z \mid (0.0,0.0,0.0)\} \mid
                                        +y,-x,-z
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                               +y+1/2,-x+1/2,+z+1/2
*******
space group: 138:2 {'Hall': '-P 4ac 2ac', 'HM': 'P 42/n c m:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y+1/2,+x,+z+1/2
+x+1/2,-y,-z+1/2
. . . . . . . . . . . . . . . . . . .
            Seitz
                                      Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                     +x,+y,+z
  \{4^+_{00z}|(0.5,0.0,0.5)\}
                                 -y+1/2,+x,+z+1/2
   \{2_{x00}|(0.5,0.0,0.5)\}
                                 +x+1/2,-y,-z+1/2
   \{2_{00z} | (0.5, 0.5, 0.0)\}
                                 -x+1/2,-y+1/2,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                                 +y+1/2,+x+1/2,-z
  \{4^-00z \mid (0.0, 0.5, 0.5)\}
                                 +y,-x+1/2,+z+1/2
   {2_0y0|(0.0,0.5,0.5)}
                                 -x, +y+1/2, -z+1/2
   \{2_x-x0|(0.0,0.0,0.0)\}
                                     -y,-x,-z
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                     -x,-y,-z
  \{-4^+_00z|(0.5,0.0,0.5)\}
                                 +y+1/2,-x,-z+1/2
                                 -x+1/2, +y, +z+1/2
   \{m_0yz \mid (0.5,0.0,0.5)\}
   \{m_xy0|(0.5,0.5,0.0)\}
                                 +x+1/2,+y+1/2,-z
   \{m_x-xz \mid (0.5,0.5,0.0)\}
                                 -y+1/2, -x+1/2, +z
  \{-4^-00z \mid (0.0, 0.5, 0.5)\}
                                 -y, +x+1/2, -z+1/2
```

+x,-y+1/2,+z+1/2

+y,+x,+z

.

 $\{m_x0z|(0.0,0.5,0.5)\}$

 $\{m_x \times z \mid (0.0, 0.0, 0.0)\}$

```
*******
space group: 139 {'Hall': ' -I 4 2', 'HM': 'I 4/m m m'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
+x,-y,-z
. . . . . . . . . . . . . . . . . . .
            Seitz
                                          Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                         +x,+y,+z
  \{4^+_{00z} | (0.0,0.0,0.0)\}
                                         -y,+x,+z
   \{2_{x00}|(0.0,0.0,0.0)\}
                                         +x,-y,-z
   \{2\_00z \mid (0.0,0.0,0.0)\}
                                         -x,-y,+z
   {2_xx0|(0.0,0.0,0.0)}
                                         +y, +x, -z
  \{4^-00z \mid (0.0,0.0,0.0)\}
                                         +y,-x,+z
   \{2_0y0|(0.0,0.0,0.0)\}
                                         -x,+y,-z
   \{2_x-x0\mid (0.0,0.0,0.0)\}
                                         -y,-x,-z
      \{-1 \mid (0.0, 0.0, 0.0)\}
                                         -x,-y,-z
  \{-4^+_00z \mid (0.0,0.0,0.0)\} \mid
                                         +y,-x,-z
   \{m_0yz \mid (0.0,0.0,0.0)\}
                                         -x,+y,+z
   \{m_xy0 | (0.0,0.0,0.0)\}
                                         +x,+y,-z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                         -y,-x,+z
  \{-4^-00z \mid (0.0,0.0,0.0)\}
                                         -y,+x,-z
   \{m_x0z | (0.0,0.0,0.0)\}
                                         +x,-y,+z
   \{m_xxz | (0.0,0.0,0.0)\}
                                         +y,+x,+z
      \{1 \mid (0.5, 0.5, 0.5)\}
                                 +x+1/2,+y+1/2,+z+1/2
  \{4^+_{00z}|(0.5,0.5,0.5)\}
                                  -y+1/2, +x+1/2, +z+1/2
   \{2_{x00}|(0.5,0.5,0.5)\}
                                  +x+1/2,-y+1/2,-z+1/2
   \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                  -x+1/2, -y+1/2, +z+1/2
   \{2_x \times 0 \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,+x+1/2,-z+1/2
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,-x+1/2,+z+1/2
   \{2 \text{ 0y0} | (0.5, 0.5, 0.5)\}
                                  -x+1/2, +y+1/2, -z+1/2
   \{2_x-x0|(0.5,0.5,0.5)\}
                                  -y+1/2,-x+1/2,-z+1/2
      \{-1 \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2, -y+1/2, -z+1/2
  \{-4^+, 00z \mid (0.5, 0.5, 0.5)\} \mid +y+1/2, -x+1/2, -z+1/2
   \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                  -x+1/2, +y+1/2, +z+1/2
   \{m_xy0|(0.5,0.5,0.5)\}
                                 +x+1/2,+y+1/2,-z+1/2
   \{m_x-xz \mid (0.5,0.5,0.5)\}
                                 -y+1/2,-x+1/2,+z+1/2
  \{-4^-00z|(0.5,0.5,0.5)\} \mid -y+1/2,+x+1/2,-z+1/2
   \{m_x0z \mid (0.5, 0.5, 0.5)\}
                                +x+1/2,-y+1/2,+z+1/2
                                +y+1/2,+x+1/2,+z+1/2
   \{m_{xxz}|(0.5,0.5,0.5)\}
*******
space group: 140 {'Hall': ' -I 4 2c', 'HM': 'I 4/m c m'}
Crystal system: Tetragonal
+x,+y,+z
-y,+x,+z
+x,-y,-z+1/2
```

```
Seitz
                                          Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                         +x,+y,+z
  \{4^+ 00z \mid (0.0,0.0,0.0)\}
                                         -y,+x,+z
   {2_x00|(0.0,0.0,0.5)}
                                       +x,-y,-z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                         -x,-y,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.5)\}
                                       +y,+x,-z+1/2
  \{4^{-}00z \mid (0.0,0.0,0.0)\}
                                         +y,-x,+z
   {2_0y0|(0.0,0.0,0.5)}
                                       -x,+y,-z+1/2
   \{2_x-x0|(0.0,0.0,0.5)\}
                                       -y,-x,-z+1/2
      \{-1 \mid (0.0, 0.0, 0.0)\}
                                         -x,-y,-z
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                         +y,-x,-z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                       -x,+y,+z+1/2
   \{m_xy0|(0.0,0.0,0.0)\}
                                         +x,+y,-z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                                       -y,-x,+z+1/2
  \{-4^-00z|(0.0,0.0,0.0)\}
                                         -y,+x,-z
   \{m_x0z \mid (0.0,0.0,0.5)\}
                                       +x,-y,+z+1/2
   \{m_xxz|(0.0,0.0,0.5)\}
                                       +y,+x,+z+1/2
      \{1 \mid (0.5, 0.5, 0.5)\}
                                  +x+1/2, +y+1/2, +z+1/2
  \{4^+_00z|(0.5,0.5,0.5)\}
                                  -y+1/2,+x+1/2,+z+1/2
   \{2_{x00} | (0.5, 0.5, 0.0)\}
                                     +x+1/2,-y+1/2,-z
   \{2_{00z} | (0.5, 0.5, 0.5)\}
                                  -x+1/2,-y+1/2,+z+1/2
   \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                                     +y+1/2,+x+1/2,-z
  \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,-x+1/2,+z+1/2
   {2_0y0|(0.5,0.5,0.0)}
                                     -x+1/2,+y+1/2,-z
   \{2_x-x0\mid (0.5,0.5,0.0)\}
                                     -y+1/2,-x+1/2,-z
      [-1|(0.5,0.5,0.5)}
                                  -x+1/2, -y+1/2, -z+1/2
  \{-4^+_{00z}|(0.5,0.5,0.5)\}
                                  +y+1/2,-x+1/2,-z+1/2
   \{m \ 0yz | (0.5, 0.5, 0.0)\}
                                     -x+1/2,+y+1/2,+z
   \{m_xy0|(0.5,0.5,0.5)\}
                                  +x+1/2, +y+1/2, -z+1/2
   \{m_x-xz\mid(0.5,0.5,0.0)\}
                                     -y+1/2, -x+1/2, +z
  \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                  -y+1/2,+x+1/2,-z+1/2
   \{m_x0z|(0.5,0.5,0.0)\}
                                     +x+1/2,-y+1/2,+z
   \{m \times xz \mid (0.5, 0.5, 0.0)\}
                                     +y+1/2,+x+1/2,+z
*******
```

```
space group: 141:1 {'Hall': ' I 4bw 2bw -1bw', 'HM': 'I 41/a m d:1'}
```

```
Setting: 1
+x,+y,+z
-y, +x+1/2, +z+1/4
+x,-y+1/2,-z+1/4
-x,-y+1/2,-z+1/4
```

```
Seitz
                                        Jones
   \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
\{4^+_{00z}|(0.0,0.5,0.25)\}
                                  -y, +x+1/2, +z+1/4
 {2_x00|(0.0,0.5,0.25)}
                                  +x,-y+1/2,-z+1/4
  \{-1 \mid (0.0, 0.5, 0.25)\}
                                  -x,-y+1/2,-z+1/4
 \{2\ 00z\mid(0.5,0.5,0.5)\}
                                -x+1/2, -y+1/2, +z+1/2
```

```
\{2_x \times 0 \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,+x+1/2,-z+1/2
  \{-4^+_00z \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,-x+1/2,-z+1/2
  \{4^-_00z \mid (0.5,0.0,0.75)\}
                                    +y+1/2,-x,+z+3/4
                                  +x+1/2, +y+1/2, +z+1/2
      \{1 \mid (0.5, 0.5, 0.5)\}
  \{4^+_{00z}|(0.5,0.0,0.75)\}
                                    -y+1/2,+x,+z+3/4
   {2_x00|(0.5,0.0,0.75)}
                                    +x+1/2,-y,-z+3/4
    \{-1 \mid (0.5, 0.0, 0.75)\}
                                    -x+1/2,-y,-z+3/4
   {2_00z|(0.0,0.0,0.0)}
                                         -x,-y,+z
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                                         +y, +x, -z
  \{-4^+ 00z \mid (0.0,0.0,0.0)\}
                                         +y,-x,-z
  \{4^-_00z \mid (0.0, 0.5, 0.25)\}
                                    +y, -x+1/2, +z+1/4
*******
space group: 141:2 {'Hall': '-I 4bd 2', 'HM': 'I 41/a m d:2'}
Crystal system: Tetragonal
Setting: 2
+x,+y,+z
-y+1/4, +x+3/4, +z+1/4
+x,-y,-z
               Seitz
                                              Jones
        \{1 \mid (0.0, 0.0, 0.0)\}
                                             +x,+y,+z
   \{4^+_{00z}|(0.25,0.75,0.25)\}
                                     -y+1/4, +x+3/4, +z+1/4
     \{2_{x00} | (0.0,0.0,0.0)\}
                                             +x,-y,-z
      \{2\ 00z\mid(0.5,0.0,0.5)\}
                                        -x+1/2,-y,+z+1/2
    {2_xx0|(0.25,0.75,0.25)}
                                     +y+1/4, +x+3/4, -z+1/4
   \{4^-_00z \mid (0.25, 0.25, 0.75)\}
                                      +y+1/4,-x+1/4,+z+3/4
      {2_0y0|(0.5,0.0,0.5)}
                                        -x+1/2,+y,-z+1/2
   \{2_x-x0\mid(0.25,0.25,0.75)\}
                                      -y+1/4, -x+1/4, -z+3/4
        \{-1 \mid (0.0, 0.0, 0.0)\}
                                             -x,-y,-z
  \{-4^+_00z \mid (0.25, 0.75, 0.25)\}
                                     +y+1/4, -x+3/4, -z+1/4
      \{m_0yz \mid (0.0,0.0,0.0)\}
                                             -x,+y,+z
      \{m_xy0|(0.5,0.0,0.5)\}
                                        +x+1/2,+y,-z+1/2
                                     -y+1/4, -x+3/4, +z+1/4
   {m_x-xz|(0.25,0.75,0.25)}
  \{-4^-_00z \mid (0.25, 0.25, 0.75)\}
                                      -y+1/4, +x+1/4, -z+3/4
      \{m_x0z \mid (0.5,0.0,0.5)\}
                                        +x+1/2,-y,+z+1/2
    \{m_xz|(0.25,0.25,0.75)\}
                                      +y+1/4, +x+1/4, +z+3/4
        \{1 \mid (0.5, 0.5, 0.5)\}
                                      +x+1/2,+y+1/2,+z+1/2
   \{4^+_{00z} | (0.75, 0.25, 0.75)\}
                                     -y+3/4, +x+1/4, +z+3/4
     \{2_{x00}|(0.5,0.5,0.5)\}
                                     +x+1/2,-y+1/2,-z+1/2
     {2_00z|(0.0,0.5,0.0)}
                                          -x,-y+1/2,+z
    \{2 \times \times 0 \mid (0.75, 0.25, 0.75)\}
                                      +y+3/4, +x+1/4, -z+3/4
   \{4^-00z \mid (0.75, 0.75, 0.25)\}
                                      +y+3/4,-x+3/4,+z+1/4
      {2_0y0|(0.0,0.5,0.0)}
                                          -x,+y+1/2,-z
   \{2_x-x0|(0.75,0.75,0.25)\}
                                     -y+3/4, -x+3/4, -z+1/4
        \{-1|(0.5,0.5,0.5)\}
                                     -x+1/2,-y+1/2,-z+1/2
  \{-4^+_00z \mid (0.75, 0.25, 0.75)\}
                                     +y+3/4,-x+1/4,-z+3/4
      \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                     -x+1/2,+y+1/2,+z+1/2
      \{m_xy0|(0.0,0.5,0.0)\}
                                          +x,+y+1/2,-z
```

-y+3/4, -x+1/4, +z+3/4

 $\{m \times -xz \mid (0.75, 0.25, 0.75)\}$

```
\{-4^{-}_{00z}|(0.75,0.75,0.25)\} \mid -y+3/4,+x+3/4,-z+1/4
     \{m_x0z \mid (0.0, 0.5, 0.0)\}
                                        +x,-y+1/2,+z
                                    +y+3/4, +x+3/4, +z+1/4
    \{m_xz|(0.75,0.75,0.25)\}
*******
space group: 142:1 {'Hall': ' I 4bw 2aw -1bw', 'HM': 'I 41/a c d:1'}
Crystal system: Tetragonal
Setting: 1
+x,+y,+z
-y, +x+1/2, +z+1/4
+x+1/2,-y,-z+1/4
-x,-y+1/2,-z+1/4
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
  \{4^+_{00z}|(0.0,0.5,0.25)\}\ |
                                   -y, +x+1/2, +z+1/4
   \{2_{x00} | (0.5, 0.0, 0.25)\}
                                   +x+1/2,-y,-z+1/4
    \{-1 \mid (0.0, 0.5, 0.25)\}
                                   -x,-y+1/2,-z+1/4
   {2_00z|(0.5,0.5,0.5)}
                                -x+1/2,-y+1/2,+z+1/2
   {2_xx0|(0.0,0.0,0.5)}
                                     +y,+x,-z+1/2
  \{-4^+_00z \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,-x+1/2,-z+1/2
  \{4^-_00z \mid (0.5, 0.0, 0.75)\}
                                   +y+1/2,-x,+z+3/4
     {1|(0.5,0.5,0.5)}
                                +x+1/2, +y+1/2, +z+1/2
  \{4^+_{00z}|(0.5,0.0,0.75)\}
                                   -y+1/2,+x,+z+3/4
   \{2_{x00}|(0.0,0.5,0.75)\}
                                   +x,-y+1/2,-z+3/4
    \{-1 \mid (0.5, 0.0, 0.75)\}
                                   -x+1/2,-y,-z+3/4
   {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
   \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                                   +y+1/2,+x+1/2,-z
  \{-4^+00z \mid (0.0,0.0,0.0)\}
                                       +y,-x,-z
  \{4^- 00z \mid (0.0, 0.5, 0.25)\}\ \mid
                                   +y,-x+1/2,+z+1/4
*******
space group: 142:2 {'Hall': '-I 4bd 2c', 'HM': 'I 41/a c d:2'}
Crystal system: Tetragonal
Setting: 2
+X,+Y,+Z
-y+1/4, +x+3/4, +z+1/4
+x,-y,-z+1/2
              Seitz
                                            Jones
        {1|(0.0,0.0,0.0)}
                                           +x,+y,+z
   \{4^+_{00z}|(0.25,0.75,0.25)\}
                                    -y+1/4, +x+3/4, +z+1/4
     \{2_{x00}|(0.0,0.0,0.5)\}
                                        +x,-y,-z+1/2
     \{2\_00z \mid (0.5,0.0,0.5)\}
                                      -x+1/2,-y,+z+1/2
    \{2_x \times 0 \mid (0.25, 0.75, 0.75)\}
                                    +y+1/4, +x+3/4, -z+3/4
   \{4^-\ 00z\ |\ (0.25,0.25,0.75)\}\ |\ +y+1/4,-x+1/4,+z+3/4
```

```
{2_0y0|(0.5,0.0,0.0)}
                                         -x+1/2,+y,-z
                                    -y+1/4, -x+1/4, -z+1/4
   \{2_x-x0|(0.25,0.25,0.25)\}
        \{-1 \mid (0.0,0.0,0.0)\}
                                           -x,-y,-z
  \{-4^+_{00z} | (0.25, 0.75, 0.25)\}
                                    +y+1/4,-x+3/4,-z+1/4
     \{m_0yz \mid (0.0,0.0,0.5)\}
                                         -x,+y,+z+1/2
     \{m_xy0|(0.5,0.0,0.5)\}
                                      +x+1/2,+y,-z+1/2
   \{m_x-xz\mid(0.25,0.75,0.75)\}
                                    -y+1/4, -x+3/4, +z+3/4
  \{-4^-00z \mid (0.25, 0.25, 0.75)\}
                                    -y+1/4, +x+1/4, -z+3/4
     \{m_x0z \mid (0.5,0.0,0.0)\}
                                         +x+1/2,-y,+z
    \{m_xxz \mid (0.25, 0.25, 0.25)\}
                                    +y+1/4, +x+1/4, +z+1/4
        \{1|(0.5,0.5,0.5)\}
                                    +x+1/2, +y+1/2, +z+1/2
   \{4^+_00z \mid (0.75, 0.25, 0.75)\}
                                    -y+3/4, +x+1/4, +z+3/4
     \{2_{x00}|(0.5,0.5,0.0)\}
                                       +x+1/2,-y+1/2,-z
     {2_00z|(0.0,0.5,0.0)}
                                         -x,-y+1/2,+z
    {2_xx0|(0.75,0.25,0.25)}
                                    +y+3/4, +x+1/4, -z+1/4
   \{4^-_00z \mid (0.75, 0.75, 0.25)\}
                                    +y+3/4,-x+3/4,+z+1/4
     {2_0y0|(0.0,0.5,0.5)}
                                      -x,+y+1/2,-z+1/2
   \{2_x-x0|(0.75,0.75,0.75)\}
                                    -y+3/4, -x+3/4, -z+3/4
        {-1|(0.5,0.5,0.5)}
                                    -x+1/2, -y+1/2, -z+1/2
  \{-4^+_00z \mid (0.75, 0.25, 0.75)\}
                                    +y+3/4,-x+1/4,-z+3/4
     \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                       -x+1/2,+y+1/2,+z
     \{m_xy0 | (0.0, 0.5, 0.0)\}
                                         +x,+y+1/2,-z
   \{m_x-xz \mid (0.75,0.25,0.25)\}
                                    -y+3/4, -x+1/4, +z+1/4
  \{-4^-_00z \mid (0.75, 0.75, 0.25)\}
                                    -y+3/4, +x+3/4, -z+1/4
     \{m_x0z \mid (0.0,0.5,0.5)\}
                                      +x,-y+1/2,+z+1/2
    \{m_xxz \mid (0.75, 0.75, 0.75)\}
                                    +y+3/4, +x+3/4, +z+3/4
*******
space group: 143 {'Hall': 'P 3', 'HM': 'P 3'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
            Seitz
                                  Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  {3^+_00z | (0.0,0.0,0.0)}
                               -y, +x-y, +z
  \{3^-00z \mid (0.0,0.0,0.0)\} \mid +y-x,-x,+z
*******
space group: 144 {'Hall': ' P 31', 'HM': 'P 31'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z+1/3
                  Seitz
                                                 Jones
```

{1|(0.0,0.0,0.0)}

+x,+y,+z

```
| \{3^+_00z | (0.0,0.0,0.33333333333)\} | -y,+x-y,+z+1/3 |
 \{3^{-}00z \mid (0.0,0.0,0.666666666667)\} \mid +y-x,-x,+z+2/3 \mid
*******
space group: 145 {'Hall': ' P 32', 'HM': 'P 32'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z+2/3
              Seitz
                                      Jones
         {1|(0.0,0.0,0.0)}
                                    +x,+y,+z
 {3^+\_00z|(0.0,0.0,0.666666666667)} \mid -y,+x-y,+z+2/3
| {3^-_00z|(0.0,0.0,0.33333333333)} | +y-x,-x,+z+1/3 |
*******
space group: 146:H {'Hall': 'R 3', 'HM': 'R 3:H'}
Crystal system: Trigonal
Setting: H
+x,+y,+z
-y, +x-y, +z
                        Seitz
Jones
                  \{1 \mid (0.0, 0.0, 0.0)\}
+x,+y,+z
                \{3^+00z \mid (0.0,0.0,0.0)\}
y,+x-y,+z
                {3^-_00z|(0.0,0.0,0.0)}
+y-x,-x,+z
   {1|(0.333333333333,0.66666666667,0.66666666667)}
                                                       +X
+1/3,+y+2/3,+z+2/3
| {3^+_00z|(0.3333333333333,0.66666666667,0.66666666667)} | -y
+1/3, +x-y+2/3, +z+2/3
+1/3, -x+2/3, +z+2/3
    {1|(0.66666666667,0.3333333333,0.33333333333)}
+2/3, +y+1/3, +z+1/3
+2/3, +x-y+1/3, +z+1/3
| {3^-_00z|(0.66666666667,0.33333333333,0.33333333333)} | +y-x
+2/3,-x+1/3,+z+1/3
```

```
******
space group: 146:R {'Hall': 'P 3*', 'HM': 'R 3:R'}
Crystal system: Trigonal
Setting: R
+x,+y,+z
+z,+x,+y
                             Jones
     {1|(0.0,0.0,0.0)}
                           +x,+y,+z
| \{3^+_xxx|(0.0,0.0,0.0)\} | +z_+x_+y_-|
| {3^-_xxx|(0.0,0.0,0.0)} | +y,+z,+x |
*******
space group: 147 {'Hall': '-P 3', 'HM': 'P -3'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
           Seitz
                               Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                             +x,+y,+z
 {3^+_00z|(0.0,0.0,0.0)}
                            -y,+x-y,+z
| {3^-_00z|(0.0,0.0,0.0)} | +y-x,-x,+z |
     \{-1 \mid (0.0, 0.0, 0.0)\}
                              -x,-y,-z
  \{-3^+_00z \mid (0.0,0.0,0.0)\} \mid +y,+y-x,-z
  \{-3^-00z \mid (0.0,0.0,0.0)\} \mid +x-y,+x,-z \mid
******
space group: 148:H {'Hall': '-R 3', 'HM': 'R -3:H'}
Crystal system: Trigonal
Setting: H
+x,+y,+z
-y, +x-y, +z
                             Seitz
Jones
                      \{1 \mid (0.0, 0.0, 0.0)\}
+x,+y,+z
                   {3^+_00z|(0.0,0.0,0.0)}
-y,+x-y,+z
                   \{3^-_00z \mid (0.0,0.0,0.0)\}
+y-x,-x,+z
```

```
\{-1 \mid (0.0, 0.0, 0.0)\}
-x,-y,-z
                    \{-3^+ 00z \mid (0.0,0.0,0.0)\}
+y,+y-x,-z
                    \{-3^-\ 00z \mid (0.0,0.0,0.0)\}
+x-y, +x, -z
      {1|(0.333333333333,0.66666666667,0.66666666667)}
                                                                  +X
+1/3, +y+2/3, +z+2/3
{3^+_00z|(0.333333333333,0.66666666667,0.66666666667)} | -y
+1/3, +x-y+2/3, +z+2/3
{3^-_00z|(0.3333333333333,0.66666666667,0.666666666667)} | +y-x
+1/3, -x+2/3, +z+2/3
     \{-1 \mid (0.33333333333333, 0.66666666667, 0.66666666667)\}
                                                                  -x
+1/3,-y+2/3,-z+2/3
| \{-3^+_00z | (0.3333333333333, 0.666666666667, 0.666666666667)\} | +y
+1/3, +v-x+2/3, -z+2/3
| {-3^-_00z|(0.33333333333333,0.666666666667,0.66666666667)} | +x-y
+1/3,+x+2/3,-z+2/3
      {1|(0.66666666667,0.33333333333,0.333333333333)}
+2/3,+y+1/3,+z+1/3
{3^+_00z|(0.6666666667,0.33333333333,0.33333333333)} | -y
+2/3, +x-y+1/3, +z+1/3
   \{3^{-}00z \mid (0.66666666667, 0.333333333333, 0.333333333333)\} \mid +y-x
+2/3,-x+1/3,+z+1/3
    \{-1 \mid (0.666666666667, 0.33333333333, 0.333333333333)\}
+2/3,-y+1/3,-z+1/3
| {-3^+_00z|(0.66666666667,0.33333333333,0.33333333333)} | +y
+2/3, +y-x+1/3, -z+1/3
-3^- 00z \mid (0.666666666667, 0.333333333333, 0.33333333333)\} \mid +x-y
+2/3,+x+1/3,-z+1/3
. . . . . . . . . . . . . . . . . . . .
*******
space group: 148:R {'Hall': '-P 3*', 'HM': 'R -3:R'}
Crystal system: Trigonal
Setting: R
+x,+y,+z
+Z,+X,+y
           Seitz
                               Jones
     {1|(0.0,0.0,0.0)}
                            | +x,+y,+z
 {3^+_xxx|(0.0,0.0,0.0)}
                            | +z,+x,+y
  {3^-_xxx|(0.0,0.0,0.0)}
                            +y,+z,+x
     \{-1 \mid (0.0, 0.0, 0.0)\}
                           -x,-y,-z
  \{-3^+ xxx \mid (0.0,0.0,0.0)\} \mid -z,-x,-y
 \{-3^-xxx|(0.0,0.0,0.0)\} \mid -y,-z,-x
```

```
space group: 149 {'Hall': 'P 3 2', 'HM': 'P 3 1 2'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
-y,-x,-z
           Seitz
                               Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                              +X,+Y,+Z
  {3^+_00z|(0.0,0.0,0.0)}
                             -y,+x-y,+z
   \{2_x-x0 \mid (0.0,0.0,0.0)\}
                             -y,-x,-z
  {3^-_00z|(0.0,0.0,0.0)} + y-x,-x,+z
   {m_2xx0|(0.0,0.0,0.0)} +x,+x-y,-z
   \{2_x2x0|(0.0,0.0,0.0)\} \mid +y-x,+y,-z
*******
space group: 150 {'Hall': 'P 3 2"', 'HM': 'P 3 2 1'}
Crystal system: Trigonal
+x,+y,+z
-y,+x-y,+z
+y,+x,-z
           Seitz
                               Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                            +X,+V,+Z
  {3^+\_00z | (0.0,0.0,0.0)} | -y,+x-y,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                              +y,+x,-z
  {3^-_00z|(0.0,0.0,0.0)} + y-x,-x,+z
   {2_0y0|(0.0,0.0,0.0)}
                           -x,+y-x,-z
   {2_x00|(0.0,0.0,0.0)}
                           +x-y,-y,-z
*******
space group: 151 {'Hall': ' P 31 2c (0,0,1)', 'HM': 'P 31 1 2'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z+1/3
-y,-x,-z+2/3
                Seitz
                                            Jones
          \{1 \mid (0.0, 0.0, 0.0)\}
                                           +x,+y,+z
  {3^+_00z|(0.0,0.0,0.333333333333)}
                                        -y,+x-y,+z+1/3
  \{2_x-x0\mid (0.0,0.0,0.666666666667)\}
                                         -y,-x,-z+2/3
  {3^-_00z|(0.0,0.0,0.66666666667)}
                                        +y-x,-x,+z+2/3
        \{m_2xx0|(0.0,0.0,0.0)\}
                                          +x,+x-y,-z
  {2_x2x0|(0.0,0.0,0.333333333333)}
                                       +y-x,+y,-z+1/3
```

******* space group: 152 {'Hall': ' P 31 2"', 'HM': 'P 31 2 1'} Crystal system: Trigonal +x,+y,+z-y, +x-y, +z+1/3+y,+x,-zSeitz Jones {1|(0.0,0.0,0.0)} +x,+y,+z{3^+_00z|(0.0,0.0,0.333333333333)} -y, +x-y, +z+1/3 $\{2_x \times 0 \mid (0.0, 0.0, 0.0)\}$ +y,+x,-z{3^-_00z|(0.0,0.0,0.66666666667)} +y-x,-x,+z+2/3{2_0y0|(0.0,0.0,0.333333333333)} -x,+y-x,-z+1/3{2_x00|(0.0,0.0,0.666666666667)} +x-y,-y,-z+2/3****** space group: 153 {'Hall': ' P 32 2c (0,0,-1)', 'HM': 'P 32 1 2'} Crystal system: Trigonal +x,+y,+z-y, +x-y, +z+2/3-y,-x,-z+1/3Seitz Jones $\{1 \mid (0.0, 0.0, 0.0)\}$ +x,+y,+z{3^+_00z|(0.0,0.0,0.666666666667)} -y, +x-y, +z+2/3 $\{2 \times -\times 0 \mid (0.0, 0.0, 0.3333333333333)\}$ -y, -x, -z+1/3{3^-_00z|(0.0,0.0,0.333333333333)} +y-x,-x,+z+1/3 ${m_2xx0|(0.0,0.0,0.0)}$ +x,+x-y,-z{2_x2x0|(0.0,0.0,0.66666666667)} +y-x, +y, -z+2/3****** space group: 154 {'Hall': ' P 32 2"', 'HM': 'P 32 2 1'} Crystal system: Trigonal +x,+y,+z-y, +x-y, +z+2/3+y,+x,-z

_		·
	Seitz	Jones
	{1 (0.0,0.0,0.0)} {3^+_00z (0.0,0.0,0.6666666666667)} {2_xx0 (0.0,0.0,0.0)} {3^00z (0.0,0.0,0.333333333333)}	+x,+y,+z -y,+x-y,+z+2/3 +y,+x,-z +y-x,-x,+z+1/3

```
\{2_0y0|(0.0,0.0,0.666666666667)\} | -x,+y-x,-z+2/3 |
   \{2_x00|(0.0,0.0,0.333333333333)\} +x-y,-y,-z+1/3 |
*******
space group: 155:H {'Hall': ' R 3 2"', 'HM': 'R 32:H'}
Crystal system: Trigonal
Setting: H
+X,+Y,+Z
-y, +x-y, +z
+y,+x,-z
                          Seitz
Jones
                    \{1 \mid (0.0, 0.0, 0.0)\}
+x,+y,+z
                 \{3^+ 00z \mid (0.0,0.0,0.0)\}
y,+x-y,+z
                  \{2 \times \times 0 \mid (0.0, 0.0, 0.0)\}
+y,+x,-z
                 \{3^- 00z \mid (0.0,0.0,0.0)\}
+y-x,-x,+z
                  {2 0y0|(0.0,0.0,0.0)}
X,+y-X,-Z
                  {2_x00|(0.0,0.0,0.0)}
+x-y,-y,-z
    {1|(0.33333333333,0.66666666667,0.66666666667)}
                                                            +X
+1/3,+y+2/3,+z+2/3
+1/3, +x-y+2/3, +z+2/3
{2_xx0|(0.33333333333,0.66666666667,0.66666666667)}
+1/3, +x+2/3, -z+2/3
\[ \{3^-_00z\] \( (0.333333333333333, 0.66666666667, 0.666666666667)\} \| \text{+y-x}
+1/3, -x+2/3, +z+2/3
{2_0y0|(0.33333333333,0.66666666667,0.66666666667)}
+1/3,+y-x+2/3,-z+2/3
{2_x00|(0.33333333333,0.66666666667,0.66666666667)}
                                                         | +x-y
+1/3,-y+2/3,-z+2/3
    {1|(0.66666666667,0.3333333333,0.33333333333)}
                                                         | +x
+2/3, +y+1/3, +z+1/3
| {3^+_00z|(0.66666666667,0.333333333333,0.33333333333)} | -y
+2/3, +x-y+1/3, +z+1/3
{2 xx0|(0.6666666667,0.33333333333,0.33333333333)}
+2/3,+x+1/3,-z+1/3
| {3^-_00z|(0.66666666667,0.33333333333,0.33333333333)} | +y-x
+2/3,-x+1/3,+z+1/3
{2_0y0|(0.6666666667,0.33333333333,0.33333333333)} | -x
+2/3, +y-x+1/3, -z+1/3
{2 x00|(0.66666666667,0.33333333333,0.33333333333)} | +x-y
```

```
+2/3,-y+1/3,-z+1/3
******
space group: 155:R {'Hall': ' P 3* 2', 'HM': 'R 32:R'}
Crystal system: Trigonal
Setting: R
+x,+y,+z
+z,+x,+y
-y,-x,-z
                           | Jones
           Seitz
    {1|(0.0,0.0,0.0)}
                           +x,+y,+z
  {3^+_xxx}|(0.0,0.0,0.0)\} | +z,+x,+y |
  \{2_x-x0\mid(0.0,0.0,0.0)\}\mid -y,-x,-z
  {3^-_xxx|(0.0,0.0,0.0)} | +y,+z,+x |
  \{2\_-x0x \mid (0.0,0.0,0.0)\} \mid -z,-y,-x \mid
  \{2_0y-y \mid (0.0,0.0,0.0)\} \mid -x,-z,-y \mid
*******
space group: 156 {'Hall': 'P 3 -2"', 'HM': 'P 3 m 1'}
Crystal system: Trigonal
+X,+Y,+Z
-y, +x-y, +z
-y,-x,+z
           Seitz
                              Jones
     {1|(0.0,0.0,0.0)}
                           +x,+y,+z
 {3^+}_{00z}|(0.0,0.0,0.0)\} | -y,+x-y,+z
  \{m_x-xz \mid (0.0,0.0,0.0)\} \mid
                             -y,-x,+z
  {3^-_00z|(0.0,0.0,0.0)} + y-x,-x,+z
  \{m_2xxz \mid (0.0,0.0,0.0)\} \mid +x,+x-y,+z
   \{m_x2xz \mid (0.0,0.0,0.0)\} \mid +y-x,+y,+z \mid
*******
space group: 157 {'Hall': 'P 3 -2', 'HM': 'P 3 1 m'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
+y,+x,+z
                              Jones
           Seitz
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                              +x,+y,+z
  {3^+\_00z | (0.0,0.0,0.0)}
                             -y,+x-y,+z
   \{m_xxz | (0.0,0.0,0.0)\}
                               +y,+x,+z
  \{3^- 00z \mid (0.0, 0.0, 0.0)\}
                              +y-x,-x,+z
   \{m_0yz \mid (0.0,0.0,0.0)\}
                             -x,+y-x,+z
   \{m_x0z \mid (0.0,0.0,0.0)\}
                             +x-y,-y,+z
*******
space group: 158 {'Hall': 'P 3 -2"c', 'HM': 'P 3 c 1'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
-y,-x,+z+1/2
            Seitz
                                  Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +x,+y,+z
  {3^+_00z|(0.0,0.0,0.0)}
                                -y, +x-y, +z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                               -y,-x,+z+1/2
  {3^-_00z|(0.0,0.0,0.0)}
                                +y-x,-x,+z
   \{m_2xxz \mid (0.0,0.0,0.5)\}
                              +x,+x-y,+z+1/2
   \{m_x2xz \mid (0.0,0.0,0.5)\} \mid +y-x,+y,+z+1/2
*******
space group: 159 {'Hall': 'P 3 -2c', 'HM': 'P 3 1 c'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
+y,+x,+z+1/2
            Seitz
                                  Jones
     {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
  {3^+_00z|(0.0,0.0,0.0)}
                                -y, +x-y, +z
   \{m_x \times z \mid (0.0, 0.0, 0.5)\}
                               +y,+x,+z+1/2
  \{3^-00z \mid (0.0,0.0,0.0)\}
                                +y-x,-x,+z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                              -x,+y-x,+z+1/2
   \{m_x0z \mid (0.0,0.0,0.5)\}
                            | +x-y,-y,+z+1/2
*******
space group: 160:H {'Hall': 'R 3 -2"', 'HM': 'R 3 m:H'}
Crystal system: Trigonal
Setting: H
+x,+y,+z
-y,+x-y,+z
-y,-x,+z
```

```
. . . . . . . . . . . . . . . . . . . .
                     Seitz
Jones
                \{1 \mid (0.0, 0.0, 0.0)\}
+x,+y,+z
              {3^+ 00z | (0.0,0.0,0.0)}
y,+x-y,+z
               \{m_x-xz \mid (0.0,0.0,0.0)\}
-y,-x,+z
              {3^-_00z|(0.0,0.0,0.0)}
+y-x,-x,+z
               \{m_2xxz \mid (0.0,0.0,0.0)\}
+x,+x-y,+z
               \{m_x2xz \mid (0.0,0.0,0.0)\}
+y-x,+y,+z
   {1|(0.333333333333,0.66666666667,0.66666666667)}
                                                +x
+1/3,+y+2/3,+z+2/3 |
+1/3, +x-y+2/3, +z+2/3
+1/3, -x+2/3, +z+2/3
| {3^-_00z|(0.333333333333,0.666666666667,0.666666666667)} | +y-x
+1/3, -x+2/3, +z+2/3
| {m 2xxz|(0.333333333333,0.66666666667,0.66666666667)}
+1/3, +x-y+2/3, +z+2/3
+1/3,+y+2/3,+z+2/3
   {1|(0.66666666667,0.33333333333,0.33333333333)}
                                             | +x
+2/3,+y+1/3,+z+1/3
\{3^+ 00z \mid (0.666666666667, 0.33333333333, 0.33333333333)\} \mid -v
+2/3,+x-y+1/3,+z+1/3
\{ m \ x-xz \mid (0.666666666667, 0.33333333333, 0.33333333333) \}
+2/3, -x+1/3, +z+1/3
+2/3,-x+1/3,+z+1/3
+2/3, +x-y+1/3, +z+1/3
+2/3,+y+1/3,+z+1/3 |
. . . . . . . . . . . . . . . . . .
*******
space group: 160:R {'Hall': 'P 3* -2', 'HM': 'R 3 m:R'}
Crystal system: Trigonal
Setting: R
+x,+y,+z
+z,+x,+y
+y,+x,+z
```

```
Seitz
                             Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                            +x,+y,+z
 {3^+_xxx|(0.0,0.0,0.0)}
                           +z,+x,+y
  \{m_xxz|(0.0,0.0,0.0)\}
                           +y,+x,+z
  {3^-_xxx|(0.0,0.0,0.0)} + y,+z,+x
   \{m_xyx | (0.0,0.0,0.0)\}
                          +z,+y,+x
   \{m \times yy \mid (0.0, 0.0, 0.0)\}
                          +x,+z,+y
*******
space group: 161:H {'Hall': 'R 3 -2"c', 'HM': 'R 3 c:H'}
Crystal system: Trigonal
Setting: H
+x,+y,+z
-y, +x-y, +z
-y, -x, +z+1/2
                           Seitz
Jones
                     {1|(0.0,0.0,0.0)}
+x,+y,+z
                  \{3^+ 00z \mid (0.0,0.0,0.0)\}
y,+x-y,+z
                   \{m_x-xz \mid (0.0,0.0,0.5)\}
y_{1}-x_{1}+z+1/2
                  \{3^- 00z \mid (0.0, 0.0, 0.0)\}
+y-x,-x,+z
                   \{m_2xxz \mid (0.0,0.0,0.5)\}
                                                                  +x,
+x-y_1+z+1/2
                   \{m_x2xz \mid (0.0,0.0,0.5)\}
                                                                  +y-
x, +y, +z+1/2
     {1|(0.333333333333,0.66666666667,0.66666666667)}
+1/3, +y+2/3, +z+2/3
+1/3, +x-y+2/3, +z+2/3
\[ \{\mathbb{m}_x - \text{xz} \| (0.33333333333333, 0.66666666667, 0.166666666667) \}
+1/3, -x+2/3, +z+1/6
| {3^-_00z|(0.3333333333333,0.666666666667,0.66666666667)} | +y-x
+1/3, -x+2/3, +z+2/3
\[ \{\mathbb{m}_2\times\text{z}\| (0.3333333333333,0.66666666667,0.166666666667)\}
+1/3, +x-y+2/3, +z+1/6
\[ \{\m_x2xz\| (0.333333333333,0.66666666667,0.16666666667)\}
                                                            | +y-x
+1/3,+y+2/3,+z+1/6
     {1|(0.66666666667,0.3333333333,0.33333333333)}
                                                              +X
+2/3,+y+1/3,+z+1/3
```

```
+2/3, +x-y+1/3, +z+1/3
+2/3,-x+1/3,+z+5/6
| \{3^- 00z | (0.66666666667, 0.33333333333333, 0.333333333333)\} | +y-x
+2/3, -x+1/3, +z+1/3
| {m_2xxz|(0.6666666667,0.33333333333,0.8333333333)}
+2/3, +x-y+1/3, +z+5/6
+2/3,+y+1/3,+z+5/6
*******
space group: 161:R {'Hall': 'P 3* -2n', 'HM': 'R 3 c:R'}
Crystal system: Trigonal
Setting: R
+x,+y,+z
+z,+x,+y
+y+1/2,+x+1/2,+z+1/2
          Seitz
                                 Jones
    {1|(0.0,0.0,0.0)}
                                +x,+y,+z
 {3^+_xxx|(0.0,0.0,0.0)} |
                               +z,+x,+y
  {m_xxz|(0.5,0.5,0.5)}
                         +y+1/2,+x+1/2,+z+1/2
 {3^-_xxx|(0.0,0.0,0.0)} |
                                +y, +z, +x
  \{m \times y \times | (0.5, 0.5, 0.5)\} + z+1/2, +y+1/2, +x+1/2
  \{m_xyy \mid (0.5, 0.5, 0.5)\}
                        +x+1/2,+z+1/2,+y+1/2
*******
space group: 162 {'Hall': '-P 3 2', 'HM': 'P -3 1 m'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
-y,-x,-z
          Seitz
                             Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                            +X,+Y,+Z
 {3^+_00z|(0.0,0.0,0.0)}
                          -y,+x-y,+z
  \{2_x-x0|(0.0,0.0,0.0)\}
                            -y,-x,-z
 \{3^-00z \mid (0.0,0.0,0.0)\}
                          +y-x,-x,+z
  \{m_2xx0|(0.0,0.0,0.0)\}
                           +x,+x-y,-z
  \{2_{x}2x0|(0.0,0.0,0.0)\}
                           +y-x,+y,-z
    \{-1 \mid (0.0, 0.0, 0.0)\}
                            -x,-y,-z
 \{-3^+,00z|(0.0,0.0,0.0)\} \mid +y,+y-x,-z \mid
  \{m_xxz | (0.0,0.0,0.0)\}
                           +y,+x,+z
 \{-3^-00z \mid (0.0,0.0,0.0)\} \mid +x-y,+x,-z \mid
  \{m_0yz \mid (0.0,0.0,0.0)\}
                          | -x,+y-x,+z |
```

```
{m_x0z|(0.0,0.0,0.0)}
                              | +x-y,-y,+z |
*******
space group: 163 {'Hall': '-P 3 2c', 'HM': 'P -3 1 c'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
-y,-x,-z+1/2
            Seitz
                                     Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{3^+ 00z \mid (0.0,0.0,0.0)\}
                                   -y, +x-y, +z
   \{2_x-x0|(0.0,0.0,0.5)\}
                                  -y,-x,-z+1/2
  \{3^-00z \mid (0.0,0.0,0.0)\}
                                   +y-x,-x,+z
   \{m_2xx0|(0.0,0.0,0.5)\}
                                 +x,+x-y,-z+1/2
   \{2_{x2x0}|(0.0,0.0,0.5)\}
                                +y-x,+y,-z+1/2
      \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{-3^+00z \mid (0.0,0.0,0.0)\}
                                   +y, +y-x, -z
   \{m_xxz | (0.0,0.0,0.5)\}
                                  +y, +x, +z+1/2
  \{-3^-00z \mid (0.0,0.0,0.0)\}
                                   +x-y, +x, -z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y-x,+z+1/2
   \{m_x0z | (0.0,0.0,0.5)\}
                                +x-y,-y,+z+1/2
*******
space group: 164 {'Hall': '-P 3 2"', 'HM': 'P -3 m 1'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
+y,+x,-z
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                  +X,+Y,+Z
  {3^+_00z|(0.0,0.0,0.0)}
                                 -y,+x-y,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                  +y, +x, -z
  \{3^-_00z \mid (0.0,0.0,0.0)\}
                                +y-x,-x,+z
   \{2_0y0|(0.0,0.0,0.0)\}
                                 -x,+y-x,-z
   {2_x00|(0.0,0.0,0.0)}
                                +x-y,-y,-z
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                 -x,-y,-z
  \{-3^+00z \mid (0.0,0.0,0.0)\}
                                +y,+y-x,-z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                  -y,-x,+z
  \{-3^-00z \mid (0.0,0.0,0.0)\}
                                 +x-y, +x, -z
   \{m_2xxz \mid (0.0,0.0,0.0)\}
                                +x,+x-y,+z
   \{m_x2xz \mid (0.0,0.0,0.0)\}
                                +y-x,+y,+z
```

```
*******
space group: 165 {'Hall': '-P 3 2"c', 'HM': 'P -3 c 1'}
Crystal system: Trigonal
+x,+y,+z
-y, +x-y, +z
+y,+x,-z+1/2
            Seitz
                                    Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {3^+_00z|(0.0,0.0,0.0)}
                                  -y, +x-y, +z
  {2_xx0|(0.0,0.0,0.5)}
                                 +y,+x,-z+1/2
 {3^-_00z|(0.0,0.0,0.0)}
                                  +y-x,-x,+z
   {2_0y0|(0.0,0.0,0.5)}
                                -x,+y-x,-z+1/2
   \{2_{x00} | (0.0,0.0,0.5)\}
                                +x-y,-y,-z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                   -x,-y,-z
  \{-3^+00z \mid (0.0,0.0,0.0)\} \mid
                                  +y, +y-x, -z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                                 -y,-x,+z+1/2
  \{-3^-00z \mid (0.0,0.0,0.0)\}
                                  +x-y,+x,-z
   \{m_2xxz \mid (0.0,0.0,0.5)\}
                              +x,+x-y,+z+1/2
   \{m_x2xz \mid (0.0,0.0,0.5)\}
                              | +y-x,+y,+z+1/2 |
*******
space group: 166:H {'Hall': '-R 3 2"', 'HM': 'R -3 m:H'}
Crystal system: Trigonal
Setting: H
+x,+y,+z
-y, +x-y, +z
+y,+x,-z
                               Seitz
Jones
                        \{1 \mid (0.0, 0.0, 0.0)\}
+x,+y,+z
                     {3^+\_00z | (0.0,0.0,0.0)}
-y, +x-y, +z
                      \{2_{xx0} | (0.0,0.0,0.0)\}
+y,+x,-z
                     {3^-_00z|(0.0,0.0,0.0)}
+y-x,-x,+z
                      {2_0y0|(0.0,0.0,0.0)}
-x,+y-x,-z
                      \{2_{x00} | (0.0,0.0,0.0)\}
+x-y,-y,-z
                        \{-1 \mid (0.0, 0.0, 0.0)\}
-x,-y,-z
                     \{-3^+ 00z \mid (0.0,0.0,0.0)\}
```

```
+y, +y-x, -z
                   \{m_x-xz \mid (0.0,0.0,0.0)\}
-y,-x,+z
                  \{-3^-\ 00z \mid (0.0,0.0,0.0)\}
+x-y, +x, -z
                   \{m_2xxz \mid (0.0,0.0,0.0)\}
+x,+x-y,+z
                   \{m_x2xz|(0.0,0.0,0.0)\}
+y-x, +y, +z
     {1|(0.33333333333,0.66666666667,0.66666666667)}
                                                           +X
+1/3,+y+2/3,+z+2/3
{3^+_00z|(0.3333333333333,0.666666666667,0.666666666667)} | -y
+1/3, +x-y+2/3, +z+2/3
   {2_xx0|(0.333333333333,0.66666666667,0.666666666667)}
+1/3, +x+2/3, -z+2/3
{3^-_00z|(0.3333333333333,0.666666666667,0.66666666667)} | +y-x
+1/3, -x+2/3, +z+2/3
   {2_0y0|(0.33333333333,0.66666666667,0.66666666667)}
+1/3,+y-x+2/3,-z+2/3
   {2_x00|(0.333333333333,0.66666666667,0.666666666667)}
                                                         | +x-y
+1/3,-y+2/3,-z+2/3
    \{-1 \mid (0.33333333333333, 0.66666666667, 0.66666666667)\}
                                                           -x
+1/3,-y+2/3,-z+2/3
-3^+00z | (0.333333333333333,0.666666666667,0.666666666667)} | +y
+1/3,+y-x+2/3,-z+2/3
{m_x-xz|(0.333333333333,0.66666666667,0.666666666667)}
+1/3, -x+2/3, +z+2/3
-3^- 00z|(0.33333333333333,0.66666666667,0.666666666667)} | +x-y
+1/3,+x+2/3,-z+2/3
| {m_2xxz|(0.3333333333333,0.66666666667,0.66666666667)} | +x
+1/3, +x-y+2/3, +z+2/3
+1/3,+y+2/3,+z+2/3
     {1|(0.66666666667,0.33333333333,0.333333333333)}
                                                           +x
+2/3,+y+1/3,+z+1/3
  \{3^+, 00z\}(0.6666666666667, 0.333333333333, 0.33333333333)\} \mid -y
+2/3, +x-y+1/3, +z+1/3
   {2_xx0|(0.66666666667,0.33333333333,0.33333333333)}
+2/3,+x+1/3,-z+1/3
  {3^-_00z|(0.66666666667,0.333333333333,0.333333333333)} + y-x
+2/3,-x+1/3,+z+1/3
   {2_0y0|(0.66666666667,0.33333333333,0.33333333333)}
+2/3,+y-x+1/3,-z+1/3
   {2_x00|(0.66666666667,0.33333333333,0.33333333333)}
+2/3,-y+1/3,-z+1/3
    \{-1 \mid (0.666666666667, 0.33333333333, 0.333333333333)\}
+2/3,-y+1/3,-z+1/3
| \{-3^+ 00z | (0.666666666667, 0.333333333333, 0.33333333333)\} | +y
+2/3,+y-x+1/3,-z+1/3
  {m_x-xz|(0.66666666667,0.33333333333,0.33333333333)}
+2/3, -x+1/3, +z+1/3
+2/3,+x+1/3,-z+1/3
  {m 2xxz|(0.66666666667,0.33333333333,0.333333333333)} | +x
```

```
+2/3, +x-y+1/3, +z+1/3
| {m_x2xz|(0.6666666667,0.333333333333,0.33333333333)} | +y-x
+2/3,+y+1/3,+z+1/3
*******
space group: 166:R {'Hall': '-P 3* 2', 'HM': 'R -3 m:R'}
Crystal system: Trigonal
Setting: R
+x,+y,+z
+z,+x,+y
-y,-x,-z
            Seitz
                                 Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
  {3^+_xxx|(0.0,0.0,0.0)}
                              | +z,+x,+y |
  \{2_x-x0\mid (0.0,0.0,0.0)\}
                              |-y,-x,-z|
  {3^-_xxx|(0.0,0.0,0.0)}
                              +y,+z,+x
   \{2_{-}\times 0\times | (0.0,0.0,0.0)\}
                                -z,-y,-x
   \{2_0y-y \mid (0.0,0.0,0.0)\}
                               -x,-z,-y
     \{-1 \mid (0.0, 0.0, 0.0)\}
                              | -x,-y,-z
  \{-3^+xxx|(0.0,0.0,0.0)\} \mid -z,-x,-y \mid
   \{m_xxz | (0.0,0.0,0.0)\}
                                +y,+x,+z
  \{-3^-xxx|(0.0,0.0,0.0)\} \mid -y,-z,-x \mid
   \{m \times y \times | (0.0, 0.0, 0.0)\}
                              +z,+y,+x
   \{m_xyy | (0.0,0.0,0.0)\}
                              | +x,+z,+y |
*******
space group: 167:H {'Hall': '-R 3 2"c', 'HM': 'R -3 c:H'}
Crystal system: Trigonal
Setting: H
+x,+y,+z
-y, +x-y, +z
+y,+x,-z+1/2
                               Seitz
Jones
                        \{1 \mid (0.0, 0.0, 0.0)\}
+x,+y,+z
                     {3^+_00z|(0.0,0.0,0.0)}
-y, +x-y, +z
                      \{2_{xx0} | (0.0, 0.0, 0.5)\}
+y,+x,-z+1/2
                     \{3^- 00z \mid (0.0, 0.0, 0.0)\}
```

```
+y-x,-x,+z
                    {2_0y0|(0.0,0.0,0.5)}
x,+y-x,-z+1/2
                    {2 x00|(0.0,0.0,0.5)}
+x-y,-y,-z+1/2
                      \{-1 \mid (0.0, 0.0, 0.0)\}
-x,-y,-z
                   \{-3^+_00z \mid (0.0,0.0,0.0)\}
+y,+y-x,-z
                   \{m \times -xz \mid (0.0,0.0,0.5)\}
y,-x,+z+1/2
                   {-3^-_00z|(0.0,0.0,0.0)}
+x-y, +x, -z
                    {m_2xxz|(0.0,0.0,0.5)}
+x,+x-y,+z+1/2
                    {m_x2xz|(0.0,0.0,0.5)}
+y-x, +y, +z+1/2
      {1|(0.33333333333,0.66666666667,0.66666666667)}
+1/3,+y+2/3,+z+2/3
| {3^+_00z|(0.333333333333,0.66666666667,0.66666666667)} | -v
+1/3, +x-y+2/3, +z+2/3
   {2_xx0|(0.333333333333,0.66666666667,0.16666666667)}
+1/3,+x+2/3,-z+1/6
{3^-_00z|(0.3333333333333,0.66666666667,0.666666666667)} | +y-x
+1/3, -x+2/3, +z+2/3
    {2_0y0|(0.333333333333,0.66666666667,0.16666666667)}
+1/3,+y-x+2/3,-z+1/6
    {2 x00|(0.333333333333,0.66666666667,0.16666666667)}
                                                            | +x-y
+1/3,-y+2/3,-z+1/6
     {-1|(0.333333333333,0.66666666667,0.66666666667)}
                                                              -x
+1/3,-y+2/3,-z+2/3
| {-3^+_00z|(0.3333333333333,0.66666666667,0.66666666667)} | +y
+1/3,+y-x+2/3,-z+2/3
   \{m \times -xz \mid (0.333333333333333, 0.666666666667, 0.166666666667)\}
+1/3, -x+2/3, +z+1/6
-3^- 00z|(0.33333333333333,0.66666666667,0.666666666667)} | +x-y
+1/3,+x+2/3,-z+2/3
+1/3, +x-y+2/3, +z+1/6
  {m_x2xz|(0.333333333333,0.66666666667,0.16666666667)}
                                                            | +y-x
+1/3,+y+2/3,+z+1/6
      {1|(0.66666666667,0.33333333333,0.33333333333)}
                                                              +X
+2/3,+y+1/3,+z+1/3
  {3^+_00z|(0.66666666667,0.33333333333,0.33333333333)} | -y
+2/3, +x-y+1/3, +z+1/3
    {2_xx0|(0.66666666667,0.33333333333,0.8333333333)}
+2/3,+x+1/3,-z+5/6
   {3^- 00z \mid (0.666666666667, 0.33333333333333333333333333333)} \mid +y-x
+2/3,-x+1/3,+z+1/3
    {2_0y0|(0.66666666667,0.33333333333,0.83333333333)}
+2/3,+y-x+1/3,-z+5/6
    {2_x00|(0.66666666667,0.33333333333,0.8333333333)}
                                                            | +x-y
+2/3,-y+1/3,-z+5/6
    \{-1 \mid (0.666666666667, 0.33333333333, 0.33333333333)\}
                                                              -x
```

```
+2/3,-y+1/3,-z+1/3
| {-3^+_00z|(0.66666666667,0.33333333333,0.33333333333)} | +y
+2/3,+y-x+1/3,-z+1/3
\{m \times x = xz \mid (0.66666666667, 0.33333333333333, 0.833333333333)\} = -y
+2/3,-x+1/3,+z+5/6
-3^- 00z \mid (0.666666666667, 0.333333333333, 0.33333333333)\} \mid +x-y
+2/3,+x+1/3,-z+1/3
[ \{\text{m_2xxz} \| (0.666666666667, 0.333333333333, 0.83333333333)}\]
+2/3, +x-y+1/3, +z+5/6
| {m x2xz|(0.6666666667,0.33333333333,0.83333333333)} | +y-x
+2/3,+y+1/3,+z+5/6
. . . . . . . . . . . . . . . . . . . .
*******
space group: 167:R {'Hall': '-P 3* 2n', 'HM': 'R -3 c:R'}
Crystal system: Trigonal
Setting: R
+x,+y,+z
+z,+x,+y
-y+1/2, -x+1/2, -z+1/2
  . . . . . . . . . . . . . . . . . .
            Seitz
                                        Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
 {3^+_xxx|(0.0,0.0,0.0)}
                                       +z,+x,+y
  \{2 \times -\times 0 \mid (0.5, 0.5, 0.5)\}
                                -y+1/2,-x+1/2,-z+1/2
  {3^-_xxx|(0.0,0.0,0.0)}
                                       +y,+z,+x
   \{2_{-x0x} | (0.5, 0.5, 0.5)\}
                                -z+1/2,-y+1/2,-x+1/2
   \{2_0y-y\mid (0.5,0.5,0.5)\}
                               -x+1/2, -z+1/2, -y+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                      -x,-y,-z
  \{-3^+ \times \times \times | (0.0, 0.0, 0.0) \} |
                                       -z,-x,-y
   \{m \times xz \mid (0.5, 0.5, 0.5)\}
                              +y+1/2,+x+1/2,+z+1/2
  \{-3^-xxx \mid (0.0,0.0,0.0)\} \mid
                                       -y, -z, -x
   \{m_xyx | (0.5, 0.5, 0.5)\}
                              +z+1/2,+y+1/2,+x+1/2
                              | +x+1/2,+z+1/2,+y+1/2
   \{m_xyy | (0.5, 0.5, 0.5)\}
*******
space group: 168 {'Hall': 'P 6', 'HM': 'P 6'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z
            Seitz
                                 Jones
     {1|(0.0,0.0,0.0)}
                             +x,+y,+z
| {6^+_00z|(0.0,0.0,0.0)} | +x-y,+x,+z |
| {3^+_00z|(0.0,0.0,0.0)} | -y,+x-y,+z |
```

 $\{2_00z \mid (0.0,0.0,0.0)\} \mid -x,-y,+z$

```
\{3^-_00z \mid (0.0,0.0,0.0)\} \mid +y-x,-x,+z \mid
  \{6^{-}00z \mid (0.0,0.0,0.0)\} \mid +y,+y-x,+z \mid
*******
space group: 169 {'Hall': ' P 61', 'HM': 'P 61'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+1/6
                 Seitz
                                              Jones
          \{1 \mid (0.0, 0.0, 0.0)\}
                                            +x,+y,+z
  {6^+_00z|(0.0,0.0,0.166666666667)}
                                       | +x-y,+x,+z+1/6
  {3^+_00z|(0.0,0.0,0.333333333333)}
                                         -y, +x-y, +z+1/3
        {2_00z|(0.0,0.0,0.5)}
                                          -x,-y,+z+1/2
  {3^-_00z|(0.0,0.0,0.666666666667)}
                                        +y-x,-x,+z+2/3
 \{6^{-}00z \mid (0.0,0.0,0.833333333333)\} \mid +y,+y-x,+z+5/6
*******
space group: 170 {'Hall': ' P 65', 'HM': 'P 65'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+5/6
                 Seitz
                                              Jones
          \{1 \mid (0.0, 0.0, 0.0)\}
                                            +x,+y,+z
 \{6^+ 00z \mid (0.0,0.0,0.833333333333)\}
                                         +x-y, +x, +z+5/6
  {3^+_00z|(0.0,0.0,0.666666666667)}
                                         -y, +x-y, +z+2/3
        {2_00z|(0.0,0.0,0.5)}
                                          -x,-y,+z+1/2
  {3^-_00z|(0.0,0.0,0.3333333333333)}
                                       | +y-x,-x,+z+1/3
  \{6^{-}00z \mid (0.0,0.0,0.16666666667)\} \mid +y,+y-x,+z+1/6
*******
space group: 171 {'Hall': ' P 62', 'HM': 'P 62'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+1/3
                 Seitz
                                              Jones
          \{1 \mid (0.0, 0.0, 0.0)\}
                                            +x,+y,+z
 \{6^+_{00z}|(0.0,0.0,0.333333333333)\} | +x-y,+x,+z+1/3
  {3^+_00z|(0.0,0.0,0.666666666667)}
                                         -y, +x-y, +z+2/3
        {2 00z|(0.0,0.0,0.0)}
                                            -x,-y,+z
```

```
| {3^-_00z|(0.0,0.0,0.333333333333)} | +y-x,-x,+z+1/3 |
 \{6^{-}00z \mid (0.0,0.0,0.666666666667)\} \mid +y,+y-x,+z+2/3 \mid
*******
space group: 172 {'Hall': ' P 64', 'HM': 'P 64'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+2/3
                 Seitz
                                              Jones
          \{1 \mid (0.0, 0.0, 0.0)\}
                                            +x,+y,+z
  {6^+_00z|(0.0,0.0,0.666666666667)}
                                       +x-y,+x,+z+2/3
  {3^+_00z|(0.0,0.0,0.333333333333)}
                                         -y, +x-y, +z+1/3
        {2_00z|(0.0,0.0,0.0)}
                                           -x,-y,+z
  {3^-_00z|(0.0,0.0,0.666666666667)}
                                        +y-x,-x,+z+2/3
 \{6^-_00z \mid (0.0,0.0,0.333333333333)\} \mid +y,+y-x,+z+1/3 \mid
*******
space group: 173 {'Hall': ' P 6c', 'HM': 'P 63'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+1/2
  . . . . . . . . . . . . . . . . . .
           Seitz
                                  Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                +x,+y,+z
 \{6^+_00z \mid (0.0,0.0,0.5)\} \mid +x-y,+x,+z+1/2
  {3^+_00z|(0.0,0.0,0.0)}
                              -y,+x-y,+z
   {2_00z|(0.0,0.0,0.5)}
                              -x,-y,+z+1/2
  \{3^-00z \mid (0.0,0.0,0.0)\} \mid
                              +y-x,-x,+z
  \{6^{-}00z \mid (0.0,0.0,0.5)\} \mid +y,+y-x,+z+1/2
*******
space group: 174 {'Hall': ' P -6', 'HM': 'P -6'}
Crystal system: Hexagonal
+x,+y,+z
+y-x,-x,-z
           Seitz
                                 Jones
     {1|(0.0,0.0,0.0)}
                              +x,+y,+z
 \{-6^+_{00z} \mid (0.0,0.0,0.0)\} \mid +y-x,-x,-z \mid
 {3^+_00z|(0.0,0.0,0.0)}
                              -y, +x-y, +z
   {m_xy0|(0.0,0.0,0.0)}
                               +x,+y,-z
```

```
| \{3^{-}00z | (0.0,0.0,0.0)\} | +y-x,-x,+z |
 \{-6^{-}00z|(0.0,0.0,0.0)\} \mid -y,+x-y,-z \mid
*******
space group: 175 {'Hall': ' -P 6', 'HM': 'P 6/m'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z
           Seitz
                                Jones
    {1|(0.0,0.0,0.0)}
                             +x,+y,+z
  \{6^+ 00z \mid (0.0, 0.0, 0.0)\}
                            +x-y, +x, +z
  {3^+_00z|(0.0,0.0,0.0)}
                            | -y, +x-y, +z |
   {2_00z|(0.0,0.0,0.0)}
                            -x,-y,+z
```

space group: 176 {'Hall': '-P 6c', 'HM': 'P 63/m'}

Crystal system: Hexagonal

+x,+y,+z

+x-y, +x, +z+1/2

.

Seitz	Jones
{1 (0.0,0.0,0.0)}	+x,+y,+z
{6^+_00z (0.0,0.0,0.5)}	+x-y,+x,+z+1/2
{3^+_00z (0.0,0.0,0.0)}	-y,+x-y,+z
{2_00z (0.0,0.0,0.5)}	-x,-y,+z+1/2
{3^00z (0.0,0.0,0.0)}	+y-x,-x,+z
{6^00z (0.0,0.0,0.0)}	+y,+y-x,+z+1/2
{-1 (0.0,0.0,0.0,0.5)}	-x,-y,-z
{-6^+_00z (0.0,0.0,0.0)}	+y-x,-x,-z+1/2
{-3^+_00z (0.0,0.0,0.0)}	+y,+y-x,-z
{m_xy0 (0.0,0.0,0.0,0.5)}	+x,+y,-z+1/2
{-3^00z (0.0,0.0,0.0,0.5)}	+x-y,+x,-z
{-6^00z (0.0,0.0,0.0,0.5)}	-y,+x-y,-z+1/2

```
space group: 177 {'Hall': 'P 6 2', 'HM': 'P 6 2 2'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z
-y,-x,-z
            Seitz
                                Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                               +X,+Y,+Z
  \{6^+00z|(0.0,0.0,0.0)\}
                              +x-y, +x, +z
   \{2_x-x0\mid(0.0,0.0,0.0)\}
                               -y,-x,-z
  {3^+_00z|(0.0,0.0,0.0)}
                              -y, +x-y, +z
   \{2_{x00}|(0.0,0.0,0.0)\}
                             +x-y,-y,-z
   {2_00z|(0.0,0.0,0.0)}
                               -x,-y,+z
   \{m \ 2xx0 | (0.0,0.0,0.0)\}
                              +x,+x-y,-z
  \{3^-00z \mid (0.0,0.0,0.0)\} \mid
                              +y-x,-x,+z
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                               +y, +x, -z
  \{6^-00z \mid (0.0,0.0,0.0)\}
                              +y,+y-x,+z
   \{2_{x}2x0|(0.0,0.0,0.0)\}
                            +y-x,+y,-z
   {2_0y0|(0.0,0.0,0.0)}
                            -x,+y-x,-z
*******
space group: 178 {'Hall': ' P 61 2 (0,0,-1)', 'HM': 'P 61 2 2'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+1/6
-y,-x,-z+-1/6
  . . . . . . . . . . . . . . . . .
                 Seitz
                                               Jones
           {1|(0.0,0.0,0.0)}
                                              +x,+y,+z
  \{6^+ 00z \mid (0.0, 0.0, 0.166666666667)\}
                                          +x-y, +x, +z+1/6
  \{2_x-x0\mid(0.0,0.0,0.8333333333333)\}
                                           -y,-x,-z+5/6
  {3^+_00z|(0.0,0.0,0.333333333333)}
                                          -y, +x-y, +z+1/3
        {2_x00|(0.0,0.0,0.0)}
                                            +x-y,-y,-z
        {2_00z|(0.0,0.0,0.5)}
                                           -x,-y,+z+1/2
  \{m_2xx0 \mid (0.0,0.0,0.166666666667)\}
                                          +x,+x-y,-z+1/6
  {3^-_00z|(0.0,0.0,0.666666666667)}
                                          +y-x,-x,+z+2/3
   {2_xx0|(0.0,0.0,0.333333333333)}
                                           +y,+x,-z+1/3
  {6^-_00z|(0.0,0.0,0.8333333333333)}
                                          +y, +y-x, +z+5/6
        \{2_{x}2x0|(0.0,0.0,0.5)\}
                                          +y-x, +y, -z+1/2
   {2_0y0|(0.0,0.0,0.666666666667)}
                                          -x,+y-x,-z+2/3
*******
space group: 179 {'Hall': ' P 65 2 (0,0,1)', 'HM': 'P 65 2 2'}
Crystal system: Hexagonal
+X,+Y,+Z
+x-y, +x, +z+5/6
```

```
-y, -x, -z+1/6
                 Seitz
                                                Jones
           {1|(0.0,0.0,0.0)}
                                               +x,+y,+z
  {6^+_00z|(0.0,0.0,0.833333333333)}
                                           +x-y, +x, +z+5/6
  \{2_x-x0 \mid (0.0,0.0,0.166666666667)\}
                                            -y,-x,-z+1/6
  {3^+_00z|(0.0,0.0,0.666666666667)}
                                           -y, +x-y, +z+2/3
        \{2_{x00} | (0.0,0.0,0.0)\}
                                             +x-y,-y,-z
        {2_00z|(0.0,0.0,0.5)}
                                            -x,-y,+z+1/2
  {m_2xx0|(0.0,0.0,0.833333333333)}
                                           +x,+x-y,-z+5/6
  {3^-_00z|(0.0,0.0,0.333333333333)}
                                           +y-x,-x,+z+1/3
   {2_xx0|(0.0,0.0,0.666666666667)}
                                            +y,+x,-z+2/3
  {6^-_00z|(0.0,0.0,0.166666666667)}
                                           +y, +y-x, +z+1/6
        \{2 \times 2 \times 0 \mid (0.0, 0.0, 0.5)\}
                                           +y-x, +y, -z+1/2
```

```
*******
```

space group: 180 {'Hall': ' P 62 2c (0,0,1)', 'HM': 'P 62 2 2'}

-x,+y-x,-z+1/3

Crystal system: Hexagonal

{2_0y0|(0.0,0.0,0.333333333333)}

+x,+y,+z

+x-y, +x, +z+1/3

-y,-x,-z+2/3

```
Seitz
                                            Jones
        {1|(0.0,0.0,0.0)}
                                           +X,+Y,+Z
{6^+_00z|(0.0,0.0,0.3333333333333)}
                                        +x-y, +x, +z+1/3
\{2_x-x0\mid (0.0,0.0,0.666666666667)\}
                                         -y, -x, -z+2/3
\{3^+ 00z \mid (0.0,0.0,0.666666666667)\}
                                        -y, +x-y, +z+2/3
      {2_x00|(0.0,0.0,0.0)}
                                          +x-y,-y,-z
      {2_00z|(0.0,0.0,0.0)}
                                           -x,-y,+z
{m_2xx0|(0.0,0.0,0.3333333333333)}
                                        +x,+x-y,-z+1/3
{3^-_00z|(0.0,0.0,0.333333333333)}
                                        +y-x, -x, +z+1/3
 {2_xx0|(0.0,0.0,0.666666666667)}
                                         +y,+x,-z+2/3
{6^-_00z|(0.0,0.0,0.666666666667)}
                                        +y,+y-x,+z+2/3
      \{2_{x}2x0|(0.0,0.0,1.0)\}
                                        +y-x, +y, -z+1/1
 {2_0y0|(0.0,0.0,0.333333333333)}
                                       -x,+y-x,-z+1/3
```

.

```
*******
```

space group: 181 {'Hall': ' P 64 2c (0,0,-1)', 'HM': 'P 64 2 2'}

Crystal system: Hexagonal

+x,+y,+z

+x-y, +x, +z+2/3

-y,-x,-z+1/3

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                               +x,+y,+z
  {6^+_00z|(0.0,0.0,0.666666666667)}
                                           +x-y, +x, +z+2/3
  \{2 \times x - x0 \mid (0.0, 0.0, 0.33333333333333)\}
                                            -y, -x, -z+1/3
  {3^+_00z|(0.0,0.0,0.333333333333)}
                                           -y, +x-y, +z+1/3
         {2_x00|(0.0,0.0,0.0)}
                                              +x-y,-y,-z
         {2_00z|(0.0,0.0,0.0)}
                                               -x,-y,+z
  {m_2xx0|(0.0,0.0,0.66666666667)}
                                           +x,+x-y,-z+2/3
  {3^-_00z|(0.0,0.0,0.666666666667)}
                                           +y-x,-x,+z+2/3
   {2 xx0|(0.0,0.0,0.333333333333)}
                                            +y,+x,-z+1/3
  {6^-_00z|(0.0,0.0,0.333333333333)}
                                           +y,+y-x,+z+1/3
         {2_x2x0|(0.0,0.0,1.0)}
                                           +y-x, +y, -z+1/1
   {2_0y0|(0.0,0.0,0.666666666667)}
                                           -x,+y-x,-z+2/3
******
space group: 182 {'Hall': ' P 6c 2c', 'HM': 'P 63 2 2'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+1/2
-y,-x,-z+1/2
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{6^+_{00z} | (0.0,0.0,0.5)\}
                               +x-y, +x, +z+1/2
   \{2 \times -\times 0 \mid (0.0, 0.0, 0.5)\}
                                -y,-x,-z+1/2
  {3^+_00z|(0.0,0.0,0.0)}
                                 -y, +x-y, +z
   \{2_{\times}00 \mid (0.0,0.0,0.0)\}
                                 +x-y,-y,-z
   \{2\_00z \mid (0.0,0.0,0.5)\}
                                -x,-y,+z+1/2
   \{m \ 2xx0 | (0.0,0.0,0.5)\}
                               +x,+x-y,-z+1/2
  \{3^- 00z \mid (0.0,0.0,0.0)\}
                                 +y-x,-x,+z
   {2_xx0|(0.0,0.0,0.0)}
                                  +y,+x,-z
  \{6^{-}00z \mid (0.0,0.0,0.5)\}
                               +y,+y-x,+z+1/2
   \{2_{x}2x0|(0.0,0.0,0.5)\}
                               +y-x, +y, -z+1/2
   {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y-x,-z
*******
space group: 183 {'Hall': 'P 6 -2', 'HM': 'P 6 m m'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z
+y, +x, +z
            Seitz
                                 Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
```

+x,+y,+z

+y, +x, +z

 $\{6^+,00z\mid (0.0,0.0,0.0)\} \mid +x-y,+x,+z$

 $\{m \times xz \mid (0.0,0.0,0.0)\}$

```
{3^+_00z|(0.0,0.0,0.0)} | -y,+x-y,+z
   \{m_x2xz \mid (0.0,0.0,0.0)\} \mid +y-x,+y,+z
   {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
   \{m \ 0 \ \forall z \ | \ (0.0, 0.0, 0.0) \}
                               -x,+y-x,+z
  \{3^-_00z \mid (0.0,0.0,0.0)\}
                               +y-x,-x,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                 -y,-x,+z
  {6^-_00z|(0.0,0.0,0.0)}
                               +y,+y-x,+z
   \{m_x0z \mid (0.0,0.0,0.0)\}
                               +x-y,-y,+z
   \{m_2xxz \mid (0.0,0.0,0.0)\} \mid +x,+x-y,+z
*******
space group: 184 {'Hall': 'P 6 -2c', 'HM': 'P 6 c c'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z
+y,+x,+z+1/2
            Seitz
                                    Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  {6^+_00z|(0.0,0.0,0.0)} |
                                 +x-y, +x, +z
   \{m_xxz | (0.0,0.0,0.5)\}
                                 +y,+x,+z+1/2
  {3^+_00z|(0.0,0.0,0.0)}
                                 -y,+x-y,+z
   \{m_x2xz \mid (0.0,0.0,0.5)\}
                                +y-x, +y, +z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
   \{m \ 0yz | (0.0,0.0,0.5)\}
                               -x,+y-x,+z+1/2
  {3^-_00z|(0.0,0.0,0.0)}
                                 +y-x,-x,+z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                                 -y,-x,+z+1/2
  \{6^{-}00z \mid (0.0,0.0,0.0)\}
                                  +y, +y-x, +z
   \{m_x0z|(0.0,0.0,0.5)\}
                              | +x-y,-y,+z+1/2
   \{m_2xxz \mid (0.0,0.0,0.5)\} \mid +x,+x-y,+z+1/2
*******
space group: 185 {'Hall': ' P 6c -2', 'HM': 'P 63 c m'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+1/2
+y,+x,+z
            Seitz
                                    Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                   +X,+Y,+Z
  \{6^+_{00z} | (0.0,0.0,0.5)\}
                               +x-y, +x, +z+1/2
   \{m_x \times z \mid (0.0, 0.0, 0.0)\}
                                   +y,+x,+z
  {3^+_00z|(0.0,0.0,0.0)}
                                  -y, +x-y, +z
   \{m_x2xz|(0.0,0.0,0.5)\}\ |\ +y-x,+y,+z+1/2
   {2_00z|(0.0,0.0,0.5)}
                                 -x,-y,+z+1/2
   \{m \ 0 \ \forall z \ | \ (0.0, 0.0, 0.0) \}
                                  -x,+y-x,+z
```

```
{3^-_00z|(0.0,0.0,0.0)} |
                                  +y-x,-x,+z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                                 -y,-x,+z+1/2
  \{6^-_00z \mid (0.0,0.0,0.5)\}
                                +y, +y-x, +z+1/2
   \{m_x0z \mid (0.0,0.0,0.0)\}
                                  +x-y,-y,+z
   \{m \ 2xxz | (0.0,0.0,0.5)\} \mid
                               +x,+x-y,+z+1/2
*******
space group: 186 {'Hall': ' P 6c -2c', 'HM': 'P 63 m c'}
Crystal system: Hexagonal
+X,+Y,+Z
+x-y, +x, +z+1/2
+y,+x,+z+1/2
            Seitz
                                    Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                   +x,+y,+z
  \{6^+_{00z} | (0.0,0.0,0.5)\}
                                +x-y, +x, +z+1/2
   \{m_x \times z \mid (0.0, 0.0, 0.5)\}
                                 +y,+x,+z+1/2
  {3^+_00z|(0.0,0.0,0.0)}
                                  -y, +x-y, +z
   \{m_x2xz \mid (0.0,0.0,0.0)\}
                                  +y-x, +y, +z
   {2_00z|(0.0,0.0,0.5)}
                                 -x,-y,+z+1/2
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                -x,+y-x,+z+1/2
  {3^-_00z|(0.0,0.0,0.0)}
                                  +y-x,-x,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                   -y,-x,+z
  \{6^-_00z \mid (0.0,0.0,0.5)\}
                                +y, +y-x, +z+1/2
   \{m \times 0z \mid (0.0, 0.0, 0.5)\}
                                +x-y,-y,+z+1/2
   \{m_2xxz \mid (0.0,0.0,0.0)\}
                                  +x,+x-y,+z
*******
space group: 187 {'Hall': ' P -6 2', 'HM': 'P -6 m 2'}
Crystal system: Hexagonal
+x,+y,+z
+y-x,-x,-z
-y,-x,-z
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                  +X,+Y,+Z
  \{-6^+,00z \mid (0.0,0.0,0.0)\} \mid
                                 +y-x,-x,-z
   \{2_x-x0\mid(0.0,0.0,0.0)\}
                                  -y,-x,-z
  {3^+_00z|(0.0,0.0,0.0)}
                                 -y, +x-y, +z
   \{m_x2xz \mid (0.0,0.0,0.0)\}
                                 +y-x, +y, +z
   \{m_xy0|(0.0,0.0,0.0)\}
                                  +x,+y,-z
   {m_2xx0|(0.0,0.0,0.0)}
                                 +x,+x-y,-z
  {3^-_00z|(0.0,0.0,0.0)}
                                 +y-x,-x,+z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                  -y,-x,+z
  \{-6^-00z \mid (0.0,0.0,0.0)\}
                                 -y, +x-y, -z
   \{2_{x}2x0|(0.0,0.0,0.0)\}
                                +y-x,+y,-z
```

```
\{m_2xxz|(0.0,0.0,0.0)\} +x,+x-y,+z 
*******
space group: 188 {'Hall': ' P -6c 2', 'HM': 'P -6 c 2'}
Crystal system: Hexagonal
+x,+y,+z
+y-x,-x,-z+1/2
-y,-x,-z
            Seitz
                                     Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{-6^+ 00z \mid (0.0,0.0,0.5)\} \mid
                                +y-x,-x,-z+1/2
   \{2_x-x0\mid (0.0,0.0,0.0)\}
                                    -y,-x,-z
                                   -y, +x-y, +z
  {3^+_00z|(0.0,0.0,0.0)}
   \{m_x2xz|(0.0,0.0,0.5)\}
                                +y-x, +y, +z+1/2
   \{m_xy0 | (0.0,0.0,0.5)\}
                                 +x,+y,-z+1/2
   \{m_2xx0 \mid (0.0,0.0,0.0)\}
                                  +x,+x-y,-z
  {3^-_00z|(0.0,0.0,0.0)}
                                  +y-x,-x,+z
   \{m_x-xz \mid (0.0,0.0,0.5)\}
                                 -y,-x,+z+1/2
  \{-6^-_00z \mid (0.0,0.0,0.5)\}
                                -y, +x-y, -z+1/2
   \{2_{x2x0} | (0.0,0.0,0.0)\}
                                  +y-x, +y, -z
   \{m_2xxz \mid (0.0,0.0,0.5)\}
                                +x, +x-y, +z+1/2
*******
space group: 189 {'Hall': ' P -6 -2', 'HM': 'P -6 2 m'}
Crystal system: Hexagonal
+x,+y,+z
+y-x,-x,-z
+y,+x,+z
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                 +X,+Y,+Z
  \{-6^+00z \mid (0.0,0.0,0.0)\}
                                +y-x,-x,-z
   \{m_xxz | (0.0,0.0,0.0)\}
                                 +y, +x, +z
  {3^+_00z|(0.0,0.0,0.0)}
                                -y, +x-y, +z
   \{2_{x00}|(0.0,0.0,0.0)\}
                                +x-y,-y,-z
   \{m_xy0|(0.0,0.0,0.0)\}
                                 +x,+y,-z
   \{m_0yz \mid (0.0,0.0,0.0)\}
                                -x,+y-x,+z
  \{3^-00z \mid (0.0,0.0,0.0)\}
                                +y-x,-x,+z
   \{2_{x} \times 0 \mid (0.0, 0.0, 0.0)\}
                                 +y, +x, -z
  \{-6^-00z \mid (0.0,0.0,0.0)\}
                                -y, +x-y, -z
   \{m_x0z | (0.0,0.0,0.0)\}
                                +x-y,-y,+z
   {2_0y0|(0.0,0.0,0.0)}
                                -x,+y-x,-z
```

```
*******
space group: 190 {'Hall': ' P -6c -2c', 'HM': 'P -6 2 c'}
Crystal system: Hexagonal
+x,+y,+z
+y-x,-x,-z+1/2
+y,+x,+z+1/2
            Seitz
                                     Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{-6^+_00z \mid (0.0,0.0,0.5)\}
                                 +y-x,-x,-z+1/2
   \{m_xz|(0.0,0.0,0.5)\}
                                  +y,+x,+z+1/2
  {3^+_00z|(0.0,0.0,0.0)}
                                   -y, +x-y, +z
   \{2_{x00} | (0.0,0.0,0.0)\}
                                   +x-y,-y,-z
   \{m_xy0|(0.0,0.0,0.5)\}
                                  +x,+y,-z+1/2
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                 -x,+y-x,+z+1/2
  \{3^-00z \mid (0.0,0.0,0.0)\}
                                   +y-x,-x,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                    +y,+x,-z
  \{-6^-00z \mid (0.0,0.0,0.5)\}
                                 -y, +x-y, -z+1/2
   \{m_x0z | (0.0,0.0,0.5)\}
                                 +x-y,-y,+z+1/2
   {2_0y0|(0.0,0.0,0.0)}
                                   -x,+y-x,-z
*******
space group: 191 {'Hall': ' -P 6 2', 'HM': 'P 6/m m m'}
Crystal system: Hexagonal
+X,+Y,+Z
+x-y, +x, +z
-y,-x,-z
            Seitz
                                   Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                  +x,+y,+z
  \{6^+_{00z} | (0.0,0.0,0.0)\}
                                 +x-y,+x,+z
   \{2_x-x0\mid(0.0,0.0,0.0)\}
                                  -y,-x,-z
  {3^+_00z|(0.0,0.0,0.0)}
                                 -y, +x-y, +z
   \{2_{x00} | (0.0,0.0,0.0)\}
                                 +x-y,-y,-z
   {2_00z|(0.0,0.0,0.0)}
                                  -x,-y,+z
   {m_2xx0|(0.0,0.0,0.0)}
                                 +x,+x-y,-z
  \{3^-_00z \mid (0.0,0.0,0.0)\}
                                 +y-x,-x,+z
   \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                  +y, +x, -z
  {6^-_00z|(0.0,0.0,0.0)}
                                 +y, +y-x, +z
   \{2_{x2x0}|(0.0,0.0,0.0)\}
                                 +y-x, +y, -z
   {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y-x,-z
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                  -x,-y,-z
  \{-6^+00z \mid (0.0,0.0,0.0)\}
                                 +y-x,-x,-z
   {m_xxz|(0.0,0.0,0.0)}
                                  +y,+x,+z
  \{-3^+,00z \mid (0.0,0.0,0.0)\}
                                 +y,+y-x,-z
   \{m_x2xz \mid (0.0,0.0,0.0)\}
                                 +y-x, +y, +z
   \{m_xy0 | (0.0,0.0,0.0)\}
                                  +x,+y,-z
   \{m \ 0 \ \forall z \ | \ (0.0, 0.0, 0.0) \}
                                 -x,+y-x,+z
```

```
\{-3^{-}00z|(0.0,0.0,0.0)\} \mid +x-y,+x,-z \mid
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                  -y,-x,+z
  \{-6^-00z \mid (0.0,0.0,0.0)\}
                                 -y,+x-y,-z
   \{m \times 0z \mid (0.0, 0.0, 0.0)\}
                                 +x-y,-y,+z
   \{m \ 2xxz | (0.0,0.0,0.0)\}
                                +x,+x-y,+z
*******
space group: 192 {'Hall': ' -P 6 2c', 'HM': 'P 6/m c c'}
Crystal system: Hexagonal
+X,+Y,+Z
+x-y, +x, +z
-y,-x,-z+1/2
            Seitz
                                      Jones
     \{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
  \{6^+_{00z} | (0.0,0.0,0.0)\}
                                   +x-y, +x, +z
   \{2_x-x0|(0.0,0.0,0.5)\}
                                  -y,-x,-z+1/2
  {3^+_00z|(0.0,0.0,0.0)}
                                   -y, +x-y, +z
   \{2_{x00} | (0.0,0.0,0.5)\}
                                 +x-y,-y,-z+1/2
   {2_00z|(0.0,0.0,0.0)}
                                    -x,-y,+z
   \{m_2xx0|(0.0,0.0,0.5)\}
                                 +x,+x-y,-z+1/2
  {3^-_00z|(0.0,0.0,0.0)}
                                   +y-x,-x,+z
   {2_xx0|(0.0,0.0,0.5)}
                                  +y,+x,-z+1/2
  \{6^-_00z \mid (0.0,0.0,0.0)\}
                                   +y, +y-x, +z
   \{2 \times 2 \times 0 \mid (0.0, 0.0, 0.5)\}
                                 +y-x,+y,-z+1/2
   {2_0y0|(0.0,0.0,0.5)}
                                 -x,+y-x,-z+1/2
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
  \{-6^+,00z \mid (0.0,0.0,0.0)\}
                                   +y-x,-x,-z
                                  +y,+x,+z+1/2
   \{m_xxz | (0.0,0.0,0.5)\}
  \{-3^+ 00z \mid (0.0,0.0,0.0)\}
                                   +y, +y-x, -z
                                 +y-x, +y, +z+1/2
   \{m_x2xz \mid (0.0,0.0,0.5)\}
   \{m_xy0 | (0.0,0.0,0.0)\}
                                    +x,+y,-z
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                 -x,+y-x,+z+1/2
  \{-3^-_00z \mid (0.0,0.0,0.0)\}
                                   +x-y, +x, -z
   \{m_x-xz\mid (0.0,0.0,0.5)\}
                                  -y,-x,+z+1/2
  \{-6^{-}00z \mid (0.0,0.0,0.0)\}
                                   -y, +x-y, -z
   \{m_x0z \mid (0.0,0.0,0.5)\}
                                 +x-y,-y,+z+1/2
   \{m_2xxz \mid (0.0,0.0,0.5)\}
                                 +x, +x-y, +z+1/2
*******
space group: 193 {'Hall': '-P 6c 2', 'HM': 'P 63/m c m'}
Crystal system: Hexagonal
+x,+y,+z
+x-y, +x, +z+1/2
-y,-x,-z
            Seitz
                                      Jones
```

```
\{1 \mid (0.0, 0.0, 0.0)\}
                                    +x,+y,+z
\{6^+_00z \mid (0.0,0.0,0.5)\}
                                +x-y, +x, +z+1/2
 \{2_x-x0 \mid (0.0,0.0,0.0)\}
                                    -y,-x,-z
{3^+_00z|(0.0,0.0,0.0)}
                                   -y, +x-y, +z
 {2_x00|(0.0,0.0,0.5)}
                                +x-y,-y,-z+1/2
 {2_00z|(0.0,0.0,0.5)}
                                 -x,-y,+z+1/2
 \{m_2xx0|(0.0,0.0,0.0)\}
                                   +x,+x-y,-z
\{3^{-}00z \mid (0.0,0.0,0.0)\}
                                   +y-x,-x,+z
 \{2_x \times 0 \mid (0.0, 0.0, 0.5)\}
                                  +y,+x,-z+1/2
\{6^-00z \mid (0.0,0.0,0.5)\}
                                +y,+y-x,+z+1/2
 \{2_{x}2x0|(0.0,0.0,0.0)\}
                                   +y-x, +y, -z
 {2_0y0|(0.0,0.0,0.5)}
                                -x,+y-x,-z+1/2
   \{-1 \mid (0.0, 0.0, 0.0)\}
                                    -x,-y,-z
\{-6^+,00^-,0.0,0.0,0.5\}
                                +y-x,-x,-z+1/2
 \{m_x \times z \mid (0.0, 0.0, 0.0)\}
                                    +y,+x,+z
\{-3^+_00z \mid (0.0,0.0,0.0)\}
                                   +y,+y-x,-z
 \{m_x2xz|(0.0,0.0,0.5)\}
                                +y-x, +y, +z+1/2
 \{m_xy0|(0.0,0.0,0.5)\}
                                  +x,+y,-z+1/2
 \{m_0yz \mid (0.0,0.0,0.0)\}
                                   -x,+y-x,+z
\{-3^-00z \mid (0.0,0.0,0.0)\}
                                   +x-y, +x, -z
 \{m_x-xz \mid (0.0,0.0,0.5)\}
                                 -y,-x,+z+1/2
\{-6^-00z \mid (0.0,0.0,0.5)\}
                                -y, +x-y, -z+1/2
 \{m_x0z \mid (0.0,0.0,0.0)\}
                                   +x-y,-y,+z
 \{m_2xxz \mid (0.0,0.0,0.5)\}
                                +x,+x-y,+z+1/2
```

```
******
```

space group: 194 {'Hall': '-P 6c 2c', 'HM': 'P 63/m m c'}

Crystal system: Hexagonal

+x,+y,+z

+x-y, +x, +z+1/2

-y, -x, -z+1/2

+	⊦
Seitz	Jones
[\ \{1 (0.0,0.0,0.0)\}	+x,+y,+z
{6^+_00z (0.0,0.0,0.5)}	+x-y,+x,+z+1/2
$\{2_x-x0 (0.0,0.0,0.5)\}$	-y,-x,-z+1/2
{3^+_00z (0.0,0.0,0.0)}	-y,+x-y,+z
$\{2_{x}00 (0.0,0.0,0.0)\}$	+x-y,-y,-z
{2_00z (0.0,0.0,0.5)}	-x,-y,+z+1/2
{m_2xx0 (0.0,0.0,0.5)}	+x,+x-y,-z+1/2
{3^00z (0.0,0.0,0.0)}	+y-x,-x,+z
{2_xx0 (0.0,0.0,0.0)}	+y,+x,-z
{6^00z (0.0,0.0,0.5)}	+y,+y-x,+z+1/2
{2_x2x0 (0.0,0.0,0.5)}	+y-x,+y,-z+1/2
{2_0y0 (0.0,0.0,0.0)}	-x,+y-x,-z
$\{-1 (0.0,0.0,0.0)\}$	-x,-y,-z
$ \{-6^+_00z (0.0,0.0,0.5)\}$	+y-x,-x,-z+1/2
{m_xxz (0.0,0.0,0.5)}	+y,+x,+z+1/2
{-3^+_00z (0.0,0.0,0.0)}	+y,+y-x,-z

```
\{m_x2xz \mid (0.0,0.0,0.0)\}
                                +y-x, +y, +z
   \{m_xy0|(0.0,0.0,0.5)\}
                               +x,+y,-z+1/2
   \{m_0yz \mid (0.0,0.0,0.5)\}
                              -x,+y-x,+z+1/2
  \{-3^-00z \mid (0.0,0.0,0.0)\}
                                +x-y, +x, -z
   \{m_x-xz \mid (0.0,0.0,0.0)\}
                                 -y,-x,+z
  \{-6^-00z \mid (0.0,0.0,0.5)\}
                              -y, +x-y, -z+1/2
   \{m_x0z|(0.0,0.0,0.5)\}
                              +x-y,-y,+z+1/2
   \{m_2xxz \mid (0.0,0.0,0.0)\}
                                +x,+x-y,+z
*******
space group: 195 {'Hall': 'P 2 2 3', 'HM': 'P 2 3'}
Crystal system: Cubic
+x,+y,+z
-x,-y,+z
+x,-y,-z
+z,+x,+y
            Seitz
                                Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                               +x,+y,+z
    {2_00z|(0.0,0.0,0.0)}
                               -x,-y,+z
    \{2_{x00}|(0.0,0.0,0.0)\}
                               +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                               +z,+x,+y
    {2_0y0|(0.0,0.0,0.0)}
                               -x,+y,-z
  {3^+_x-x-x}(0.0,0.0,0.0)
                               -z,-x,+y
 {3^+-xx-x|(0.0,0.0,0.0)}
                               +z,-x,-y
  {3^+_-x^-x^+ | (0.0,0.0,0.0)}
                               -z,+x,-y
   {3^-_xxx|(0.0,0.0,0.0)}
                               +y,+z,+x
  \{3^--x-xx\mid (0.0,0.0,0.0)\}
                               +y,-z,-x
  \{3^-x-x-x|(0.0,0.0,0.0)\}
                               -y, +z, -x
  {3^--xx-x|(0.0,0.0,0.0)} | -y,-z,+x
*******
space group: 196 {'Hall': 'F 2 2 3', 'HM': 'F 2 3'}
Crystal system: Cubic
+x,+y,+z
-x,-y,+z
+x,-y,-z
+z,+x,+y
            Seitz
                                     Jones
      {1|(0.0,0.0,0.0)}
                                    +x,+y,+z
    {2_00z|(0.0,0.0,0.0)}
                                   -x,-y,+z
    {2_x00|(0.0,0.0,0.0)}
                                    +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                   +z,+x,+y
    {2_0y0|(0.0,0.0,0.0)}
```

 ${3^+_x-x-x|(0.0,0.0,0.0)}$

-x,+y,-z

-z,-x,+y

```
+z,-x,-y
  {3^+_-x^-x^-|(0.0,0.0,0.0)}
                                    -z,+x,-y
   {3^-_xxx|(0.0,0.0,0.0)}
                                    +y,+z,+x
  \{3^--x-xx \mid (0.0,0.0,0.0)\}
                                    +y,-z,-x
  {3^-_x-x-x|(0.0,0.0,0.0)}
                                    -y,+z,-x
  {3^-_xx-x|(0.0,0.0,0.0)}
                                    -y,-z,+x
      \{1 \mid (0.0, 0.5, 0.5)\}
                                +x,+y+1/2,+z+1/2
    {2_00z|(0.0,0.5,0.5)}
                                -x,-y+1/2,+z+1/2
    \{2_{x00}|(0.0,0.5,0.5)\}
                                +x,-y+1/2,-z+1/2
   {3^+_xxx|(0.0,0.5,0.5)}
                                +z,+x+1/2,+y+1/2
    {2_0y0|(0.0,0.5,0.5)}
                                -x, +y+1/2, -z+1/2
  {3^+_x-x-x|(0.0,0.5,0.5)}
                                -z, -x+1/2, +y+1/2
  {3^+_-xx-x|(0.0,0.5,0.5)}
                                +z,-x+1/2,-y+1/2
  \{3^+-x-xx\mid(0.0,0.5,0.5)\}
                                -z, +x+1/2, -y+1/2
   \{3^-xxx|(0.0,0.5,0.5)\}
                                +y, +z+1/2, +x+1/2
  \{3^--x-xx\mid(0.0,0.5,0.5)\}
                                +y,-z+1/2,-x+1/2
  \{3^-x-x-x|(0.0,0.5,0.5)\}
                                -y, +z+1/2, -x+1/2
  {3^--xx-x|(0.0,0.5,0.5)}
                                -y, -z+1/2, +x+1/2
      \{1|(0.5,0.0,0.5)\}
                                +x+1/2, +y, +z+1/2
                                -x+1/2,-y,+z+1/2
    {2_00z|(0.5,0.0,0.5)}
    \{2_{x00}|(0.5,0.0,0.5)\}
                                +x+1/2,-y,-z+1/2
   {3^+_xxx|(0.5,0.0,0.5)}
                                +z+1/2,+x,+y+1/2
    \{2_0y0|(0.5,0.0,0.5)\}
                                -x+1/2,+y,-z+1/2
  {3^+_x-x-x|(0.5,0.0,0.5)}
                                -z+1/2,-x,+y+1/2
  \{3^+-xx-x\mid(0.5,0.0,0.5)\}
                                +z+1/2,-x,-y+1/2
  {3^+_-x^-x^-|(0.5,0.0,0.5)}
                                -z+1/2,+x,-y+1/2
   {3^-_xxx|(0.5,0.0,0.5)}
                                +y+1/2,+z,+x+1/2
  \{3^--x-xx\mid(0.5,0.0,0.5)\}
                                +y+1/2,-z,-x+1/2
  {3^-_x-x-x|(0.5,0.0,0.5)}
                                -y+1/2,+z,-x+1/2
  {3^--xx-x|(0.5,0.0,0.5)}
                                -y+1/2,-z,+x+1/2
      {1|(0.5,0.5,0.0)}
                                +x+1/2,+y+1/2,+z
    \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                -x+1/2, -y+1/2, +z
    \{2_{x00}|(0.5,0.5,0.0)\}
                                +x+1/2,-y+1/2,-z
   {3^+_xxx|(0.5,0.5,0.0)}
                                +z+1/2,+x+1/2,+y
    {2_0y0|(0.5,0.5,0.0)}
                                -x+1/2,+y+1/2,-z
                                -z+1/2, -x+1/2, +y
  \{3^+x^-x^-x^-\}
                                +z+1/2,-x+1/2,-y
  {3^+_-xx-x|(0.5,0.5,0.0)}
  {3^+_-x^-x^-|(0.5,0.5,0.0)}
                                -z+1/2,+x+1/2,-y
   {3^-_xxx|(0.5,0.5,0.0)}
                                +y+1/2,+z+1/2,+x
  {3^-_x-x\times | (0.5,0.5,0.0)}
                                +y+1/2,-z+1/2,-x
  {3^-_x-x-x|(0.5,0.5,0.0)}
                                -y+1/2,+z+1/2,-x
  {3^--xx-x|(0.5,0.5,0.0)}
                                -y+1/2,-z+1/2,+x
*******
space group: 197 {'Hall': 'I 2 2 3', 'HM': 'I 2 3'}
Crystal system: Cubic
+x,+y,+z
-x,-y,+z
+x,-y,-z
+z,+x,+y
 . . . . . . . . . . . . . . . . . . .
```

 ${3^+-xx-x|(0.0,0.0,0.0)}$

```
Seitz
                                      Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                     +x,+y,+z
  {2_00z|(0.0,0.0,0.0)}
                                     -x,-y,+z
  \{2_{x00} | (0.0,0.0,0.0)\}
                                     +x,-y,-z
 {3^+_xxx|(0.0,0.0,0.0)}
                                     +z,+x,+y
  {2_0y0|(0.0,0.0,0.0)}
                                     -x,+y,-z
{3^+_x-x-x|(0.0,0.0,0.0)}
                                     -z,-x,+y
{3^+-xx-x|(0.0,0.0,0.0)}
                                     +z,-x,-y
{3^+_-x^-x^-|(0.0,0.0,0.0)}
                                     -z,+x,-y
 \{3^-xxx|(0.0,0.0,0.0)\}
                                     +y,+z,+x
{3^-_-x-xx|(0.0,0.0,0.0)}
                                     +y,-z,-x
{3^-_x-x-x|(0.0,0.0,0.0)}
                                     -y,+z,-x
{3^-_xx-x|(0.0,0.0,0.0)}
                                     -y,-z,+x
    \{1 \mid (0.5, 0.5, 0.5)\}
                              +x+1/2, +y+1/2, +z+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                              -x+1/2,-y+1/2,+z+1/2
                              +x+1/2,-y+1/2,-z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
 \{3^+ xxx \mid (0.5, 0.5, 0.5)\}
                              +z+1/2,+x+1/2,+y+1/2
                              -x+1/2, +y+1/2, -z+1/2
  {2_0y0|(0.5,0.5,0.5)}
{3^+_x-x-x|(0.5,0.5,0.5)}
                              -z+1/2,-x+1/2,+y+1/2
{3^+-xx-x|(0.5,0.5,0.5)}
                              +z+1/2, -x+1/2, -y+1/2
{3^+-x-xx|(0.5,0.5,0.5)}
                              -z+1/2,+x+1/2,-y+1/2
 \{3^-xxx|(0.5,0.5,0.5)\}
                              +y+1/2,+z+1/2,+x+1/2
\{3^--x-xx\mid(0.5,0.5,0.5)\}
                              +y+1/2,-z+1/2,-x+1/2
{3^-_x-x-x|(0.5,0.5,0.5)}
                              -y+1/2,+z+1/2,-x+1/2
\{3^--xx-x|(0.5,0.5,0.5)\}
                              -y+1/2,-z+1/2,+x+1/2
```

space group: 198 {'Hall': ' P 2ac 2ab 3', 'HM': 'P 21 3'}

Crystal system: Cubic

+x,+y,+z

-x+1/2, -y, +z+1/2

+x+1/2,-y+1/2,-z

+z,+x,+y

.

Seitz	Jones
	+x,+y,+z -x+1/2,-y,+z+1/2 +x+1/2,-y+1/2,-z +z,+x,+y -x,+y+1/2,-z+1/2 -z+1/2,-x,+y+1/2 +z+1/2,-x+1/2,-y -z,+x+1/2,-y+1/2 +y,+z,+x +y+1/2,-z+1/2,-x -y,+z+1/2,-x+1/2

```
*******
space group: 199 {'Hall': ' I 2b 2c 3', 'HM': 'I 21 3'}
Crystal system: Cubic
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z+1/2
+z,+x,+y
             Seitz
                                        Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
    {2_00z|(0.0,0.5,0.0)}
                                     -x,-y+1/2,+z
    \{2_{x00} | (0.0, 0.0, 0.5)\}
                                     +x,-y,-z+1/2
   \{3^+ xxx \mid (0.0,0.0,0.0)\}
                                       +z,+x,+y
    {2_0y0|(0.0,0.5,0.5)}
                                   -x,+y+1/2,-z+1/2
  {3^+_x-x-x}(0.0,0.5,0.0)
                                     -z, -x+1/2, +y
  {3^+_-xx-x|(0.0,0.0,0.5)}
                                     +z,-x,-y+1/2
  {3^+_-x^-x^-|(0.0,0.5,0.5)}
                                   -z, +x+1/2, -y+1/2
   {3^-_xxx|(0.0,0.0,0.0)}
                                       +y, +z, +x
  \{3^--x-xx\mid (0.0,0.0,0.5)\}
                                     +y,-z,-x+1/2
  \{3^-x-x-x|(0.5,0.0,0.0)\}
                                     -y+1/2,+z,-x
  {3^-_xx-x|(0.5,0.0,0.5)}
                                   -y+1/2,-z,+x+1/2
      \{1|(0.5,0.5,0.5)\}
                                +x+1/2,+y+1/2,+z+1/2
    \{2\_00z \mid (0.5,0.0,0.5)\}
                                  -x+1/2,-y,+z+1/2
                                   +x+1/2,-y+1/2,-z
    \{2_{x00} | (0.5, 0.5, 0.0)\}
   \{3^+ xxx \mid (0.5, 0.5, 0.5)\}
                                +z+1/2, +x+1/2, +y+1/2
    {2_0y0|(0.5,0.0,0.0)}
                                     -x+1/2,+y,-z
  {3^+_x-x-x|(0.5,0.0,0.5)}
                                   -z+1/2, -x, +y+1/2
  {3^+_-xx-x|(0.5,0.5,0.0)}
                                  +z+1/2,-x+1/2,-y
  {3^+_-x^-x^-|(0.5,0.0,0.0)}
                                     -z+1/2,+x,-y
   {3^-_xxx|(0.5,0.5,0.5)}
                                +y+1/2,+z+1/2,+x+1/2
  \{3^--x-xx\mid(0.5,0.5,0.0)\}
                                   +y+1/2,-z+1/2,-x
  \{3^-x-x-x|(0.0,0.5,0.5)\}
                                   -y, +z+1/2, -x+1/2
  \{3^--xx-x \mid (0.0,0.5,0.0)\}
                                     -y, -z+1/2, +x
******
space group: 200 {'Hall': '-P 2 2 3', 'HM': 'P m -3'}
Crystal system: Cubic
+x,+y,+z
-x,-y,+z
+x,-y,-z
+z,+x,+y
             Seitz
                                   Jones
      {1|(0.0,0.0,0.0)}
                                 +x,+y,+z
    {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
    {2_x00|(0.0,0.0,0.0)}
                                 +x,-y,-z
   \{3^+ \times \times \times | (0.0,0.0,0.0)\}
                                 +z,+x,+y
```

```
{2_0y0|(0.0,0.0,0.0)}
                             | -x,+y,-z |
\{3^+_x-x-x|(0.0,0.0,0.0)\}
                              -z,-x,+y
\{3^+_-xx^-x \mid (0.0,0.0,0.0)\}
                             +z,-x,-y
 {3^+_-x-xx|(0.0,0.0,0.0)}
                              -z,+x,-y
   \{3^-xxx|(0.0,0.0,0.0)\}
                             +y,+z,+x
 \{3^--x-xx\mid (0.0,0.0,0.0)\}
                             | +y,-z,-x |
| \{3^-x-x-x|(0.0,0.0,0.0)\}|
                             | -y,+z,-x |
 \{3^{-}-xx-x \mid (0.0,0.0,0.0)\}
                               -y,-z,+x
      \{-1 \mid (0.0, 0.0, 0.0)\}
                               -x,-y,-z
    \{m_xy0|(0.0,0.0,0.0)\}
                              | +x,+y,-z |
    \{m_0yz \mid (0.0,0.0,0.0)\}
                             |-x,+y,+z|
   \{-3^+ xxx \mid (0.0,0.0,0.0)\}
                               -z,-x,-y
    \{m_x0z \mid (0.0,0.0,0.0)\}
                              | +x,-y,+z |
 \{-3^+x^-x^-x^-|(0.0,0.0,0.0)\}
                             | +z,+x,-y |
 \{-3^+-xx-x \mid (0.0,0.0,0.0)\} \mid -z,+x,+y \mid
 \{-3^-x-x-x|(0.0,0.0,0.0)\} \mid +y,-z,+x \mid
| {-3^-_-xx-x|(0.0,0.0,0.0)} | +y,+z,-x |
. . . . . . . . . . . . . . . . . . . .
*******
space group: 201:1 {'Hall': ' P 2 2 3 -1n', 'HM': 'P n -3:1'}
Crystal system: Cubic
Setting: 1
+x,+y,+z
+x,-y,-z
```

-x,-y,+z

+z,+x,+y

-x+1/2,-y+1/2,-z+1/2

.

+	++
Seitz	Jones
+	
{1 (0.0,0.0,0.0)}	+x,+y,+z
$\{2_00z \mid (0.0,0.0,0.0)\}\$	-x,-y,+z
{2_x00 (0.0,0.0,0.0)}	+x,-y,-z
{3^+_xxx (0.0,0.0,0.0)}	+z,+x,+y
$ \{-1 (0.5,0.5,0.5)\} $	-x+1/2,-y+1/2,-z+1/2
{2_0y0 (0.0,0.0,0.0)}	-x,+y,-z
$ \{3^+_x-x^- (0.0,0.0,0.0)\} $	-z,-x,+y
{m_xy0 (0.5,0.5,0.5)}	+x+1/2,+y+1/2,-z+1/2
$ \{3^+_{xx-x} (0.0,0.0,0.0)\} $	+z,-x,-y
$ \{m_0yz (0.5, 0.5, 0.5)\} $	-x+1/2,+y+1/2,+z+1/2
$ \{3^+x^-x^-\} \{0.0,0.0,0.0\} $	-z,+x,-y
{m_x0z (0.5,0.5,0.5)}	+x+1/2,-y+1/2,+z+1/2

.

```
*******
```

space group: 201:2 {'Hall': '-P 2ab 2bc 3', 'HM': 'P n -3:2'}

Crystal system: Cubic

```
Setting: 2
+x,+y,+z
-x+1/2,-y+1/2,+z
+x,-y+1/2,-z+1/2
+z,+x,+y
               Seitz
       \{1 \mid (0.0, 0.0, 0.0)\}
     \{2\_00z \mid (0.5, 0.5, 0.0)\}
```

-x+1/2,-y+1/2,+z+x,-y+1/2,-z+1/2 $\{2_{x00}|(0.0,0.5,0.5)\}$ {3^+_xxx|(0.0,0.0,0.0)} +z,+x,+y{2_0y0|(0.5,0.0,0.5)} -x+1/2,+y,-z+1/2 ${3^+_x-x-x|(0.5,0.5,0.0)}$ -z+1/2, -x+1/2, +y ${3^+-xx-x|(0.0,0.5,0.5)}$ +z,-x+1/2,-y+1/2 ${3^+_-x^-x^-|(0.5,0.0,0.5)}$ -z+1/2,+x,-y+1/2+y,+z,+x {3^-_xxx|(0.0,0.0,0.0)} $\{3^--x-xx\mid(0.0,0.5,0.5)\}$ +y,-z+1/2,-x+1/2 ${3^-_x-x-x|(0.5,0.0,0.5)}$ -y+1/2,+z,-x+1/2 ${3^-_xx-x|(0.5,0.5,0.0)}$ -y+1/2,-z+1/2,+x $\{-1 \mid (0.0, 0.0, 0.0)\}$ -x,-y,-z $\{m_xy0|(0.5,0.5,0.0)\}$ +x+1/2, +y+1/2, -z $\{m_0yz \mid (0.0,0.5,0.5)\}$ -x, +y+1/2, +z+1/2 $\{-3^+ xxx | (0.0,0.0,0.0)\}$ -z,-x,-y $\{m_x0z | (0.5,0.0,0.5)\}$ +x+1/2,-y,+z+1/2 $\{-3^+x^-x^-x^- (0.5,0.5,0.0)\}$ +z+1/2, +x+1/2, -y $\{-3^+-xx-x|(0.0,0.5,0.5)\}$ -z, +x+1/2, +y+1/2 $\{-3^+-x-xx\mid(0.5,0.0,0.5)\}$ +z+1/2,-x,+y+1/2 $\{-3^-xxx|(0.0,0.0,0.0)\}$ -y, -z, -x $\{-3^--x-xx\mid(0.0,0.5,0.5)\}$ -y, +z+1/2, +x+1/2 $\{-3^-x-x-x|(0.5,0.0,0.5)\}$ +y+1/2,-z,+x+1/2 $\{-3^--xx-x|(0.5,0.5,0.0)\}$ +y+1/2,+z+1/2,-x

Jones

+X,+Y,+Z

.

```
*******
```

space group: 202 {'Hall': '-F 2 2 3', 'HM': 'F m -3'}

Crystal system: Cubic

+x,+y,+z

-x,-y,+z

+x,-y,-z

+z,+x,+y

±	
Seitz	Jones
{1 (0.0,0.0,0.0)} {2_00z (0.0,0.0,0.0)} {2_x00 (0.0,0.0,0.0)} {3^+_xxx (0.0,0.0,0.0)} {2_0y0 (0.0,0.0,0.0)} {3^+_x-x-x (0.0,0.0,0.0)} {3^+_x-x-x (0.0,0.0,0.0)}	+x,+y,+z -x,-y,+z +x,-y,-z +z,+x,+y -x,+y,-z -z,-x,+y +z,-x,-y

```
{3^+_-x^-x^-|(0.0,0.0,0.0)}
                                    -z,+x,-y
 {3^-_xxx|(0.0,0.0,0.0)}
                                    +y,+z,+x
\{3^--x-xx\mid (0.0,0.0,0.0)\}
                                    +y,-z,-x
\{3^-x-x-x|(0.0,0.0,0.0)\}
                                    -y,+z,-x
\{3^--xx-x \mid (0.0,0.0,0.0)\}
                                    -y,-z,+x
    {-1|(0.0,0.0,0.0)}
                                    -x,-y,-z
  {m_xy0|(0.0,0.0,0.0)}
                                    +x,+y,-z
  {m_0yz|(0.0,0.0,0.0)}
                                    -x,+y,+z
 \{-3^+ \times \times | (0.0,0.0,0.0)\}
                                    -z,-x,-y
  {m_x0z|(0.0,0.0,0.0)}
                                    +x,-y,+z
\{-3^+x^-x^-x^-\}
                                    +z,+x,-y
\{-3^+-xx-x \mid (0.0,0.0,0.0)\}
                                    -z,+x,+y
\{-3^+-x-xx \mid (0.0,0.0,0.0)\}
                                    +z,-x,+y
 {-3^-_xxx|(0.0,0.0,0.0)}
                                    -y,-z,-x
\{-3^--x-xx \mid (0.0,0.0,0.0)\}
                                    -y,+z,+x
\{-3^-x-x-x|(0.0,0.0,0.0)\}
                                    +y,-z,+x
\{-3^--xx-x \mid (0.0,0.0,0.0)\}
                                    +y,+z,-x
    {1|(0.0,0.5,0.5)}
                                +x,+y+1/2,+z+1/2
  {2_00z|(0.0,0.5,0.5)}
                                -x,-y+1/2,+z+1/2
                                +x,-y+1/2,-z+1/2
  {2_x00|(0.0,0.5,0.5)}
 {3^+_xxx|(0.0,0.5,0.5)}
                                +z, +x+1/2, +y+1/2
  {2_0y0|(0.0,0.5,0.5)}
                                -x, +y+1/2, -z+1/2
{3^+_x-x-x}(0.0,0.5,0.5)
                                -z, -x+1/2, +y+1/2
{3^+-xx-x|(0.0,0.5,0.5)}
                                +z,-x+1/2,-y+1/2
\{3^+-x-x^+ (0.0,0.5,0.5)\}
                                -z,+x+1/2,-y+1/2
 {3^-_xxx|(0.0,0.5,0.5)}
                                +y, +z+1/2, +x+1/2
\{3^--x-xx\mid(0.0,0.5,0.5)\}
                                +y,-z+1/2,-x+1/2
\{3^-x-x-x|(0.0,0.5,0.5)\}
                                -y, +z+1/2, -x+1/2
{3^--xx-x|(0.0,0.5,0.5)}
                                -y, -z+1/2, +x+1/2
    \{-1|(0.0,0.5,0.5)\}
                                -x,-y+1/2,-z+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                               +x,+y+1/2,-z+1/2
  {m_0yz|(0.0,0.5,0.5)}
                                -x,+y+1/2,+z+1/2
 \{-3^+ xxx | (0.0, 0.5, 0.5)\}
                                -z, -x+1/2, -y+1/2
                                +x,-y+1/2,+z+1/2
  \{m_x0z \mid (0.0,0.5,0.5)\}
\{-3^+_x-x-x|(0.0,0.5,0.5)\}
                                +z,+x+1/2,-y+1/2
\{-3^+-xx-x|(0.0,0.5,0.5)\}
                                -z, +x+1/2, +y+1/2
\{-3^+-x-xx|(0.0,0.5,0.5)\}
                                +z,-x+1/2,+y+1/2
 \{-3^-xxx|(0.0,0.5,0.5)\}
                                -y, -z+1/2, -x+1/2
\{-3^--x-xx|(0.0,0.5,0.5)\}
                                -y, +z+1/2, +x+1/2
\{-3^-x-x-x|(0.0,0.5,0.5)\}
                                +y,-z+1/2,+x+1/2
\{-3^--xx-x \mid (0.0,0.5,0.5)\}
                                +y, +z+1/2, -x+1/2
    {1|(0.5,0.0,0.5)}
                                +x+1/2,+y,+z+1/2
  {2_00z|(0.5,0.0,0.5)}
                                -x+1/2,-y,+z+1/2
  {2_x00|(0.5,0.0,0.5)}
                                +x+1/2,-y,-z+1/2
 {3^+_xxx|(0.5,0.0,0.5)}
                                +z+1/2,+x,+y+1/2
  {2_0y0|(0.5,0.0,0.5)}
                                -x+1/2,+y,-z+1/2
{3^+_x-x-x}(0.5,0.0,0.5)
                                -z+1/2, -x, +y+1/2
\{3^+-xx-x\mid(0.5,0.0,0.5)\}
                                +z+1/2,-x,-y+1/2
\{3^+-x-x^+ | (0.5,0.0,0.5)\}
                                -z+1/2,+x,-y+1/2
 {3^-_xxx|(0.5,0.0,0.5)}
                                +y+1/2,+z,+x+1/2
{3^-_x-xx|(0.5,0.0,0.5)}
                                +y+1/2,-z,-x+1/2
{3^-_x-x-x|(0.5,0.0,0.5)}
                                -y+1/2,+z,-x+1/2
{3^--xx-x|(0.5,0.0,0.5)}
                                -y+1/2,-z,+x+1/2
    \{-1|(0.5,0.0,0.5)\}
                               -x+1/2,-y,-z+1/2
```

```
-x+1/2,+y,+z+1/2
    \{m_0yz \mid (0.5,0.0,0.5)\}
   \{-3^+ \times \times | (0.5, 0.0, 0.5)\}
                                  -z+1/2,-x,-y+1/2
    \{m_x0z \mid (0.5,0.0,0.5)\}
                                  +x+1/2, -y, +z+1/2
  \{-3^+x^-x^-x^- (0.5,0.0,0.5)\}
                                  +z+1/2,+x,-y+1/2
  \{-3^+-xx-x \mid (0.5,0.0,0.5)\}
                                  -z+1/2,+x,+y+1/2
  \{-3^+-x-xx|(0.5,0.0,0.5)\}
                                  +z+1/2,-x,+y+1/2
   \{-3^-xxx|(0.5,0.0,0.5)\}
                                  -y+1/2,-z,-x+1/2
  \{-3^--x-xx \mid (0.5,0.0,0.5)\}
                                  -y+1/2,+z,+x+1/2
  \{-3^-x-x-x|(0.5,0.0,0.5)\}
                                  +y+1/2,-z,+x+1/2
  \{-3^--xx-x \mid (0.5,0.0,0.5)\}
                                  +y+1/2,+z,-x+1/2
      {1|(0.5,0.5,0.0)}
                                  +x+1/2,+y+1/2,+z
    {2_00z|(0.5,0.5,0.0)}
                                  -x+1/2,-y+1/2,+z
    {2_x00|(0.5,0.5,0.0)}
                                  +x+1/2,-y+1/2,-z
   {3^+_xxx|(0.5,0.5,0.0)}
                                  +z+1/2,+x+1/2,+y
    {2_0y0|(0.5,0.5,0.0)}
                                  -x+1/2,+y+1/2,-z
                                  -z+1/2, -x+1/2, +y
  \{3^+x^-x^-x^-\}
  \{3^+-xx-x\mid(0.5,0.5,0.0)\}
                                  +z+1/2,-x+1/2,-y
  {3^+_-x^-x^+|(0.5,0.5,0.0)}
                                  -z+1/2,+x+1/2,-y
   {3^-_xxx|(0.5,0.5,0.0)}
                                  +y+1/2,+z+1/2,+x
  {3^-_x-x\times|(0.5,0.5,0.0)}
                                  +y+1/2,-z+1/2,-x
  {3^-_x-x-x|(0.5,0.5,0.0)}
                                  -y+1/2,+z+1/2,-x
  \{3^--xx-x \mid (0.5,0.5,0.0)\}
                                  -y+1/2,-z+1/2,+x
                                  -x+1/2,-y+1/2,-z
      \{-1 \mid (0.5, 0.5, 0.0)\}
    \{m_xy0|(0.5,0.5,0.0)\}
                                  +x+1/2, +y+1/2, -z
    \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                  -x+1/2,+y+1/2,+z
   \{-3^+ xxx | (0.5, 0.5, 0.0)\}
                                  -z+1/2, -x+1/2, -y
    \{m_x0z \mid (0.5,0.5,0.0)\}
                                  +x+1/2,-y+1/2,+z
  \{-3^+x^-x^-x^-(0.5,0.5,0.0)\}
                                  +z+1/2,+x+1/2,-y
  \{-3^+-xx-x \mid (0.5,0.5,0.0)\}
                                  -z+1/2,+x+1/2,+y
  \{-3^+-x-xx|(0.5,0.5,0.0)\}
                                  +z+1/2,-x+1/2,+y
   \{-3^-xxx|(0.5,0.5,0.0)\}
                                  -y+1/2,-z+1/2,-x
  \{-3^--x-xx|(0.5,0.5,0.0)\}
                                  -y+1/2,+z+1/2,+x
  \{-3^-x-x-x|(0.5,0.5,0.0)\}
                                  +y+1/2,-z+1/2,+x
  \{-3^--xx-x \mid (0.5,0.5,0.0)\}
                                 +y+1/2,+z+1/2,-x
*******
space group: 203:1 {'Hall': ' F 2 2 3 -1d', 'HM': 'F d -3:1'}
Crystal system: Cubic
Setting: 1
+x,+y,+z
-x,-y,+z
+x,-y,-z
+z,+x,+y
-x+1/4, -y+1/4, -z+1/4
             Seitz
                                         Jones
      {1|(0.0,0.0,0.0)}
                                       +x,+y,+z
    {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
    \{2_{x00} | (0.0,0.0,0.0)\}
                                       +x,-y,-z
```

+x+1/2,+y,-z+1/2

 $\{m_xy0|(0.5,0.0,0.5)\}$

```
{3^+_xxx|(0.0,0.0,0.0)}
                                     +z,+x,+y
                              -x+1/4, -y+1/4, -z+1/4
  \{-1 \mid (0.25, 0.25, 0.25)\}
  {2_0y0|(0.0,0.0,0.0)}
                                     -x,+y,-z
{3^+_x-x-x|(0.0,0.0,0.0)}
                                     -z,-x,+y
 {m_xy0|(0.75,0.75,0.25)}
                              +x+3/4, +y+3/4, -z+1/4
{3^+_-xx-x|(0.0,0.0,0.0)}
                                     +z,-x,-y
 \{m_0yz \mid (0.25, 0.75, 0.75)\}
                              -x+1/4, +y+3/4, +z+3/4
\{3^+-x-x^+ \mid (0.0,0.0,0.0)\}
                                     -z,+x,-y
 \{m_x0z \mid (0.75, 0.25, 0.75)\}
                              +x+3/4,-y+1/4,+z+3/4
    {1|(0.0,0.5,0.5)}
                                 +x,+y+1/2,+z+1/2
  {2_00z|(0.0,0.5,0.5)}
                                 -x,-y+1/2,+z+1/2
  {2_x00|(0.0,0.5,0.5)}
                                 +x,-y+1/2,-z+1/2
 {3^+_xxx|(0.0,0.5,0.5)}
                                 +z, +x+1/2, +y+1/2
  \{-1 \mid (0.25, 0.75, 0.75)\}
                               -x+1/4, -y+3/4, -z+3/4
  {2_0y0|(0.0,0.5,0.5)}
                                 -x,+y+1/2,-z+1/2
\{3^+x^-x^-x^-\}
                                 -z, -x+1/2, +y+1/2
 \{m_xy0|(0.75,0.25,0.75)\}
                              +x+3/4,+y+1/4,-z+3/4
\{3^+-xx-x\mid(0.0,0.5,0.5)\}
                                 +z,-x+1/2,-y+1/2
 {m_0yz|(0.25,0.25,0.25)}
                              -x+1/4, +y+1/4, +z+1/4
{3^+_-x^-x^-|(0.0,0.5,0.5)}
                                 -z, +x+1/2, -y+1/2
 \{m_x0z|(0.75,0.75,0.25)\}
                               +x+3/4, -y+3/4, +z+1/4
    \{1 \mid (0.5, 0.0, 0.5)\}
                                 +x+1/2,+y,+z+1/2
  {2_00z|(0.5,0.0,0.5)}
                                 -x+1/2,-y,+z+1/2
  {2_x00|(0.5,0.0,0.5)}
                                 +x+1/2,-y,-z+1/2
 \{3^+ xxx \mid (0.5, 0.0, 0.5)\}
                                 +z+1/2,+x,+y+1/2
  \{-1 \mid (0.75, 0.25, 0.75)\}
                               -x+3/4, -y+1/4, -z+3/4
  {2_0y0|(0.5,0.0,0.5)}
                                 -x+1/2,+y,-z+1/2
{3^+_x-x-x|(0.5,0.0,0.5)}
                                 -z+1/2,-x,+y+1/2
 {m_xy0|(0.25,0.75,0.75)}
                               +x+1/4, +y+3/4, -z+3/4
{3^+_-xx-x|(0.5,0.0,0.5)}
                                 +z+1/2,-x,-y+1/2
 {m_0yz|(0.75,0.75,0.25)}
                               -x+3/4, +y+3/4, +z+1/4
{3^+_-x^-x^-|(0.5,0.0,0.5)}
                                 -z+1/2,+x,-y+1/2
 {m_x0z|(0.25,0.25,0.25)}
                               +x+1/4, -y+1/4, +z+1/4
    {1|(0.5,0.5,0.0)}
                                 +x+1/2, +y+1/2, +z
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                 -x+1/2,-y+1/2,+z
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                                 +x+1/2,-y+1/2,-z
 {3^+_xxx|(0.5,0.5,0.0)}
                                 +z+1/2,+x+1/2,+y
  \{-1 \mid (0.75, 0.75, 0.25)\}
                               -x+3/4, -y+3/4, -z+1/4
  {2_0y0|(0.5,0.5,0.0)}
                                 -x+1/2,+y+1/2,-z
\{3^+x^-x^-x^-\}
                                 -z+1/2, -x+1/2, +y
                               +x+1/4, +y+1/4, -z+1/4
 \{m_xy0|(0.25,0.25,0.25)\}
{3^+-xx-x|(0.5,0.5,0.0)}
                                 +z+1/2,-x+1/2,-y
 {m_0yz|(0.75,0.25,0.75)}
                              -x+3/4, +y+1/4, +z+3/4
\{3^+-x-xx\mid(0.5,0.5,0.0)\}
                                 -z+1/2,+x+1/2,-y
 \{m_x0z|(0.25,0.75,0.75)\}
                              +x+1/4,-y+3/4,+z+3/4
```

```
******
```

```
space group: 203:2 {'Hall': '-F 2uv 2vw 3', 'HM': 'F d -3:2'}
Crystal system: Cubic
Setting: 2
+x,+y,+z
-x+1/4,-y+1/4,+z
```

Seitz 	Jones
Seitz	Jones +x,+y,+z -x+1/4,-y+1/4,+z +z,+x,+y -x+1/4,+y,-z+1/4 -z+1/4,-x+1/4,+y +z,-x+1/4,-y+1/4 -z+1/4,+x,-y+1/4 -z+1/4,+x,-y+1/4 -y+1/4,-z,-x+1/4 -y+1/4,-z+1/4,-z -x,-y,-z +x+1/4,+y+1/4,-z -x,-y,-z +x+1/4,-y+1/4,-z -x,-y,-z +x+1/4,-y+1/4,-z -x,-y+1/4,-z+1/4 -z,-x,-y +x+1/4,-y+1/4 +z+1/4,-x,+y+1/4 +z+1/4,-x,+y+1/4 +z+1/4,-x,+y+1/4 +y+1/4,-z,+x+1/4 +y+1/4,-z,+x+1/4 +y+1/4,-z,+x+1/4 +y+1/4,-z+1/2,-z+3/4 -x,+y+1/2,-z+3/4 -z+1/4,-y+3/4,-z+1/2 -x,-y+3/4,-z+3/4 -z+1/4,-x+3/4,-y+3/4 -z+1/4,-x+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-x+3/4 -y+1/4,-z+3/4,-z+1/2 -x,-y+1/2,-z+1/2 +x+1/4,-y+1/2,-z+3/4 -z,-x+1/2,-y+1/2 +x+1/4,-y+1/2,-z+3/4 -z,-x+1/2,-y+1/2 -x,-y+1/2,-z+1/2 -x,-y+1/2,-z+3/4 -z,-x+1/2,-y+1/2 -x,-y+1/2,-z+1/2 -x,-y+1/2,-z+

```
{1|(0.5,0.0,0.5)}
                                    +x+1/2,+y,+z+1/2
  {2_00z|(0.75,0.25,0.5)}
                                  -x+3/4,-y+1/4,+z+1/2
                                  +x+1/2,-y+1/4,-z+3/4
  {2_x00|(0.5,0.25,0.75)}
  {3^+_xxx|(0.5,0.0,0.5)}
                                    +z+1/2,+x,+y+1/2
  {2_0y0|(0.75,0.0,0.75)}
                                    -x+3/4,+y,-z+3/4
\{3^+x^-x^-x^-\}(0.75,0.25,0.5)\}
                                  -z+3/4,-x+1/4,+y+1/2
                                  +z+1/2,-x+1/4,-y+3/4
\{3^+-xx-x|(0.5,0.25,0.75)\}
{3^+_-x^-x^+|(0.75,0.0,0.75)}
                                    -z+3/4,+x,-y+3/4
  \{3^-xxx|(0.5,0.0,0.5)\}
                                    +y+1/2,+z,+x+1/2
{3^-_x-xx|(0.5,0.25,0.75)}
                                  +y+1/2,-z+1/4,-x+3/4
{3^-_x-x-x|(0.75,0.0,0.75)}
                                    -y+3/4,+z,-x+3/4
\{3^--xx-x|(0.75,0.25,0.5)\}
                                  -y+3/4, -z+1/4, +x+1/2
                                    -x+1/2,-y,-z+1/2
     {-1|(0.5,0.0,0.5)}
  {m_xy0|(0.75,0.25,0.5)}
                                  +x+3/4, +y+1/4, -z+1/2
  \{m_0yz \mid (0.5, 0.25, 0.75)\}
                                  -x+1/2, +y+1/4, +z+3/4
  \{-3^+ \times \times | (0.5, 0.0, 0.5)\}
                                    -z+1/2, -x, -y+1/2
  \{m_x0z|(0.75,0.0,0.75)\}
                                    +x+3/4, -y, +z+3/4
\{-3^+x^-x^-x^-(0.75,0.25,0.5)\}
                                  +z+3/4, +x+1/4, -y+1/2
\{-3^+-xx-x \mid (0.5,0.25,0.75)\}
                                  -z+1/2,+x+1/4,+y+3/4
\{-3^+-x-xx|(0.75,0.0,0.75)\}
                                    +z+3/4,-x,+y+3/4
  \{-3^-xxx|(0.5,0.0,0.5)\}
                                    -y+1/2,-z,-x+1/2
\{-3^--x-xx|(0.5,0.25,0.75)\}
                                  -y+1/2, +z+1/4, +x+3/4
\{-3^-x-x-x|(0.75,0.0,0.75)\}
                                    +y+3/4,-z,+x+3/4
      _-xx-x|(0.75,0.25,0.5)}
                                  +y+3/4,+z+1/4,-x+1/2
     {1|(0.5,0.5,0.0)}
                                    +x+1/2,+y+1/2,+z
  {2_00z|(0.75,0.75,0.0)}
                                    -x+3/4, -y+3/4, +z
  {2_x00|(0.5,0.75,0.25)}
                                  +x+1/2,-y+3/4,-z+1/4
  \{3^+ xxx \mid (0.5, 0.5, 0.0)\}
                                    +z+1/2,+x+1/2,+y
  {2_0y0|(0.75,0.5,0.25)}
                                  -x+3/4,+y+1/2,-z+1/4
{3^+_x-x-x|(0.75,0.75,0.0)}
                                    -z+3/4, -x+3/4, +y
{3^+-xx-x|(0.5,0.75,0.25)}
                                  +z+1/2,-x+3/4,-y+1/4
{3^+-x-xx|(0.75,0.5,0.25)}
                                  -z+3/4,+x+1/2,-y+1/4
  {3^-_xxx|(0.5,0.5,0.0)}
                                    +y+1/2,+z+1/2,+x
\{3^--x-xx\mid(0.5,0.75,0.25)\}
                                  +y+1/2,-z+3/4,-x+1/4
\{3^-x-x-x|(0.75,0.5,0.25)\}
                                  -y+3/4, +z+1/2, -x+1/4
\{3^--xx-x|(0.75,0.75,0.0)\}
                                    -y+3/4,-z+3/4,+x
     \{-1 \mid (0.5, 0.5, 0.0)\}
                                    -x+1/2,-y+1/2,-z
  {m_xy0|(0.75,0.75,0.0)}
                                    +x+3/4, +y+3/4, -z
  \{m_0yz \mid (0.5, 0.75, 0.25)\}
                                  -x+1/2,+y+3/4,+z+1/4
  \{-3^+ \times \times | (0.5, 0.5, 0.0)\}
                                    -z+1/2, -x+1/2, -y
  {m_x0z|(0.75,0.5,0.25)}
                                  +x+3/4,-y+1/2,+z+1/4
\{-3^+x^-x^-x^-(0.75,0.75,0.0)\}
                                    +z+3/4,+x+3/4,-y
\{-3^+-xx-x|(0.5,0.75,0.25)\}
                                  -z+1/2,+x+3/4,+y+1/4
\{-3^+-x-xx|(0.75,0.5,0.25)\}
                                  +z+3/4,-x+1/2,+y+1/4
  \{-3^-xxx|(0.5,0.5,0.0)\}
                                    -y+1/2,-z+1/2,-x
\{-3^--x-xx|(0.5,0.75,0.25)\}
                                  -y+1/2, +z+3/4, +x+1/4
\{-3^-x-x-x|(0.75,0.5,0.25)\}
                                  +y+3/4,-z+1/2,+x+1/4
\{-3^--xx-x|(0.75,0.75,0.0)\}
                                    +y+3/4,+z+3/4,-x
```

space group: 204 {'Hall': '-I 2 2 3', 'HM': 'I m -3'} Crystal system: Cubic

```
+x,+y,+z
-x,-y,+z
+x,-y,-z
+z,+x,+y
```

```
\{-3^-x-x-x|(0.5,0.5,0.5)\} | +y+1/2,-z+1/2,+x+1/2 |
  \{-3^--xx-x|(0.5,0.5,0.5)\} | +y+1/2,+z+1/2,-x+1/2 |
*******
space group: 205 {'Hall': '-P 2ac 2ab 3', 'HM': 'P a -3'}
Crystal system: Cubic
+x,+y,+z
-x+1/2,-y,+z+1/2
+x+1/2,-y+1/2,-z
+Z,+X,+y
             Seitz
                                       Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
    {2_00z|(0.5,0.0,0.5)}
                                 -x+1/2,-y,+z+1/2
    \{2_{x00} | (0.5, 0.5, 0.0)\}
                                 +x+1/2,-y+1/2,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                      +z,+x,+y
    {2_0y0|(0.0,0.5,0.5)}
                                 -x, +y+1/2, -z+1/2
                                 -z+1/2,-x,+y+1/2
  {3^+_x-x-x|(0.5,0.0,0.5)}
  \{3^+-xx-x\mid(0.5,0.5,0.0)\}
                                 +z+1/2,-x+1/2,-y
  {3^+_-x^-x^-|(0.0,0.5,0.5)}
                                 -z, +x+1/2, -y+1/2
   {3^-_xxx|(0.0,0.0,0.0)}
                                      +y,+z,+x
  {3^-_x-xx|(0.5,0.5,0.0)}
                                 +y+1/2,-z+1/2,-x
  {3^-_x-x-x|(0.0,0.5,0.5)}
                                 -y, +z+1/2, -x+1/2
  {3^--xx-x|(0.5,0.0,0.5)}
                                 -y+1/2,-z,+x+1/2
      \{-1 \mid (0.0, 0.0, 0.0)\}
                                      -x,-y,-z
    \{m_xy0|(0.5,0.0,0.5)\}
                                 +x+1/2, +y, -z+1/2
    \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                 -x+1/2,+y+1/2,+z
   \{-3^+ \times \times | (0.0,0.0,0.0)\}
                                      -z,-x,-y
    \{m_x0z | (0.0,0.5,0.5)\}
                                 +x,-y+1/2,+z+1/2
  \{-3^+x^-x^-x^-|(0.5,0.0,0.5)\}
                                 +z+1/2, +x, -y+1/2
  \{-3^+-xx-x \mid (0.5,0.5,0.0)\}
                                 -z+1/2,+x+1/2,+y
  \{-3^+-x-xx|(0.0,0.5,0.5)\}
                                 +z, -x+1/2, +y+1/2
   \{-3^-xxx \mid (0.0,0.0,0.0)\}
                                      -y,-z,-x
  \{-3^--x-xx|(0.5,0.5,0.0)\}
                                 -y+1/2,+z+1/2,+x
  \{-3^-x-x-x|(0.0,0.5,0.5)\}
                                 +y,-z+1/2,+x+1/2
  \{-3^--xx-x|(0.5,0.0,0.5)\} | +y+1/2,+z,-x+1/2
. . . . . . . . . . . . . . . . . . . .
*******
space group: 206 {'Hall': '-I 2b 2c 3', 'HM': 'I a -3'}
Crystal system: Cubic
+x,+y,+z
-x,-y+1/2,+z
+x,-y,-z+1/2
+z,+x,+y
             Seitz
                                         Jones
```

```
{1|(0.0,0.0,0.0)}
                                      +x,+y,+z
  {2_00z|(0.0,0.5,0.0)}
                                    -x,-y+1/2,+z
  \{2_{x00} | (0.0,0.0,0.5)\}
                                    +x,-y,-z+1/2
 {3^+_xxx|(0.0,0.0,0.0)}
                                      +z,+x,+y
  {2_0y0|(0.0,0.5,0.5)}
                                  -x,+y+1/2,-z+1/2
\{3^+x^-x^-x^-\}
                                    -z, -x+1/2, +y
{3^+_-xx-x|(0.0,0.0,0.5)}
                                    +z,-x,-y+1/2
{3^+_-x^-x^+|(0.0,0.5,0.5)}
                                  -z, +x+1/2, -y+1/2
 {3^-_xxx|(0.0,0.0,0.0)}
                                      +y, +z, +x
{3^-_x-xx|(0.0,0.0,0.5)}
                                    +y,-z,-x+1/2
{3^-_x-x-x|(0.5,0.0,0.0)}
                                    -y+1/2,+z,-x
\{3^--xx-x \mid (0.5,0.0,0.5)\}
                                  -y+1/2,-z,+x+1/2
    {-1|(0.0,0.0,0.0)}
                                      -x,-y,-z
  {m_xy0|(0.0,0.5,0.0)}
                                    +x,+y+1/2,-z
  \{m_0yz \mid (0.0,0.0,0.5)\}
                                    -x,+y,+z+1/2
 \{-3^+ \times \times | (0.0, 0.0, 0.0) \}
                                      -z,-x,-y
  {m_x0z|(0.0,0.5,0.5)}
                                  +x,-y+1/2,+z+1/2
\{-3^+x^-x^-x^-\}
                                    +z, +x+1/2, -y
\{-3^+-xx-x \mid (0.0,0.0,0.5)\}
                                    -z,+x,+y+1/2
\{-3^+-x-xx|(0.0,0.5,0.5)\}
                                  +z,-x+1/2,+y+1/2
 \{-3^-xxx|(0.0,0.0,0.0)\}
                                      -y,-z,-x
\{-3^--x-xx|(0.0,0.0,0.5)\}
                                    -y, +z, +x+1/2
\{-3^-x-x-x \mid (0.5,0.0,0.0)\}
                                    +y+1/2,-z,+x
\{-3^--xx-x \mid (0.5,0.0,0.5)\}
                                  +y+1/2,+z,-x+1/2
    \{1|(0.5,0.5,0.5)\}
                                +x+1/2,+y+1/2,+z+1/2
  {2_00z|(0.5,0.0,0.5)}
                                  -x+1/2,-y,+z+1/2
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                                  +x+1/2,-y+1/2,-z
 \{3^+ xxx \mid (0.5, 0.5, 0.5)\}
                               +z+1/2,+x+1/2,+y+1/2
  {2_0y0|(0.5,0.0,0.0)}
                                    -x+1/2,+y,-z
{3^+_x-x-x|(0.5,0.0,0.5)}
                                  -z+1/2, -x, +y+1/2
{3^+_-xx-x|(0.5,0.5,0.0)}
                                  +z+1/2,-x+1/2,-y
{3^+_-x^-x^+|(0.5,0.0,0.0)}
                                    -z+1/2,+x,-y
 {3^-_xxx|(0.5,0.5,0.5)}
                                +y+1/2,+z+1/2,+x+1/2
\{3^--x-xx\mid(0.5,0.5,0.0)\}
                                  +y+1/2,-z+1/2,-x
{3^-_x-x-x|(0.0,0.5,0.5)}
                                  -y, +z+1/2, -x+1/2
                                    -y, -z+1/2, +x
\{3^--xx-x \mid (0.0,0.5,0.0)\}
    \{-1|(0.5,0.5,0.5)\}
                                -x+1/2,-y+1/2,-z+1/2
  {m_xy0|(0.5,0.0,0.5)}
                                  +x+1/2,+y,-z+1/2
  \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                  -x+1/2,+y+1/2,+z
 \{-3^+ xxx \mid (0.5, 0.5, 0.5)\}
                                -z+1/2,-x+1/2,-y+1/2
  {m_x0z|(0.5,0.0,0.0)}
                                    +x+1/2,-y,+z
\{-3^+x^-x^-x^-\}
                                  +z+1/2,+x,-y+1/2
\{-3^+-xx-x|(0.5,0.5,0.0)\}
                                  -z+1/2,+x+1/2,+y
\{-3^+-x-xx|(0.5,0.0,0.0)\}
                                    +z+1/2,-x,+y
 \{-3^-xxx|(0.5,0.5,0.5)\}
                               -y+1/2,-z+1/2,-x+1/2
\{-3^--x-xx|(0.5,0.5,0.0)\}
                                  -y+1/2,+z+1/2,+x
\{-3^-x-x-x|(0.0,0.5,0.5)\}
                                  +y,-z+1/2,+x+1/2
\{-3^--xx-x \mid (0.0,0.5,0.0)\}
                                    +y,+z+1/2,-x
```

space group: 207 {'Hall': 'P 4 2 3', 'HM': 'P 4 3 2'}
Crystal system: Cubic

```
+x,+y,+z
-y,+x,+z
+x,-y,-z
+z,+x,+y
             Seitz
                                 Jones
      {1|(0.0,0.0,0.0)}
                                +x,+y,+z
   {4^+_00z|(0.0,0.0,0.0)}
                                -y,+x,+z
    {2_x00|(0.0,0.0,0.0)}
                                +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                +z,+x,+y
    {2_00z|(0.0,0.0,0.0)}
                                -x,-y,+z
    {2_xx0|(0.0,0.0,0.0)}
                                +y,+x,-z
    \{2_0yy \mid (0.0,0.0,0.0)\}
                                -x,+z,+y
   {4^-_00z|(0.0,0.0,0.0)}
                                +y,-x,+z
    {2_0y0|(0.0,0.0,0.0)}
                                -x,+y,-z
  {3^+_x-x-x}(0.0,0.0,0.0)
                                -z,-x,+y
    {2_x-x0|(0.0,0.0,0.0)}
                                -y,-x,-z
   {4^+_x00|(0.0,0.0,0.0)}
                                +x,-z,+y
  {3^+_-xx-x|(0.0,0.0,0.0)}
                                +z,-x,-y
    \{2_0y-y \mid (0.0,0.0,0.0)\}
                                -x,-z,-y
  {3^+_-x^-x^+|(0.0,0.0,0.0)}
                                -z,+x,-y
   {4^-_x00|(0.0,0.0,0.0)}
                                +x,+z,-y
    \{2_x0x|(0.0,0.0,0.0)\}
                                +z,-y,+x
   {3^-_xxx|(0.0,0.0,0.0)}
                                +y,+z,+x
   {4^-_0y0|(0.0,0.0,0.0)}
                                -z,+y,+x
   {4^+_0y0|(0.0,0.0,0.0)}
                                +z,+y,-x
  \{3^--x-xx\mid (0.0,0.0,0.0)\}
                                +y,-z,-x
    \{2_{-}\times 0\times | (0.0,0.0,0.0)\}
                                -z,-y,-x
  {3^-_x-x-x|(0.0,0.0,0.0)}
                                -y,+z,-x
  \{3^--xx-x \mid (0.0,0.0,0.0)\}
                                -y,-z,+x
*******
space group: 208 {'Hall': ' P 4n 2 3', 'HM': 'P 42 3 2'}
Crystal system: Cubic
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x,-y,-z
+Z,+X,+y
             Seitz
                                        Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
   \{4^+_{00z}|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,+z+1/2
    {2_x00|(0.0,0.0,0.0)}
                                       +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                       +z,+x,+y
```

-x,-y,+z

+y+1/2,+x+1/2,-z+1/2

-x+1/2,+z+1/2,+y+1/2

| +y+1/2, -x+1/2, +z+1/2 |

{2_00z|(0.0,0.0,0.0)}

 $\{2_{xx0}|(0.5,0.5,0.5)\}$

 $\{2_{0yy} | (0.5, 0.5, 0.5)\}$

 $\{4^-_00z \mid (0.5, 0.5, 0.5)\}$

```
{2_0y0|(0.0,0.0,0.0)}
                                    -x,+y,-z
{3^+_x-x-x|(0.0,0.0,0.0)}
                                    -z,-x,+y
  \{2_x-x0|(0.5,0.5,0.5)\}
                              -y+1/2, -x+1/2, -z+1/2
 \{4^+_x00|(0.5,0.5,0.5)\}
                              +x+1/2,-z+1/2,+y+1/2
{3^+-xx-x|(0.0,0.0,0.0)}
                                    +z,-x,-y
  \{2_0y-y\mid (0.5,0.5,0.5)\}
                             -x+1/2,-z+1/2,-y+1/2
{3^+_-x^-x^+|(0.0,0.0,0.0)}
                                    -z,+x,-y
 \{4^-x00|(0.5,0.5,0.5)\}
                              +x+1/2,+z+1/2,-y+1/2
  \{2_x0x \mid (0.5, 0.5, 0.5)\}
                              +z+1/2,-y+1/2,+x+1/2
 {3^-_xxx|(0.0,0.0,0.0)}
                                    +y, +z, +x
 \{4^-_0y0|(0.5,0.5,0.5)\}
                              -z+1/2, +y+1/2, +x+1/2
 {4^+_0y0|(0.5,0.5,0.5)}
                              +z+1/2, +y+1/2, -x+1/2
{3^-_x-x}(0.0,0.0,0.0)
                                    +y,-z,-x
  \{2\_-x0x \mid (0.5,0.5,0.5)\}
                             -z+1/2,-y+1/2,-x+1/2
{3^-_x-x-x|(0.0,0.0,0.0)}
                                    -y, +z, -x
{3^-_-xx-x|(0.0,0.0,0.0)} |
                                    -y,-z,+x
```

space group: 209 {'Hall': 'F 4 2 3', 'HM': 'F 4 3 2'}

Crystal system: Cubic

+x,+y,+z

-y,+x,+z

+x,-y,-z

+z,+x,+y

.

Seitz	Jones
[\ \{1 (0.0,0.0,0.0)\}	+x,+y,+z
{4^+_00z (0.0,0.0,0.0)}	-y,+x,+z
{2_x00 (0.0,0.0,0.0)}	+x,-y,-z
{3^+_xxx (0.0,0.0,0.0)}	+z,+x,+y
{2_00z (0.0,0.0,0.0)}	-x,-y,+z
{2_xx0 (0.0,0.0,0.0)}	+y,+x,-z
{2_0yy (0.0,0.0,0.0)}	-x,+z,+y
{4^00z (0.0,0.0,0.0)}	+y,-x,+z
$\{2\overline{0}y0 (0.0,0.0,0.0)\}$	-x,+y,-z
{3^+_x-x-x (0.0,0.0,0.0)}	-z,-x,+y
$\{2_x-x0\mid (0.0,0.0,0.0)\}$	-y,-x,-z
{4^+_x00 (0.0,0.0,0.0)}	+x,-z,+y
{3^+xx-x (0.0,0.0,0.0)}	+z,-x,-y
$\{2_0y-y\mid (0.0,0.0,0.0)\}$	-x,-z,-y
{3^+x-xx (0.0,0.0,0.0)}	-z,+x,-y
{4^x00 (0.0,0.0,0.0)}	+x,+z,-y
$\{2_{x0x} (0.0,0.0,0.0)\}$	+z,-y,+x
{3^xxx (0.0,0.0,0.0)}	+y,+z,+x
{4^0y0 (0.0,0.0,0.0)}	-z,+y,+x
{4^+_0y0 (0.0,0.0,0.0)}	+z,+y,-x
{3^x-xx (0.0,0.0,0.0)}	+y,-z,-x
$\{2-x0x \mid (0.0,0.0,0.0)\}$	-z,-y,-x
{3^x-x-x (0.0,0.0,0.0)}	-y,+z,-x
{3^xx-x (0.0,0.0,0.0)}	-y,-z,+x

```
{1|(0.0,0.5,0.5)}
                              +x,+y+1/2,+z+1/2
 \{4^+_{00z}|(0.0,0.5,0.5)\}
                              -y, +x+1/2, +z+1/2
  {2_x00|(0.0,0.5,0.5)}
                              +x,-y+1/2,-z+1/2
 {3^+_xxx|(0.0,0.5,0.5)}
                              +z, +x+1/2, +y+1/2
  {2_00z|(0.0,0.5,0.5)}
                              -x,-y+1/2,+z+1/2
  \{2_x \times 0 \mid (0.0, 0.5, 0.5)\}
                              +y, +x+1/2, -z+1/2
  {2_0yy|(0.0,0.5,0.5)}
                              -x, +z+1/2, +y+1/2
 {4^-_00z|(0.0,0.5,0.5)}
                              +y,-x+1/2,+z+1/2
  {2_0y0|(0.0,0.5,0.5)}
                              -x, +y+1/2, -z+1/2
{3^+_x-x-x}(0.0,0.5,0.5)
                              -z,-x+1/2,+y+1/2
  {2_x-x0|(0.0,0.5,0.5)}
                              -y, -x+1/2, -z+1/2
 {4^+_x00|(0.0,0.5,0.5)}
                              +x,-z+1/2,+y+1/2
\{3^+-xx-x\mid(0.0,0.5,0.5)\}
                              +z,-x+1/2,-y+1/2
  {2_0y-y|(0.0,0.5,0.5)}
                              -x, -z+1/2, -y+1/2
{3^+_-x^-x^-|(0.0,0.5,0.5)}
                              -z, +x+1/2, -y+1/2
 {4^-_x00|(0.0,0.5,0.5)}
                              +x,+z+1/2,-y+1/2
  \{2_x0x|(0.0,0.5,0.5)\}
                              +z,-y+1/2,+x+1/2
 {3^-_xxx|(0.0,0.5,0.5)}
                              +y, +z+1/2, +x+1/2
 {4^-_0y0|(0.0,0.5,0.5)}
                              -z, +y+1/2, +x+1/2
 {4^+_0y0|(0.0,0.5,0.5)}
                              +z, +y+1/2, -x+1/2
\{3^--x-xx\mid(0.0,0.5,0.5)\}
                              +y,-z+1/2,-x+1/2
  \{2\_-x0x \mid (0.0,0.5,0.5)\}
                              -z,-y+1/2,-x+1/2
{3^-_x-x-x|(0.0,0.5,0.5)}
                              -y, +z+1/2, -x+1/2
    _-xx-x|(0.0,0.5,0.5)}
                              -y, -z+1/2, +x+1/2
    {1|(0.5,0.0,0.5)}
                              +x+1/2,+y,+z+1/2
 {4^+_00z|(0.5,0.0,0.5)}
                              -y+1/2,+x,+z+1/2
  {2_x00|(0.5,0.0,0.5)}
                              +x+1/2,-y,-z+1/2
 {3^+_xxx|(0.5,0.0,0.5)}
                              +z+1/2,+x,+y+1/2
  {2_00z|(0.5,0.0,0.5)}
                              -x+1/2,-y,+z+1/2
  \{2_x \times 0 \mid (0.5, 0.0, 0.5)\}
                              +y+1/2,+x,-z+1/2
  {2_0yy|(0.5,0.0,0.5)}
                              -x+1/2,+z,+y+1/2
 {4^-_00z|(0.5,0.0,0.5)}
                              +y+1/2,-x,+z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                              -x+1/2,+y,-z+1/2
{3^+_x-x-x|(0.5,0.0,0.5)}
                              -z+1/2, -x, +y+1/2
  \{2_x-x0|(0.5,0.0,0.5)\}
                              -y+1/2,-x,-z+1/2
 {4^+_x00|(0.5,0.0,0.5)}
                              +x+1/2,-z,+y+1/2
{3^+-xx-x|(0.5,0.0,0.5)}
                              +z+1/2,-x,-y+1/2
  {2_0y-y|(0.5,0.0,0.5)}
                              -x+1/2,-z,-y+1/2
{3^+_-x^-x^+|(0.5,0.0,0.5)}
                              -z+1/2,+x,-y+1/2
 {4^-_x00|(0.5,0.0,0.5)}
                              +x+1/2,+z,-y+1/2
  \{2_x0x \mid (0.5,0.0,0.5)\}
                              +z+1/2,-y,+x+1/2
 {3^-_xxx|(0.5,0.0,0.5)}
                              +y+1/2,+z,+x+1/2
 {4^-_0y0|(0.5,0.0,0.5)}
                              -z+1/2,+y,+x+1/2
 {4^+_0y0|(0.5,0.0,0.5)}
                              +z+1/2,+y,-x+1/2
\{3^--x-xx\mid(0.5,0.0,0.5)\}
                              +y+1/2,-z,-x+1/2
  \{2\_-x0x \mid (0.5,0.0,0.5)\}
                              -z+1/2,-y,-x+1/2
{3^-_x-x-x|(0.5,0.0,0.5)}
                              -y+1/2,+z,-x+1/2
\{3^--xx-x \mid (0.5,0.0,0.5)\}
                              -y+1/2,-z,+x+1/2
    {1|(0.5,0.5,0.0)}
                              +x+1/2,+y+1/2,+z
 {4^+_00z|(0.5,0.5,0.0)}
                              -y+1/2,+x+1/2,+z
  {2_x00|(0.5,0.5,0.0)}
                              +x+1/2,-y+1/2,-z
 {3^+_xxx|(0.5,0.5,0.0)}
                              +z+1/2,+x+1/2,+y
                              -x+1/2,-y+1/2,+z
  {2_00z|(0.5,0.5,0.0)}
  \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                              +y+1/2,+x+1/2,-z
```

```
{2_0yy|(0.5,0.5,0.0)}
                                -x+1/2,+z+1/2,+y
   {4^-_00z|(0.5,0.5,0.0)}
                                 +y+1/2,-x+1/2,+z
    {2_0y0|(0.5,0.5,0.0)}
                                 -x+1/2,+y+1/2,-z
  \{3^+x^-x^-x^-\}
                                -z+1/2, -x+1/2, +y
    \{2_x-x0|(0.5,0.5,0.0)\}
                                -y+1/2, -x+1/2, -z
   {4^+_x00|(0.5,0.5,0.0)}
                                +x+1/2,-z+1/2,+y
  {3^+_-xx-x|(0.5,0.5,0.0)}
                                +z+1/2,-x+1/2,-y
    \{2_0y-y\mid (0.5,0.5,0.0)\}
                                -x+1/2, -z+1/2, -y
  \{3^+-x-x^+ \mid (0.5,0.5,0.0)\}
                                -z+1/2,+x+1/2,-y
   \{4^-x00|(0.5,0.5,0.0)\}
                                 +x+1/2,+z+1/2,-y
    \{2_{x0x} | (0.5, 0.5, 0.0)\}
                                 +z+1/2,-y+1/2,+x
   {3^-_xxx|(0.5,0.5,0.0)}
                                 +y+1/2,+z+1/2,+x
   {4^-_0y0|(0.5,0.5,0.0)}
                                -z+1/2,+y+1/2,+x
   {4^+_0y0|(0.5,0.5,0.0)}
                                +z+1/2,+y+1/2,-x
  \{3^--x-xx\mid(0.5,0.5,0.0)\}
                                 +y+1/2,-z+1/2,-x
    \{2_{-}\times 0\times | (0.5, 0.5, 0.0)\}
                                -z+1/2,-y+1/2,-x
  \{3^-x-x-x|(0.5,0.5,0.0)\}
                                -y+1/2,+z+1/2,-x
  \{3^--xx-x\mid (0.5,0.5,0.0)\}
                                -y+1/2,-z+1/2,+x
*******
space group: 210 {'Hall': ' F 4d 2 3', 'HM': 'F 41 3 2'}
Crystal system: Cubic
+x,+y,+z
-y+1/4,+x+1/4,+z+1/4
+x,-y,-z
+z,+x,+y
             Seitz
                                         Jones
      {1|(0.0,0.0,0.0)}
                                        +x,+y,+z
  \{4^+_{00z} | (0.25, 0.25, 0.25)\}
                                  -y+1/4, +x+1/4, +z+1/4
    {2_x00|(0.0,0.0,0.0)}
                                        +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                        +z,+x,+y
    {2_00z|(0.0,0.5,0.5)}
                                    -x,-y+1/2,+z+1/2
                                  +y+1/4, +x+1/4, -z+1/4
   {2_xx0|(0.25,0.25,0.25)}
                                  -x+1/4, +z+1/4, +y+1/4
   {2_0yy|(0.25,0.25,0.25)}
  {4^-_00z|(0.75,0.25,0.75)}
                                  +y+3/4,-x+1/4,+z+3/4
    {2_0y0|(0.0,0.5,0.5)}
                                    -x,+y+1/2,-z+1/2
  {3^+_x-x-x|(0.0,0.5,0.5)}
                                    -z, -x+1/2, +y+1/2
  \{2_x-x0|(0.75,0.25,0.75)\}
                                  -y+3/4, -x+1/4, -z+3/4
  {4^+_x00|(0.75,0.25,0.75)}
                                  +x+3/4,-z+1/4,+y+3/4
  {3^+_-xx-x|(0.0,0.0,0.0)}
                                        +z,-x,-y
  \{2_0y-y\mid (0.25,0.75,0.75)\}
                                  -x+1/4, -z+3/4, -y+3/4
  {3^+_-x^-x^+|(0.0,0.5,0.5)}
                                    -z, +x+1/2, -y+1/2
  \{4^-x00|(0.75,0.75,0.25)\}
                                  +x+3/4, +z+3/4, -y+1/4
   \{2_x0x \mid (0.25, 0.25, 0.25)\}
                                  +z+1/4, -y+1/4, +x+1/4
   {3^-_xxx|(0.0,0.0,0.0)}
                                        +y,+z,+x
  {4^-_0y0|(0.25,0.25,0.25)}
                                  -z+1/4, +y+1/4, +x+1/4
                                  +z+3/4, +y+3/4, -x+1/4
  \{4^+_0y0|(0.75,0.75,0.25)\}
  {3^-_x - x - xx | (0.5, 0.0, 0.5)}
                                    +y+1/2,-z,-x+1/2
  \{2_{-}\times 0\times | (0.75, 0.75, 0.25)\}
                                 -z+3/4,-y+3/4,-x+1/4
```

```
\{3^-x-x-x|(0.0,0.0,0.0)\}
                                       -y,+z,-x
\{3^--xx-x \mid (0.5,0.0,0.5)\}
                                   -y+1/2,-z,+x+1/2
    \{1|(0.0,0.5,0.5)\}
                                   +x,+y+1/2,+z+1/2
\{4^+ 00z \mid (0.25, 0.75, 0.75)\}
                                 -y+1/4, +x+3/4, +z+3/4
  \{2_{x00}|(0.0,0.5,0.5)\}
                                   +x,-y+1/2,-z+1/2
 \{3^+ xxx \mid (0.0, 0.5, 0.5)\}
                                   +z, +x+1/2, +y+1/2
  {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
                                 +y+1/4, +x+3/4, -z+3/4
 {2_xx0|(0.25,0.75,0.75)}
 {2_0yy|(0.25,0.75,0.75)}
                                 -x+1/4, +z+3/4, +y+3/4
{4^-_00z|(0.75,0.75,0.25)}
                                 +y+3/4,-x+3/4,+z+1/4
  {2_0y0|(0.0,0.0,0.0)}
                                       -x, +y, -z
{3^+_x-x-x|(0.0,0.0,0.0)}
                                       -z,-x,+y
\{2_x-x0|(0.75,0.75,0.25)\}
                                 -y+3/4, -x+3/4, -z+1/4
{4^+_x00|(0.75,0.75,0.25)}
                                 +x+3/4,-z+3/4,+y+1/4
{3^+-xx-x|(0.0,0.5,0.5)}
                                   +z, -x+1/2, -y+1/2
\{2_0y-y\mid (0.25,0.25,0.25)\}
                                 -x+1/4, -z+1/4, -y+1/4
\{3^+-x-xx\mid (0.0,0.0,0.0)\}
                                       -z,+x,-y
{4^-_x00|(0.75,0.25,0.75)}
                                 +x+3/4, +z+1/4, -y+3/4
 \{2_x0x \mid (0.25, 0.75, 0.75)\}
                                 +z+1/4,-y+3/4,+x+3/4
 {3^-_xxx|(0.0,0.5,0.5)}
                                   +y, +z+1/2, +x+1/2
\{4^-_0y0|(0.25,0.75,0.75)\}
                                 -z+1/4, +y+3/4, +x+3/4
\{4^+_0y0|(0.75,0.25,0.75)\}
                                 +z+3/4, +y+1/4, -x+3/4
                                   +y+1/2,-z+1/2,-x
\{3^--x-xx\mid(0.5,0.5,0.0)\}
\{2\_-x0x|(0.75,0.25,0.75)\}
                                 -z+3/4,-y+1/4,-x+3/4
\{3^-x-x-x|(0.0,0.5,0.5)\}
                                   -y, +z+1/2, -x+1/2
\{3^--xx-x \mid (0.5,0.5,0.0)\}
                                   -y+1/2,-z+1/2,+x
    {1|(0.5,0.0,0.5)}
                                   +x+1/2, +y, +z+1/2
\{4^+_{00z}|(0.75,0.25,0.75)\}
                                 -y+3/4, +x+1/4, +z+3/4
  \{2 \times 00 \mid (0.5, 0.0, 0.5)\}
                                   +x+1/2,-y,-z+1/2
 \{3^+ xxx \mid (0.5, 0.0, 0.5)\}
                                   +z+1/2, +x, +y+1/2
  {2_00z|(0.5,0.5,0.0)}
                                   -x+1/2,-y+1/2,+z
 \{2_x \times 0 \mid (0.75, 0.25, 0.75)\}
                                 +y+3/4, +x+1/4, -z+3/4
 {2_0yy|(0.75,0.25,0.75)}
                                 -x+3/4, +z+1/4, +y+3/4
\{4^- 00z \mid (0.25, 0.25, 0.25)\}
                                 +y+1/4,-x+1/4,+z+1/4
  {2_0y0|(0.5,0.5,0.0)}
                                   -x+1/2, +y+1/2, -z
{3^+_x-x-x|(0.5,0.5,0.0)}
                                   -z+1/2, -x+1/2, +y
\{2_x-x0|(0.25,0.25,0.25)\}
                                 -y+1/4, -x+1/4, -z+1/4
                                 +x+1/4,-z+1/4,+y+1/4
{4^+_x00|(0.25,0.25,0.25)}
{3^+-xx-x|(0.5,0.0,0.5)}
                                   +z+1/2,-x,-y+1/2
\{2_0y-y|(0.75,0.75,0.25)\}
                                 -x+3/4, -z+3/4, -y+1/4
{3^+_-x^-x^+|(0.5,0.5,0.0)}
                                   -z+1/2,+x+1/2,-y
                                 +x+1/4,+z+3/4,-y+3/4
\{4^-x00|(0.25,0.75,0.75)\}
 \{2_{x}0x | (0.75, 0.25, 0.75)\}
                                 +z+3/4,-y+1/4,+x+3/4
 {3^-_xxx|(0.5,0.0,0.5)}
                                   +y+1/2,+z,+x+1/2
{4^-_0y0|(0.75,0.25,0.75)}
                                 -z+3/4,+y+1/4,+x+3/4
{4^+_0y0|(0.25,0.75,0.75)}
                                 +z+1/4, +y+3/4, -x+3/4
\{3^--x-xx\mid (0.0,0.0,0.0)\}
                                       +y,-z,-x
\{2\_-x0x \mid (0.25, 0.75, 0.75)\}
                                 -z+1/4,-y+3/4,-x+3/4
                                   -y+1/2,+z,-x+1/2
\{3^-x-x-x|(0.5,0.0,0.5)\}
     _-xx-x|(0.0,0.0,0.0)}
                                       -y,-z,+x
    {1|(0.5,0.5,0.0)}
                                   +x+1/2,+y+1/2,+z
\{4^+_00z|(0.75,0.75,0.25)\}
                                 -y+3/4,+x+3/4,+z+1/4
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                                   +x+1/2,-y+1/2,-z
 \{3^+ xxx \mid (0.5, 0.5, 0.0)\}
                                   +z+1/2,+x+1/2,+y
```

```
{2_00z|(0.5,0.0,0.5)}
                                  -x+1/2,-y,+z+1/2
 \{2_x \times 0 \mid (0.75, 0.75, 0.25)\}
                               +y+3/4,+x+3/4,-z+1/4
 \{2_0yy | (0.75, 0.75, 0.25)\}
                               -x+3/4, +z+3/4, +y+1/4
\{4^{-}00z \mid (0.25, 0.75, 0.75)\}
                               +y+1/4,-x+3/4,+z+3/4
  {2_0y0|(0.5,0.0,0.5)}
                                  -x+1/2, +y, -z+1/2
{3^+_x-x-x|(0.5,0.0,0.5)}
                                  -z+1/2,-x,+y+1/2
\{2_x-x0|(0.25,0.75,0.75)\}
                               -y+1/4,-x+3/4,-z+3/4
                                +x+1/4,-z+3/4,+y+3/4
{4^+_x00|(0.25,0.75,0.75)}
{3^+-xx-x|(0.5,0.5,0.0)}
                                  +z+1/2,-x+1/2,-y
\{2_0y-y\mid (0.75,0.25,0.75)\}
                                -x+3/4, -z+1/4, -y+3/4
{3^+_-x-xx|(0.5,0.0,0.5)}
                                  -z+1/2,+x,-y+1/2
                                +x+1/4, +z+1/4, -y+1/4
\{4^-x00|(0.25,0.25,0.25)\}
 \{2_{x}0x | (0.75, 0.75, 0.25)\}
                               +z+3/4,-y+3/4,+x+1/4
 {3^-_xxx|(0.5,0.5,0.0)}
                                  +y+1/2,+z+1/2,+x
\{4^{-}0y0|(0.75,0.75,0.25)\}
                                -z+3/4,+y+3/4,+x+1/4
{4^+_0y0|(0.25,0.25,0.25)}
                               +z+1/4, +y+1/4, -x+1/4
{3^-_x-x}(0.0,0.5,0.5)
                                  +y,-z+1/2,-x+1/2
\{2_{-x0x}|(0.25,0.25,0.25)\}
                                -z+1/4, -y+1/4, -x+1/4
{3^-_x-x-x|(0.5,0.5,0.0)}
                                  -y+1/2,+z+1/2,-x
{3^--xx-x|(0.0,0.5,0.5)}
                                  -y, -z+1/2, +x+1/2
```

space group: 211 {'Hall': 'I 4 2 3', 'HM': 'I 4 3 2'}

Crystal system: Cubic

+x,+y,+z

-y,+x,+z

+x,-y,-z

+z,+x,+y

•		
	Seitz	Jones
		+x,+y,+z
	{4^+_00z (0.0,0.0,0.0)}	-y,+x,+z
	{2_x00 (0.0,0.0,0.0)}	+x,-y,-z
	{3^+_xxx (0.0,0.0,0.0)}	+z,+x,+y
	{2_00z (0.0,0.0,0.0)}	-x,-y,+z
	{2_xx0 (0.0,0.0,0.0)}	+y,+x,-z
	{2_0yy (0.0,0.0,0.0)}	-x,+z,+y
	$\{4^{-}00z (0.0,0.0,0.0)\}$	+y,-x,+z
	{2_0y0 (0.0,0.0,0.0)}	-x,+y,-z
	{3^+_x-x-x (0.0,0.0,0.0)}	-z,-x,+y
	{2_x-x0 (0.0,0.0,0.0)}	-y,-x,-z
	{4^+_x00 (0.0,0.0,0.0)}	+x,-z,+y
	{3^+xx-x (0.0,0.0,0.0)}	+z,-x,-y
	{2_0y-y (0.0,0.0,0.0)}	-x,-z,-y
	{3^+x-xx (0.0,0.0,0.0)}	-z,+x,-y
	{4^x00 (0.0,0.0,0.0)}	+x,+z,-y
	{2_x0x (0.0,0.0,0.0)}	+z,-y,+x
	{3^xxx (0.0,0.0,0.0)}	+y,+z,+x
	{4^0y0 (0.0,0.0,0.0)}	-z,+y,+x
	{4^+_0y0 (0.0,0.0,0.0)}	+z,+y,-x

```
\{3^--x-xx\mid (0.0,0.0,0.0)\}
                                        +y,-z,-x
    \{2\_-x0x \mid (0.0,0.0,0.0)\}
                                        -z,-y,-x
  \{3^-x-x-x|(0.0,0.0,0.0)\}
                                        -y, +z, -x
  {3^--xx-x | (0.0,0.0,0.0)}
                                        -y,-z,+x
       {1|(0.5,0.5,0.5)}
                                 +x+1/2, +y+1/2, +z+1/2
   \{4^+_00z|(0.5,0.5,0.5)\}
                                 -y+1/2,+x+1/2,+z+1/2
                                 +x+1/2,-y+1/2,-z+1/2
    \{2_{x00}|(0.5,0.5,0.5)\}
   \{3^+ xxx \mid (0.5, 0.5, 0.5)\}
                                 +z+1/2,+x+1/2,+y+1/2
    \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                 -x+1/2,-y+1/2,+z+1/2
                                 +y+1/2,+x+1/2,-z+1/2
    \{2_x \times 0 \mid (0.5, 0.5, 0.5)\}
    \{2_{0yy} | (0.5, 0.5, 0.5)\}
                                 -x+1/2,+z+1/2,+y+1/2
   \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                 +y+1/2,-x+1/2,+z+1/2
    {2_0y0|(0.5,0.5,0.5)}
                                 -x+1/2,+y+1/2,-z+1/2
  \{3^+x^-x^-x^-(0.5,0.5,0.5)\}
                                 -z+1/2, -x+1/2, +y+1/2
    \{2_x-x0\mid(0.5,0.5,0.5)\}
                                 -y+1/2, -x+1/2, -z+1/2
   {4^+_x00|(0.5,0.5,0.5)}
                                 +x+1/2,-z+1/2,+y+1/2
  {3^+-xx-x|(0.5,0.5,0.5)}
                                 +z+1/2,-x+1/2,-y+1/2
    \{2_0y-y|(0.5,0.5,0.5)\}
                                 -x+1/2,-z+1/2,-y+1/2
                                 -z+1/2,+x+1/2,-y+1/2
  {3^+_-x^-x^+|(0.5,0.5,0.5)}
   {4^-_x00|(0.5,0.5,0.5)}
                                 +x+1/2,+z+1/2,-y+1/2
    \{2_{x0x} | (0.5, 0.5, 0.5)\}
                                 +z+1/2,-y+1/2,+x+1/2
   {3^-_xxx|(0.5,0.5,0.5)}
                                 +y+1/2,+z+1/2,+x+1/2
   \{4^-_0y0|(0.5,0.5,0.5)\}
                                 -z+1/2,+y+1/2,+x+1/2
   {4^+_0y0|(0.5,0.5,0.5)}
                                 +z+1/2, +y+1/2, -x+1/2
  \{3^--x-xx\mid (0.5,0.5,0.5)\}
                                 +y+1/2,-z+1/2,-x+1/2
    \{2_{-x0x} | (0.5, 0.5, 0.5)\}
                                 -z+1/2, -y+1/2, -x+1/2
  \{3^-x-x-x|(0.5,0.5,0.5)\}
                                 -y+1/2,+z+1/2,-x+1/2
  \{3^--xx-x \mid (0.5,0.5,0.5)\}
                                 -y+1/2,-z+1/2,+x+1/2
*******
space group: 212 {'Hall': ' P 4acd 2ab 3', 'HM': 'P 43 3 2'}
Crystal system: Cubic
+x,+y,+z
-y+3/4, +x+1/4, +z+3/4
+x+1/2,-y+1/2,-z
+Z,+X,+y
             Seitz
                                          Jones
      {1|(0.0,0.0,0.0)}
                                         +x,+y,+z
  \{4^+_{00z} | (0.75, 0.25, 0.75)\}
                                  -y+3/4, +x+1/4, +z+3/4
    {2_x00|(0.5,0.5,0.0)}
                                    +x+1/2,-y+1/2,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                         +z,+x,+y
    \{2\_00z \mid (0.5,0.0,0.5)\}
                                    -x+1/2,-y,+z+1/2
   {2_xx0|(0.25,0.75,0.75)}
                                  +y+1/4, +x+3/4, -z+3/4
   {2_0yy|(0.75,0.25,0.75)}
                                  -x+3/4, +z+1/4, +y+3/4
  {4^-_00z|(0.75,0.75,0.25)}
                                  +y+3/4,-x+3/4,+z+1/4
    {2_0y0|(0.0,0.5,0.5)}
                                    -x,+y+1/2,-z+1/2
  {3^+_x-x-x|(0.5,0.0,0.5)}
                                    -z+1/2, -x, +y+1/2
```

{2_x-x0|(0.25,0.25,0.25)} {4^+_x00|(0.75,0.75,0.25)} -y+1/4, -x+1/4, -z+1/4

+x+3/4,-z+3/4,+y+1/4

```
{3^+-xx-x|(0.5,0.5,0.0)}
                                 +z+1/2,-x+1/2,-y
\{2_0y-y|(0.25,0.25,0.25)\}
                               -x+1/4, -z+1/4, -y+1/4
\{3^+_-x^-x^-\}
                                 -z, +x+1/2, -y+1/2
\{4^-x00|(0.25,0.75,0.25)\}
                               +x+1/4, +z+3/4, -y+1/4
 \{2_x0x|(0.75,0.75,0.25)\}
                               +z+3/4,-y+3/4,+x+1/4
 \{3^-xxx|(0.0,0.0,0.0)\}
                                     +y,+z,+x
{4^-_0y0|(0.75,0.25,0.75)}
                               -z+3/4,+y+1/4,+x+3/4
{4^+_0y0|(0.25,0.75,0.75)}
                               +z+1/4, +y+3/4, -x+3/4
\{3^--x-xx\mid(0.5,0.5,0.0)\}
                                 +y+1/2,-z+1/2,-x
\{2_-x0x \mid (0.25, 0.25, 0.25)\}
                               -z+1/4, -y+1/4, -x+1/4
\{3^-x-x-x|(0.0,0.5,0.5)\}
                                 -y, +z+1/2, -x+1/2
{3^--xx-x|(0.5,0.0,0.5)}
                                 -y+1/2,-z,+x+1/2
```

```
*******
```

space group: 213 {'Hall': ' P 4bd 2ab 3', 'HM': 'P 41 3 2'}

Crystal system: Cubic

+x,+y,+z

-y+1/4, +x+3/4, +z+1/4

+x+1/2,-y+1/2,-z

+z,+x,+y

```
Seitz
                                       Jones
    \{1 \mid (0.0, 0.0, 0.0)\}
                                      +x,+y,+z
\{4^+_{00z} | (0.25, 0.75, 0.25)\}
                               -y+1/4, +x+3/4, +z+1/4
  \{2_{x00}|(0.5,0.5,0.0)\}
                                  +x+1/2,-y+1/2,-z
 {3^+_xxx|(0.0,0.0,0.0)}
                                      +z,+x,+y
  \{2\_00z \mid (0.5,0.0,0.5)\}
                                  -x+1/2,-y,+z+1/2
 {2_xx0|(0.75,0.25,0.25)}
                               +y+3/4, +x+1/4, -z+1/4
 {2_0yy|(0.25,0.75,0.25)}
                               -x+1/4, +z+3/4, +y+1/4
\{4^-_00z \mid (0.25, 0.25, 0.75)\}
                               +y+1/4,-x+1/4,+z+3/4
  {2_0y0|(0.0,0.5,0.5)}
                                  -x,+y+1/2,-z+1/2
\{3^+x^-x^-x^-\}
                                  -z+1/2,-x,+y+1/2
\{2_x-x0|(0.75,0.75,0.75)\}
                               -y+3/4, -x+3/4, -z+3/4
                               +x+1/4,-z+1/4,+y+3/4
{4^+_x00|(0.25,0.25,0.75)}
{3^+-xx-x|(0.5,0.5,0.0)}
                                  +z+1/2,-x+1/2,-y
\{2_0y-y\mid (0.75,0.75,0.75)\}
                               -x+3/4, -z+3/4, -y+3/4
\{3^+_-x^-x^-\}
                                  -z, +x+1/2, -y+1/2
                               +x+3/4, +z+1/4, -y+1/4
\{4^-x00|(0.75,0.25,0.25)\}
 \{2_{x0x} | (0.25, 0.25, 0.75)\}
                               +z+1/4,-y+1/4,+x+3/4
 {3^-_xxx|(0.0,0.0,0.0)}
                                      +y, +z, +x
{4^-_0y0|(0.25,0.75,0.25)}
                               -z+1/4, +y+3/4, +x+1/4
\{4^+_0y0|(0.75,0.25,0.25)\}
                               +z+3/4, +y+1/4, -x+1/4
\{3^--x-xx\mid(0.5,0.5,0.0)\}
                                  +y+1/2,-z+1/2,-x
\{2_-x0x|(0.75,0.75,0.75)\}
                               -z+3/4,-y+3/4,-x+3/4
\{3^-x-x-x|(0.0,0.5,0.5)\}
                                  -y, +z+1/2, -x+1/2
{3^-_xx-x|(0.5,0.0,0.5)}
                                  -y+1/2,-z,+x+1/2
```

```
space group: 214 {'Hall': ' I 4bd 2c 3', 'HM': 'I 41 3 2'}
Crystal system: Cubic
+x,+y,+z
-y+1/4,+x+3/4,+z+1/4
+x,-y,-z+1/2
+z,+x,+y
                                           Jones
             Seitz
      \{1 \mid (0.0, 0.0, 0.0)\}
                                          +x,+y,+z
  \{4^+_{00z} | (0.25, 0.75, 0.25)\}
                                   -y+1/4, +x+3/4, +z+1/4
    {2_x00|(0.0,0.0,0.5)}
                                       +x,-y,-z+1/2
   {3^+_xxx|(0.0,0.0,0.0)}
                                          +Z,+X,+y
    \{2\_00z \mid (0.5,0.0,0.5)\}
                                     -x+1/2, -y, +z+1/2
   \{2_x \times 0 \mid (0.25, 0.75, 0.75)\}
                                   +y+1/4, +x+3/4, -z+3/4
   \{2_{0yy} | (0.25, 0.75, 0.25)\}
                                   -x+1/4, +z+3/4, +y+1/4
  \{4^-00z \mid (0.25, 0.25, 0.75)\}
                                   +y+1/4,-x+1/4,+z+3/4
                                       -x+1/2, +y, -z
    {2_0y0|(0.5,0.0,0.0)}
  \{3^+x^-x^-x^-\}
                                     -z+1/2,-x,+y+1/2
  \{2_x-x0|(0.25,0.25,0.25)\}
                                   -y+1/4, -x+1/4, -z+1/4
  \{4^+x00|(0.25,0.25,0.75)\}
                                   +x+1/4,-z+1/4,+y+3/4
  \{3^+-xx-x\mid(0.0,0.0,0.5)\}
                                       +z,-x,-y+1/2
  \{2_0y-y\mid (0.25,0.25,0.25)\}
                                   -x+1/4, -z+1/4, -y+1/4
  \{3^+-x-x^+ (0.5,0.0,0.0)\}
                                       -z+1/2,+x,-y
  \{4^-x00|(0.25,0.75,0.75)\}
                                   +x+1/4,+z+3/4,-y+3/4
   \{2_x0x \mid (0.25, 0.25, 0.75)\}
                                   +z+1/4,-y+1/4,+x+3/4
   \{3^-xxx|(0.0,0.0,0.0)\}
                                          +y, +z, +x
  \{4^- 0 \lor 0 \mid (0.75, 0.25, 0.75)\}
                                   -z+3/4, +y+1/4, +x+3/4
  \{4^+_0y0|(0.75,0.25,0.25)\}
                                   +z+3/4, +y+1/4, -x+1/4
  {3^-_x-x}(0.5,0.5,0.0)
                                     +y+1/2,-z+1/2,-x
  \{2_{-}\times 0\times | (0.25, 0.25, 0.25)\}
                                   -z+1/4, -y+1/4, -x+1/4
  \{3^-x-x-x|(0.5,0.0,0.0)\}
                                       -y+1/2,+z,-x
  \{3^- -xx-x \mid (0.0,0.5,0.0)\}
                                       -y, -z+1/2, +x
       {1|(0.5,0.5,0.5)}
                                   +x+1/2,+y+1/2,+z+1/2
  \{4^+_{00z}|(0.75,0.25,0.75)\}
                                   -y+3/4,+x+1/4,+z+3/4
    \{2_{x00} | (0.5, 0.5, 0.0)\}
                                     +x+1/2,-y+1/2,-z
   {3^+_xxx|(0.5,0.5,0.5)}
                                   +z+1/2,+x+1/2,+y+1/2
    {2_00z|(0.0,0.5,0.0)}
                                       -x,-y+1/2,+z
   {2_xx0|(0.75,0.25,0.25)}
                                   +y+3/4, +x+1/4, -z+1/4
   \{2_{0yy} \mid (0.75, 0.25, 0.75)\}
                                   -x+3/4, +z+1/4, +y+3/4
  \{4^-_00z \mid (0.75, 0.75, 0.25)\}
                                   +y+3/4,-x+3/4,+z+1/4
                                     -x,+y+1/2,-z+1/2
    {2_0y0|(0.0,0.5,0.5)}
  \{3^+_x-x-x|(0.0,0.5,0.0)\}
                                       -z, -x+1/2, +y
  \{2_x-x0|(0.75,0.75,0.75)\}
                                   -y+3/4, -x+3/4, -z+3/4
  {4^+_x00|(0.75,0.75,0.25)}
                                   +x+3/4,-z+3/4,+y+1/4
  {3^+-xx-x|(0.5,0.5,0.0)}
                                     +z+1/2,-x+1/2,-y
  \{2_0y-y|(0.75,0.75,0.75)\}
                                   -x+3/4, -z+3/4, -y+3/4
  {3^+_-x^-x^-|(0.0,0.5,0.5)}
                                     -z, +x+1/2, -y+1/2
  {4^-_x00|(0.75,0.25,0.25)}
                                   +x+3/4,+z+1/4,-y+1/4
   {2_x0x|(0.75,0.75,0.25)}
                                   +z+3/4,-y+3/4,+x+1/4
   \{3^-xxx|(0.5,0.5,0.5)\}
                                   +y+1/2,+z+1/2,+x+1/2
  \{4^-_0y0|(0.25,0.75,0.25)\}
                                   -z+1/4, +y+3/4, +x+1/4
  \{4^+ 0_0 | (0.25, 0.75, 0.75)\}
                                 +z+1/4,+y+3/4,-x+3/4
```

```
{3^-_x-x\times|(0.0,0.0,0.5)}
                                      +y,-z,-x+1/2
                                  -z+3/4,-y+3/4,-x+3/4
  \{2_{-}\times 0\times | (0.75, 0.75, 0.75)\}
  {3^-_x-x-x|(0.0,0.5,0.5)}
                                    -y, +z+1/2, -x+1/2
  {3^--xx-x|(0.5,0.0,0.5)}
                                    -y+1/2,-z,+x+1/2
*******
space group: 215 {'Hall': ' P -4 2 3', 'HM': 'P -4 3 m'}
Crystal system: Cubic
+x,+y,+z
+y,-x,-z
+x,-y,-z
+z,+x,+y
             Seitz
                                  Jones
      {1|(0.0,0.0,0.0)}
                                +x,+y,+z
   {-4^+_00z|(0.0,0.0,0.0)} |
                                +y,-x,-z
    \{2_{\times}00 \mid (0.0, 0.0, 0.0)\}
                                 +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                 +z,+x,+y
    {2_00z|(0.0,0.0,0.0)}
                                 -x,-y,+z
    \{m_x-xz \mid (0.0,0.0,0.0)\}
                                 -y,-x,+z
    \{m_xy-y \mid (0.0,0.0,0.0)\}
                                 +x,-z,-y
   \{-4^-_00z \mid (0.0,0.0,0.0)\}
                                 -y,+x,-z
    {2_0y0|(0.0,0.0,0.0)}
                                 -x,+y,-z
  {3^+_x-x-x|(0.0,0.0,0.0)}
                                 -z,-x,+y
    \{m_xxz | (0.0,0.0,0.0)\}
                                 +y,+x,+z
   {-4^+_x00|(0.0,0.0,0.0)}
                                 -x,+z,-y
  {3^+_-xx-x|(0.0,0.0,0.0)}
                                 +z,-x,-y
    \{m_xyy \mid (0.0,0.0,0.0)\}
                                 +x,+z,+y
  {3^+_-x^-x^+|(0.0,0.0,0.0)}
                                 -z,+x,-y
   \{-4^-x00 \mid (0.0,0.0,0.0)\}
                                 -x,-z,+y
    \{m_-xyz \mid (0.0,0.0,0.0)\}
                                 -z,+y,-x
   \{3^-xxx|(0.0,0.0,0.0)\}
                                 +y,+z,+x
   \{-4^-_0y0|(0.0,0.0,0.0)\}
                                 +z,-y,-x
   {-4^+_0y0|(0.0,0.0,0.0)}
                                 -z,-y,+x
  {3^-_x - x - xx | (0.0, 0.0, 0.0)} |
                                 +y,-z,-x
    \{m_xyx | (0.0,0.0,0.0)\}
                               +z,+y,+x
  {3^-_x-x-x}(0.0,0.0,0.0) | -y,+z,-x
  \{3^--xx-x \mid (0.0,0.0,0.0)\} \mid -y,-z,+x
. . . . . . . . . . . . . . . . . . . .
*******
space group: 216 {'Hall': ' F -4 2 3', 'HM': 'F -4 3 m'}
Crystal system: Cubic
+x,+y,+z
+y,-x,-z
+x,-y,-z
+z,+x,+y
 . . . . . . . . . . . . . . . . . . .
```

Seitz	Jones
{1 (0.0,0.0,0.0)} {-4^++_00z (0.0,0.0,0.0)} {2_x00 (0.0,0.0,0.0)} {3^++_xxx (0.0,0.0,0.0)} {m_x-xz (0.0,0.0,0.0)} {m_xy-y (0.0,0.0,0.0)} {1-4^00z (0.0,0.0,0.0)} {2_0y0 (0.0,0.0,0.0)} {1-4^00z (0.0,0.0,0.0)} {1-4^+-x00 (0.0,0.0,0.0)} {1-4^++x00 (0.0,0.0,0.0)} {1-4^+-x00 (0.0,0.0,0.0)} {1-4^+-x00 (0.0,0.0,0.0)} {1-4^x00 (0.0,0.0,0.0)} {1-4^x00 (0.0,0.0,0.0)} {1-4^x00 (0.0,0.0,0.0)} {1-4^y00 (0.0,0.0,0.0)} {1-4^y00 (0.0,0.0,0.0)} {1-4^y00 (0.0,0.0,0.0)} {1-4^x00 (0.0,0.0,0.0)} {1-4^x00 (0.0,0.0,0.0)} {1-4^x00 (0.0,0.0,0.0)} {1-4^y00 (0.0,0.0,0.0)} {1-4^y00 (0.0,0.0,0.0)} {1-4^y00 (0.0,0.0,0.0)} {1-4^y00 (0.0,0.0,0.0)} {1-4^xxxx (0.0,0.0,0.0)} {1-4^xxxx (0.0,0.0,0.0)} {1-4^xxxx (0.0,0.0,0.0)} {1-4^xxxx (0.0,0.0,0.0)} {1-4^xxxx (0.0,0.0,0.0)} {1-4^xxxx (0.0,0.0,0.0)} {1-4^xxxxx (0.0,0.0,0.0)} {1-4^xxxxxx (0.0,0.0,0.0)} {1-4^xxxxxx (0.0,0.0,0.0)}	+x,+y,+z +y,-x,-z +x,-y,-z +z,+x,+y -x,-y,+z -y,-x,+z +x,-z,-y -y,+x,-z -x,+y,-z -z,-x,+y +y,+x,+z -x,+z,-y +z,-x,-y +x,+z,+y -z,+x,-y -z,+y,-x +y,+z,+x +z,-y,-x +y,-z,-x +y,-z,-x +y,-z,-x +y,-z,-x +y,-z,-x +y,-z,-x +y,-z,-x +z,+y,+x +y,-z,-x +z,+y,+x +y,-z,-x +z,+y,+x +y,-z,-x +z,+y,+x -y,-z,+x +x,+y+1/2,-z+1/2 +x,-y+1/2,-z+1/2 +x,-y+1/2,-z+1/2 -x,-y+1/2,-z+1/2 -x,-y+1/2,-z+1/2 -y,-x+1/2,-z+1/2 -y,-x+1/2,-z+1/2 -y,-x+1/2,-z+1/2 -y,+x+1/2,-z+1/2 -y,+x+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+z+1/2,-y+1/2 -x,+z+1/2,-y+1/2
<pre>{3^+_xxx (0.0,0.5,0.5)} {2_00z (0.0,0.5,0.5)} {m_x-xz (0.0,0.5,0.5)} {m_xy-y (0.0,0.5,0.5)} {-4^00z (0.0,0.5,0.5)} {2_0y0 (0.0,0.5,0.5)} {3^+_x-x-x (0.0,0.5,0.5)} {m_xxz (0.0,0.5,0.5)} {4-4^+_x00 (0.0,0.5,0.5)} {3^+xx-x (0.0,0.5,0.5)} {m_xyy (0.0,0.5,0.5)} {3^+x-xx (0.0,0.5,0.5)} {3^+x-xx (0.0,0.5,0.5)} {4xyy (0.0,0.5,0.5)} {4xyz (0.0,0.5,0.5)} {3xxx (0.0,0.5,0.5)} {3xxx (0.0,0.5,0.5)}</pre>	+z,+x+1/2,+y+1/2 -x,-y+1/2,+z+1/2 -y,-x+1/2,+z+1/2 +x,-z+1/2,-y+1/2 -y,+x+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -z,-x+1/2,+y+1/2 +y,+x+1/2,-y+1/2 +z,-x+1/2,-y+1/2 +z,-x+1/2,-y+1/2 -z,+x+1/2,-y+1/2 -z,+x+1/2,-y+1/2 -z,+x+1/2,-y+1/2 -z,+y+1/2,-x+1/2 +y,+z+1/2,+x+1/2 +y,+z+1/2,+x+1/2
{-4^0y0 (0.0,0.5,0.5)} {-4^+_0y0 (0.0,0.5,0.5)} {3^x-xx (0.0,0.5,0.5)} {m_xyx (0.0,0.5,0.5)} {3^x-x-x (0.0,0.5,0.5)} {3^xx-x (0.0,0.5,0.5)} {1 (0.5,0.0,0.5)} {-4^+_00z (0.5,0.0,0.5)} {2_x00 (0.5,0.0,0.5)} {3^+_xxx (0.5,0.0,0.5)}	+z,-y+1/2,-x+1/2 -z,-y+1/2,+x+1/2 +y,-z+1/2,-x+1/2 +z,+y+1/2,+x+1/2 -y,+z+1/2,-x+1/2 -y,-z+1/2,+x+1/2 +x+1/2,+y,+z+1/2 +y+1/2,-x,-z+1/2 +z+1/2,-y,-z+1/2 +z+1/2,+x,+y+1/2

```
{2_00z|(0.5,0.0,0.5)}
                              -x+1/2,-y,+z+1/2
  \{m_x-xz\mid(0.5,0.0,0.5)\}
                              -y+1/2,-x,+z+1/2
  {m_xy-y|(0.5,0.0,0.5)}
                              +x+1/2,-z,-y+1/2
 \{-4^-_00z \mid (0.5,0.0,0.5)\}
                              -y+1/2,+x,-z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                              -x+1/2,+y,-z+1/2
{3^+_x-x-x|(0.5,0.0,0.5)}
                              -z+1/2,-x,+y+1/2
  \{m_{xxz} | (0.5, 0.0, 0.5)\}
                              +y+1/2,+x,+z+1/2
 {-4^+_x00|(0.5,0.0,0.5)}
                              -x+1/2,+z,-y+1/2
\{3^+-xx-x\mid(0.5,0.0,0.5)\}
                              +z+1/2,-x,-y+1/2
  {m_xyy|(0.5,0.0,0.5)}
                              +x+1/2,+z,+y+1/2
\{3^+_-x^-x^-\}
                              -z+1/2,+x,-y+1/2
 \{-4^- \times 00 \mid (0.5, 0.0, 0.5)\}
                              -x+1/2,-z,+y+1/2
  \{m_-xyz \mid (0.5,0.0,0.5)\}
                              -z+1/2,+y,-x+1/2
 {3^-_xxx|(0.5,0.0,0.5)}
                              +y+1/2,+z,+x+1/2
                              +z+1/2,-y,-x+1/2
 \{-4^-_0y0|(0.5,0.0,0.5)\}
 {-4^+_0y0|(0.5,0.0,0.5)}
                              -z+1/2,-y,+x+1/2
\{3^--x-xx\mid(0.5,0.0,0.5)\}
                              +y+1/2,-z,-x+1/2
  {m_xyx|(0.5,0.0,0.5)}
                              +z+1/2, +y, +x+1/2
{3^-_x-x-x|(0.5,0.0,0.5)}
                              -y+1/2,+z,-x+1/2
{3^-_-xx-x|(0.5,0.0,0.5)}
                              -y+1/2,-z,+x+1/2
    {1|(0.5,0.5,0.0)}
                              +x+1/2, +y+1/2, +z
 \{-4^+_00z|(0.5,0.5,0.0)\}
                              +y+1/2,-x+1/2,-z
  {2_x00|(0.5,0.5,0.0)}
                              +x+1/2,-y+1/2,-z
 {3^+_xxx|(0.5,0.5,0.0)}
                              +z+1/2,+x+1/2,+y
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                              -x+1/2,-y+1/2,+z
  \{m_x-xz\mid(0.5,0.5,0.0)\}
                              -y+1/2,-x+1/2,+z
  \{m_xy-y \mid (0.5,0.5,0.0)\}
                              +x+1/2,-z+1/2,-y
 \{-4^-00z \mid (0.5, 0.5, 0.0)\}
                              -y+1/2,+x+1/2,-z
  {2_0y0|(0.5,0.5,0.0)}
                              -x+1/2,+y+1/2,-z
{3^+_x-x-x|(0.5,0.5,0.0)}
                              -z+1/2, -x+1/2, +y
  \{m_{xxz} | (0.5, 0.5, 0.0)\}
                              +y+1/2,+x+1/2,+z
 {-4^+_x00|(0.5,0.5,0.0)}
                              -x+1/2,+z+1/2,-y
{3^+_-xx-x|(0.5,0.5,0.0)}
                              +z+1/2,-x+1/2,-y
  {m_xyy|(0.5,0.5,0.0)}
                              +x+1/2,+z+1/2,+y
{3^+_-x^-x^+|(0.5,0.5,0.0)}
                              -z+1/2,+x+1/2,-y
 \{-4^-x00|(0.5,0.5,0.0)\}
                              -x+1/2, -z+1/2, +y
  \{m_-xyz \mid (0.5,0.5,0.0)\}
                              -z+1/2,+y+1/2,-x
 {3^-_xxx|(0.5,0.5,0.0)}
                              +y+1/2,+z+1/2,+x
                              +z+1/2,-y+1/2,-x
 {-4^-_0y0|(0.5,0.5,0.0)}
 {-4^+_0y0|(0.5,0.5,0.0)}
                              -z+1/2,-y+1/2,+x
\{3^--x-xx\mid (0.5,0.5,0.0)\}
                              +y+1/2,-z+1/2,-x
  \{m_xyx|(0.5,0.5,0.0)\}
                              +z+1/2,+y+1/2,+x
\{3^-x-x-x|(0.5,0.5,0.0)\}
                              -y+1/2,+z+1/2,-x
\{3^--xx-x\mid(0.5,0.5,0.0)\}
                              -y+1/2,-z+1/2,+x
```

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Crystal system: Cubic +x,+y,+z +y,-x,-z +x,-y,-z +z,+x,+y
```

<u>+</u>				
Seitz	Jones			
{1 (0.0,0.0,0.0)}	+x,+y,+z			
$ \{-4^+_00z (0.0,0.0,0.0)\} $	+y,-x,-z			
{2_x00 (0.0,0.0,0.0)}	+x,-y,-z			
{3^+_xxx (0.0,0.0,0.0)}	+z,+x,+y			
{2_00z (0.0,0.0,0.0)}	-x,-y,+z			
$\{m_x-xz\mid (0.0,0.0,0.0)\}\$	-y,-x,+z			
$\{m_xy-y \mid (0.0,0.0,0.0)\}$	+x,-z,-y			
$\{-4^{-}00z (0.0,0.0,0.0)\}$	-y,+x,-z			
{2_0y0 (0.0,0.0,0.0)}	-x,+y,-z			
{3^+_x-x-x (0.0,0.0,0.0)}	-z,-x,+y			
{m_xxz (0.0,0.0,0.0)}	+y,+x,+z			
$\{-4^+ \times 00 \mid (0.0, 0.0, 0.0)\}\$	-x,+z,-y			
[\[\langle 3^+xx-x \] \[\langle 0.0,0.0,0.0 \] \[\langle \]	+z,-x,-y			
{m_xyy (0.0,0.0,0.0)}	+x,+z,+y			
{3^+x-xx (0.0,0.0,0.0)} {-4^x00 (0.0,0.0,0.0)}	-z,+x,-y			
\{\text{mxyz} (0.0,0.0,0.0)}	-X,-Z,+y			
{3^xxx (0.0,0.0,0.0)}	-z,+y,-x			
-4^0y0 (0.0,0.0,0.0)}	+y,+z,+x			
-4^+_0y0 (0.0,0.0,0.0)}	+z,-y,-x -z,-y,+x			
{3^x-xx (0.0,0.0,0.0)}	+y,-z,-x			
{m_xyx (0.0,0.0,0.0)}	+z,+y,+x			
{3^x-x-x (0.0,0.0,0.0)}	-y,+z,-x			
{3^xx-x (0.0,0.0,0.0)}	-y,-z,+x			
$\{1 (0.5,0.5,0.5)\}$	+x+1/2,+y+1/2,+z+1/2			
$\{-4^+_00z (0.5,0.5,0.5)\}$	+y+1/2,-x+1/2,-z+1/2			
$\{2_{\times}00 (0.5,0.5,0.5)\}$	+x+1/2,-y+1/2,-z+1/2			
$\{3^+ \times \times (0.5, 0.5, 0.5)\}$	+z+1/2,+x+1/2,+y+1/2			
$\{2_00z \mid (0.5, 0.5, 0.5)\}$	-x+1/2, -y+1/2, +z+1/2			
$\{m_x-xz\mid(0.5,0.5,0.5)\}\$	-y+1/2,-x+1/2,+z+1/2			
$ \{m_xy-y (0.5,0.5,0.5)\} $	+x+1/2,-z+1/2,-y+1/2			
$ \{-4^00z (0.5,0.5,0.5)\} $	-y+1/2,+x+1/2,-z+1/2			
{2_0y0 (0.5,0.5,0.5)}	-x+1/2,+y+1/2,-z+1/2			
$ \{3^+_x - x - x (0.5, 0.5, 0.5)\} $	-z+1/2, -x+1/2, +y+1/2			
$\{m_xxz (0.5,0.5,0.5)\}$	+y+1/2,+x+1/2,+z+1/2			
$\{-4^+ \times 00 \mid (0.5, 0.5, 0.5)\}$	-x+1/2,+z+1/2,-y+1/2			
{3^+xx-x (0.5,0.5,0.5)}	+z+1/2, -x+1/2, -y+1/2			
{m_xyy (0.5,0.5,0.5)}	+x+1/2,+z+1/2,+y+1/2			
{3^+x-xx (0.5,0.5,0.5)}	-z+1/2, +x+1/2, -y+1/2			
$\{-4^{-} \times 00 \mid (0.5, 0.5, 0.5)\}\$	-x+1/2, -z+1/2, +y+1/2			
$\{mxyz (0.5,0.5,0.5)\}\$	-z+1/2, +y+1/2, -x+1/2			
{3^xxx (0.5,0.5,0.5)}	+y+1/2,+z+1/2,+x+1/2			
$\{-4^{-}_{0},0,0,0,5,0,5,0,5,0,5,0,5,0,5,0,5,0,5,0$	+z+1/2,-y+1/2,-x+1/2			
-4^+_0y0 (0.5,0.5,0.5)}	-z+1/2,-y+1/2,+x+1/2			
{3^x-xx (0.5,0.5,0.5)}	+y+1/2,-z+1/2,-x+1/2			
{m_xyx (0.5,0.5,0.5)} {3^x-x-x (0.5,0.5,0.5)}	+z+1/2,+y+1/2,+x+1/2 -y+1/2,+z+1/2,-x+1/2			
{3^x=x=x (0.5,0.5,0.5)}	-y+1/2,-z+1/2,-x+1/2 -y+1/2,-z+1/2,+x+1/2			
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space group: 218 {'Hall': ' P -4n 2 3', 'HM': 'P -4 3 n'}
Crystal system: Cubic
+x,+y,+z
+y+1/2,-x+1/2,-z+1/2
+x,-y,-z
+z,+x,+y
             Seitz
                                        Jones
      {1|(0.0,0.0,0.0)}
                                       +x,+y,+z
   \{-4^+_00z|(0.5,0.5,0.5)\}
                                +y+1/2,-x+1/2,-z+1/2
    \{2_{\times}00 \mid (0.0, 0.0, 0.0)\}
                                       +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                       +z,+x,+y
    {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
    \{m_x-xz\mid(0.5,0.5,0.5)\}
                                -y+1/2, -x+1/2, +z+1/2
    \{m_xy-y \mid (0.5,0.5,0.5)\}
                                +x+1/2,-z+1/2,-y+1/2
   \{-4^-00z|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,-z+1/2
    {2_0y0|(0.0,0.0,0.0)}
                                       -x,+y,-z
  {3^+_x-x-x|(0.0,0.0,0.0)}
                                       -z,-x,+y
    \{m_xxz \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,+x+1/2,+z+1/2
   {-4^+_x00|(0.5,0.5,0.5)}
                                -x+1/2,+z+1/2,-y+1/2
  {3^+_-xx-x|(0.0,0.0,0.0)}
                                       +z,-x,-y
    \{m_xyy | (0.5, 0.5, 0.5)\}
                                +x+1/2,+z+1/2,+y+1/2
  {3^+_-x^-x^-|(0.0,0.0,0.0)}
                                       -z,+x,-y
   \{-4^-x00|(0.5,0.5,0.5)\}
                                -x+1/2,-z+1/2,+y+1/2
    \{m_-xyz \mid (0.5, 0.5, 0.5)\}
                                -z+1/2,+y+1/2,-x+1/2
   \{3^-xxx|(0.0,0.0,0.0)\}
                                       +y, +z, +x
   \{-4^-_0y0|(0.5,0.5,0.5)\}
                                +z+1/2,-y+1/2,-x+1/2
   \{-4^+_0y0|(0.5,0.5,0.5)\}
                                -z+1/2,-y+1/2,+x+1/2
  \{3^--x-xx\mid (0.0,0.0,0.0)\}
                                       +y,-z,-x
    \{m_xyx \mid (0.5, 0.5, 0.5)\}
                                +z+1/2, +y+1/2, +x+1/2
  {3^-_x-x-x|(0.0,0.0,0.0)}
                                       -y,+z,-x
  \{3^--xx-x \mid (0.0,0.0,0.0)\} \mid
                                       -y,-z,+x
******
space group: 219 {'Hall': ' F -4c 2 3', 'HM': 'F -4 3 c'}
Crystal system: Cubic
+x,+y,+z
+y,-x,-z+1/2
+x,-y,-z
+z,+x,+y
             Seitz
                                        Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
   \{-4^+_{00z}|(0.0,0.0,0.5)\}
                                     +y,-x,-z+1/2
    {2_x00|(0.0,0.0,0.0)}
                                       +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                       +z,+x,+y
```

```
{2_00z|(0.0,0.0,0.0)}
                                      -x,-y,+z
  \{m_x-xz\mid(0.0,0.0,0.5)\}
                                    -y, -x, +z+1/2
  {m_xy-y|(0.0,0.0,0.5)}
                                    +x,-z,-y+1/2
 \{-4^-_00z \mid (0.0,0.0,0.5)\}
                                    -y, +x, -z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                      -x,+y,-z
{3^+_x-x-x|(0.0,0.0,0.0)}
                                      -z,-x,+y
  \{m_x \times z \mid (0.0, 0.0, 0.5)\}
                                    +y,+x,+z+1/2
 {-4^+_x00|(0.0,0.0,0.5)}
                                    -x,+z,-y+1/2
\{3^+-xx-x\mid (0.0,0.0,0.0)\}
                                      +z,-x,-y
  \{m_xyy | (0.0,0.0,0.5)\}
                                    +x,+z,+y+1/2
\{3^+_-x^-x^-\}
                                      -z,+x,-y
 \{-4^- \times 00 \mid (0.0, 0.0, 0.5)\}
                                    -x,-z,+y+1/2
  \{m_-xyz \mid (0.5,0.0,0.0)\}
                                    -z+1/2,+y,-x
 {3^-_xxx|(0.0,0.0,0.0)}
                                      +y,+z,+x
 \{-4^-_0y0|(0.5,0.0,0.0)\}
                                    +z+1/2,-y,-x
 \{-4^+_0y0 | (0.5,0.0,0.0)\}
                                    -z+1/2,-y,+x
\{3^--x-xx\mid (0.0,0.0,0.0)\}
                                      +y,-z,-x
  {m_xyx|(0.5,0.0,0.0)}
                                    +z+1/2,+y,+x
{3^-_x-x-x|(0.0,0.0,0.0)}
                                      -y,+z,-x
{3^--xx-x|(0.0,0.0,0.0)}
                                      -y,-z,+x
    {1|(0.0,0.5,0.5)}
                                  +x,+y+1/2,+z+1/2
 \{-4^+_00z \mid (0.0,0.5,0.0)\}
                                    +y,-x+1/2,-z
  {2_x00|(0.0,0.5,0.5)}
                                  +x,-y+1/2,-z+1/2
 {3^+_xxx|(0.0,0.5,0.5)}
                                  +z, +x+1/2, +y+1/2
  {2_00z|(0.0,0.5,0.5)}
                                  -x,-y+1/2,+z+1/2
  \{m_x-xz\mid(0.0,0.5,0.0)\}
                                    -y, -x+1/2, +z
  \{m_xy-y \mid (0.0,0.5,0.0)\}
                                    +x,-z+1/2,-y
 \{-4^-00z \mid (0.0,0.5,0.0)\}
                                    -y, +x+1/2, -z
  {2_0y0|(0.0,0.5,0.5)}
                                  -x,+y+1/2,-z+1/2
{3^+_x-x-x|(0.0,0.5,0.5)}
                                  -z, -x+1/2, +y+1/2
  \{m_{xxz} | (0.0, 0.5, 0.0)\}
                                    +y,+x+1/2,+z
 {-4^+_x00|(0.0,0.5,0.0)}
                                    -x,+z+1/2,-y
{3^+_-xx-x|(0.0,0.5,0.5)}
                                  +z,-x+1/2,-y+1/2
  {m_xyy|(0.0,0.5,0.0)}
                                    +x,+z+1/2,+y
{3^+_-x^-x^-|(0.0,0.5,0.5)}
                                  -z, +x+1/2, -y+1/2
 \{-4^-x00|(0.0,0.5,0.0)\}
                                    -x, -z+1/2, +y
  \{m_-xyz \mid (0.5,0.5,0.5)\}
                               -z+1/2,+y+1/2,-x+1/2
 {3^-_xxx|(0.0,0.5,0.5)}
                                  +y, +z+1/2, +x+1/2
 \{-4^-_0y0|(0.5,0.5,0.5)\}
                               +z+1/2,-y+1/2,-x+1/2
 \{-4^+_0y0|(0.5,0.5,0.5)\}
                               -z+1/2,-y+1/2,+x+1/2
\{3^--x-xx\mid(0.0,0.5,0.5)\}
                                  +y,-z+1/2,-x+1/2
  {m_xyx|(0.5,0.5,0.5)}
                               +z+1/2, +y+1/2, +x+1/2
{3^-_x-x-x|(0.0,0.5,0.5)}
                                  -y, +z+1/2, -x+1/2
\{3^--xx-x\mid (0.0,0.5,0.5)\}
                                  -y, -z+1/2, +x+1/2
                                  +x+1/2, +y, +z+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
 {-4^+_00z|(0.5,0.0,0.0)}
                                    +y+1/2,-x,-z
  \{2_{x00}|(0.5,0.0,0.5)\}
                                  +x+1/2,-y,-z+1/2
 \{3^+ xxx \mid (0.5, 0.0, 0.5)\}
                                  +z+1/2,+x,+y+1/2
  \{2\_00z \mid (0.5,0.0,0.5)\}
                                  -x+1/2, -y, +z+1/2
  \{m_x-xz\mid(0.5,0.0,0.0)\}
                                    -y+1/2,-x,+z
  \{m_xy-y \mid (0.5,0.0,0.0)\}
                                    +x+1/2,-z,-y
 \{-4^-00z \mid (0.5,0.0,0.0)\}
                                    -y+1/2,+x,-z
  {2_0y0|(0.5,0.0,0.5)}
                                  -x+1/2,+y,-z+1/2
{3^+_x-x-x|(0.5,0.0,0.5)}
                                  -z+1/2, -x, +y+1/2
```

```
\{m_{xxz} | (0.5,0.0,0.0)\}
                                      +y+1/2,+x,+z
   {-4^+_x00|(0.5,0.0,0.0)}
                                      -x+1/2,+z,-y
  {3^+_-xx-x|(0.5,0.0,0.5)}
                                    +z+1/2,-x,-y+1/2
    \{m_xyy \mid (0.5,0.0,0.0)\}
                                      +x+1/2,+z,+y
  {3^+_-x^-x^-|(0.5,0.0,0.5)}
                                   -z+1/2,+x,-y+1/2
   \{-4^- \times 00 \mid (0.5, 0.0, 0.0)\}
                                      -x+1/2,-z,+y
    \{m_-xyz \mid (0.0,0.0,0.5)\}
                                      -z,+y,-x+1/2
   {3^-_xxx|(0.5,0.0,0.5)}
                                    +y+1/2,+z,+x+1/2
   \{-4^-_0y0|(0.0,0.0,0.5)\}
                                      +z,-y,-x+1/2
   \{-4^+ 0 \lor 0 \mid (0.0, 0.0, 0.5)\}
                                      -z,-y,+x+1/2
  \{3^--x-xx\mid(0.5,0.0,0.5)\}
                                    +y+1/2,-z,-x+1/2
    {m_xyx|(0.0,0.0,0.5)}
                                      +z,+y,+x+1/2
  {3^-_x-x-x|(0.5,0.0,0.5)}
                                    -y+1/2,+z,-x+1/2
  \{3^--xx-x\mid (0.5,0.0,0.5)\}
                                    -y+1/2,-z,+x+1/2
                                    +x+1/2, +y+1/2, +z
      \{1 \mid (0.5, 0.5, 0.0)\}
   \{-4^+_00z|(0.5,0.5,0.5)\}
                                 +y+1/2,-x+1/2,-z+1/2
    \{2_{x00}|(0.5,0.5,0.0)\}
                                   +x+1/2,-y+1/2,-z
   {3^+_xxx|(0.5,0.5,0.0)}
                                    +z+1/2,+x+1/2,+y
    \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                    -x+1/2, -y+1/2, +z
    \{m_x-xz|(0.5,0.5,0.5)\}
                                 -y+1/2,-x+1/2,+z+1/2
    \{m_xy-y \mid (0.5,0.5,0.5)\}
                                 +x+1/2,-z+1/2,-y+1/2
   \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                 -y+1/2,+x+1/2,-z+1/2
    {2_0y0|(0.5,0.5,0.0)}
                                    -x+1/2,+y+1/2,-z
  {3^+_x-x-x|(0.5,0.5,0.0)}
                                   -z+1/2, -x+1/2, +y
    \{m_xxz \mid (0.5,0.5,0.5)\}
                                 +y+1/2,+x+1/2,+z+1/2
                                 -x+1/2, +z+1/2, -y+1/2
   {-4^+_x00|(0.5,0.5,0.5)}
  {3^+-xx-x|(0.5,0.5,0.0)}
                                   +z+1/2,-x+1/2,-y
    \{m_xyy \mid (0.5, 0.5, 0.5)\}
                                 +x+1/2,+z+1/2,+y+1/2
  \{3^+-x-xx\mid(0.5,0.5,0.0)\}
                                   -z+1/2,+x+1/2,-y
   \{-4^-x00|(0.5,0.5,0.5)\}
                                 -x+1/2,-z+1/2,+y+1/2
    \{m_-xyz \mid (0.0,0.5,0.0)\}
                                      -z, +y+1/2, -x
   \{3^-xxx|(0.5,0.5,0.0)\}
                                    +y+1/2,+z+1/2,+x
   \{-4^-_0y0|(0.0,0.5,0.0)\}
                                      +z,-y+1/2,-x
   \{-4^+_0y0|(0.0,0.5,0.0)\}
                                      -z, -y+1/2, +x
  {3^-_x-x\times|(0.5,0.5,0.0)}
                                    +y+1/2,-z+1/2,-x
    \{m_xyx | (0.0,0.5,0.0)\}
                                      +z,+y+1/2,+x
                                    -y+1/2,+z+1/2,-x
  {3^-_x-x-x|(0.5,0.5,0.0)}
  \{3^--xx-x\mid(0.5,0.5,0.0)\}
                                    -y+1/2,-z+1/2,+x
*******
space group: 220 {'Hall': ' I -4bd 2c 3', 'HM': 'I -4 3 d'}
Crystal system: Cubic
+x,+y,+z
+y+1/4,-x+3/4,-z+1/4
+x,-y,-z+1/2
+Z,+X,+y
              Seitz
                                           Jones
        \{1 \mid (0.0, 0.0, 0.0)\}
                                          +X,+Y,+Z
 \{-4^+,00z|(0.25,0.75,0.25)\} | +y+1/4,-x+3/4,-z+1/4 |
```

```
\{2 \times 00 \mid (0.0, 0.0, 0.5)\}
                                       +x,-y,-z+1/2
  {3^+_xxx|(0.0,0.0,0.0)}
                                         +z,+x,+y
   {2_00z|(0.0,0.5,0.0)}
                                       -x,-y+1/2,+z
 {m_x-xz|(0.25,0.75,0.75)}
                                  -y+1/4,-x+3/4,+z+3/4
 \{m_xy-y \mid (0.25,0.75,0.25)\}
                                  +x+1/4,-z+3/4,-y+1/4
\{-4^-_00z \mid (0.75, 0.75, 0.25)\}
                                  -y+3/4,+x+3/4,-z+1/4
                                    -x,+y+1/2,-z+1/2
   {2_0y0|(0.0,0.5,0.5)}
 {3^+_x-x-x}(0.0,0.5,0.0)
                                       -z, -x+1/2, +y
  \{m_xz|(0.75,0.75,0.75)\}
                                  +y+3/4,+x+3/4,+z+3/4
\{-4^+ \times 00 \mid (0.75, 0.75, 0.25)\}
                                  -x+3/4, +z+3/4, -y+1/4
 {3^+_-xx-x|(0.0,0.0,0.5)}
                                       +z,-x,-y+1/2
                                  +x+1/4, +z+1/4, +y+1/4
  {m_xyy|(0.25,0.25,0.25)}
 {3^+_-x-xx|(0.0,0.5,0.5)}
                                    -z, +x+1/2, -y+1/2
\{-4^- \times 00 \mid (0.75, 0.25, 0.25)\}
                                  -x+3/4, -z+1/4, +y+1/4
 \{m_-xyz \mid (0.25, 0.25, 0.75)\}
                                  -z+1/4, +y+1/4, -x+3/4
  {3^-_xxx|(0.0,0.0,0.0)}
                                         +y,+z,+x
\{-4^-_0y0|(0.75,0.25,0.75)\}
                                  +z+3/4,-y+1/4,-x+3/4
\{-4^+_0y0|(0.25,0.75,0.75)\}
                                  -z+1/4,-y+3/4,+x+3/4
 \{3^--x-xx\mid (0.0,0.0,0.5)\}
                                       +y,-z,-x+1/2
                                  +z+3/4, +y+3/4, +x+3/4
  \{m_xyx | (0.75, 0.75, 0.75)\}
 {3^-_x-x-x|(0.5,0.0,0.0)}
                                       -y+1/2,+z,-x
 \{3^--xx-x \mid (0.5,0.0,0.5)\}
                                    -y+1/2,-z,+x+1/2
     \{1 \mid (0.5, 0.5, 0.5)\}
                                  +x+1/2,+y+1/2,+z+1/2
\{-4^+_{00z} | (0.75, 0.25, 0.75)\}
                                  +y+3/4,-x+1/4,-z+3/4
   \{2_{x00} | (0.5, 0.5, 0.0)\}
                                    +x+1/2,-y+1/2,-z
                                  +z+1/2,+x+1/2,+y+1/2
  {3^+_xxx|(0.5,0.5,0.5)}
   {2_00z|(0.5,0.0,0.5)}
                                    -x+1/2, -y, +z+1/2
 \{m_x-xz\mid(0.75,0.25,0.25)\}
                                  -y+3/4, -x+1/4, +z+1/4
                                  +x+3/4,-z+1/4,-y+3/4
 \{m_xy-y \mid (0.75,0.25,0.75)\}
\{-4^-_00z \mid (0.25, 0.25, 0.75)\}
                                  -y+1/4,+x+1/4,-z+3/4
   {2_0y0|(0.5,0.0,0.0)}
                                       -x+1/2,+y,-z
 {3^+_x-x-x|(0.5,0.0,0.5)}
                                    -z+1/2,-x,+y+1/2
  \{m_xxz \mid (0.25, 0.25, 0.25)\}
                                  +y+1/4, +x+1/4, +z+1/4
\{-4^+ \times 00 \mid (0.25, 0.25, 0.75)\}
                                  -x+1/4, +z+1/4, -y+3/4
 {3^+_-xx-x|(0.5,0.5,0.0)}
                                    +z+1/2,-x+1/2,-y
  \{m_xyy \mid (0.75, 0.75, 0.75)\}
                                  +x+3/4,+z+3/4,+y+3/4
 {3^+_-x^-x^+|(0.5,0.0,0.0)}
                                       -z+1/2,+x,-y
\{-4^-x00|(0.25,0.75,0.75)\}
                                  -x+1/4, -z+3/4, +y+3/4
 \{m_-xyz \mid (0.75, 0.75, 0.25)\}
                                  -z+3/4,+y+3/4,-x+1/4
  \{3^-xxx|(0.5,0.5,0.5)\}
                                  +y+1/2,+z+1/2,+x+1/2
\{-4^-_0y0|(0.25,0.75,0.25)\}
                                  +z+1/4,-y+3/4,-x+1/4
\{-4^+_0y0|(0.75,0.25,0.25)\}
                                  -z+3/4,-y+1/4,+x+1/4
 \{3^--x-xx\mid (0.5,0.5,0.0)\}
                                    +y+1/2,-z+1/2,-x
  {m_xyx|(0.25,0.25,0.25)}
                                  +z+1/4, +y+1/4, +x+1/4
 {3^-_x-x-x|(0.0,0.5,0.5)}
                                    -y, +z+1/2, -x+1/2
 {3^--xx-x|(0.0,0.5,0.0)}
                                       -y,-z+1/2,+x
```

.....

```
*******
space group: 222:1 {'Hall': ' P 4 2 3 -1n', 'HM': 'P n -3 n:1'}
Crystal system: Cubic
Setting: 1
+x,+y,+z
-y,+x,+z
+x,-y,-z
+z,+x,+y
-x+1/2, -y+1/2, -z+1/2
             Seitz
                                        Jones
      \{1 \mid (0.0, 0.0, 0.0)\}
                                       +x,+y,+z
   {4^+_00z|(0.0,0.0,0.0)}
                                       -y,+x,+z
    \{2_{\times}00 \mid (0.0, 0.0, 0.0)\}
                                       +x,-y,-z
                                       +z,+x,+y
   {3^+_xxx|(0.0,0.0,0.0)}
      \{-1|(0.5,0.5,0.5)\}
                                -x+1/2,-y+1/2,-z+1/2
    {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
    \{2_x \times 0 \mid (0.0, 0.0, 0.0)\}
                                       +y,+x,-z
    {2_0yy|(0.0,0.0,0.0)}
                                       -x,+z,+y
   \{-4^+_00z|(0.5,0.5,0.5)\}
                                +y+1/2,-x+1/2,-z+1/2
   {4^-_00z|(0.0,0.0,0.0)}
                                       +y,-x,+z
    {2_0y0|(0.0,0.0,0.0)}
                                       -x,+y,-z
  {3^+_x-x-x|(0.0,0.0,0.0)}
                                       -z,-x,+y
    \{m_xy0|(0.5,0.5,0.5)\}
                                +x+1/2,+y+1/2,-z+1/2
    \{2_x-x0|(0.0,0.0,0.0)\}
                                       -y,-x,-z
   {4^+_x00|(0.0,0.0,0.0)}
                                       +x,-z,+y
   \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                -y+1/2,+x+1/2,-z+1/2
  {3^+_-xx-x|(0.0,0.0,0.0)}
                                       +z,-x,-y
    \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                -x+1/2,+y+1/2,+z+1/2
    \{2_0y-y \mid (0.0,0.0,0.0)\}
                                       -x,-z,-y
    \{m_{xxz} | (0.5, 0.5, 0.5)\}
                                +y+1/2,+x+1/2,+z+1/2
  {3^+_-x^-x^+|(0.0,0.0,0.0)}
                                       -z,+x,-y
    \{m_x0z \mid (0.5, 0.5, 0.5)\}
                                +x+1/2,-y+1/2,+z+1/2
   {4^-_x00|(0.0,0.0,0.0)}
                                       +x,+z,-y
    \{m_x-xz \mid (0.5,0.5,0.5)\}
                                -y+1/2, -x+1/2, +z+1/2
*******
space group: 222:2 {'Hall': '-P 4a 2bc 3', 'HM': 'P n -3 n:2'}
Crystal system: Cubic
Setting: 2
+X,+Y,+Z
-y+1/2,+x,+z
+x,-y+1/2,-z+1/2
+z,+x,+y
             Seitz
                                         Jones
```

```
{1|(0.0,0.0,0.0)}
                                       +x,+y,+z
 \{4^+00z|(0.5,0.0,0.0)\}
                                     -y+1/2,+x,+z
  \{2_{x00} | (0.0, 0.5, 0.5)\}
                                   +x,-y+1/2,-z+1/2
 {3^+_xxx|(0.0,0.0,0.0)}
                                       +z,+x,+y
  \{2\_00z \mid (0.5, 0.5, 0.0)\}
                                   -x+1/2,-y+1/2,+z
  \{2_{xx0}|(0.0,0.0,0.5)\}
                                     +y,+x,-z+1/2
                                     -x+1/2,+z,+y
  {2_0yy|(0.5,0.0,0.0)}
 \{4^-_00z \mid (0.0, 0.5, 0.0)\}
                                     +y,-x+1/2,+z
  {2_0y0|(0.5,0.0,0.5)}
                                   -x+1/2,+y,-z+1/2
\{3^+x^-x^-x^-\}
                                   -z+1/2, -x+1/2, +y
  \{2_x-x0|(0.5,0.5,0.5)\}
                                -y+1/2,-x+1/2,-z+1/2
 {4^+_x00|(0.0,0.5,0.0)}
                                     +x,-z+1/2,+y
\{3^+-xx-x|(0.0,0.5,0.5)\}
                                   +z,-x+1/2,-y+1/2
  \{2_0y-y\mid (0.5,0.5,0.5)\}
                                -x+1/2, -z+1/2, -y+1/2
\{3^+_-x^-x^-\}
                                   -z+1/2,+x,-y+1/2
 \{4^-x00|(0.0,0.0,0.5)\}
                                     +x,+z,-y+1/2
  \{2_x0x|(0.0,0.5,0.0)\}
                                     +z,-y+1/2,+x
 {3^-_xxx|(0.0,0.0,0.0)}
                                       +y, +z, +x
 {4^-_0y0|(0.5,0.0,0.0)}
                                     -z+1/2,+y,+x
 {4^+_0y0|(0.0,0.0,0.5)}
                                     +z,+y,-x+1/2
\{3^--x-xx\mid(0.0,0.5,0.5)\}
                                   +y,-z+1/2,-x+1/2
  \{2_-x0x \mid (0.5,0.5,0.5)\}
                                -z+1/2,-y+1/2,-x+1/2
{3^-_x-x-x|(0.5,0.0,0.5)}
                                   -y+1/2,+z,-x+1/2
{3^-_xx-x|(0.5,0.5,0.0)}
                                   -y+1/2,-z+1/2,+x
    \{-1 \mid (0.0,0.0,0.0)\}
                                       -x,-y,-z
 \{-4^+_00z \mid (0.5,0.0,0.0)\}
                                     +y+1/2,-x,-z
  \{m_0yz \mid (0.0,0.5,0.5)\}
                                   -x, +y+1/2, +z+1/2
 \{-3^+ \times \times | (0.0,0.0,0.0)\}
                                       -z,-x,-y
  \{m_xy0|(0.5,0.5,0.0)\}
                                   +x+1/2, +y+1/2, -z
  \{m_x-xz\mid(0.0,0.0,0.5)\}
                                     -y,-x,+z+1/2
                                     +x+1/2,-z,-y
  \{m_xy-y \mid (0.5,0.0,0.0)\}
 \{-4^-00z \mid (0.0,0.5,0.0)\}
                                     -y, +x+1/2, -z
                                   +x+1/2,-y,+z+1/2
  \{m_x0z \mid (0.5,0.0,0.5)\}
\{-3^+x^-x^-x^- (0.5, 0.5, 0.0)\}
                                   +z+1/2, +x+1/2, -y
  \{m_xxz|(0.5,0.5,0.5)\}
                                +y+1/2,+x+1/2,+z+1/2
 {-4^+_x00|(0.0,0.5,0.0)}
                                     -x,+z+1/2,-y
\{-3^+-xx-x|(0.0,0.5,0.5)\}
                                   -z, +x+1/2, +y+1/2
  \{m_xyy | (0.5, 0.5, 0.5)\}
                                +x+1/2,+z+1/2,+y+1/2
\{-3^+-x-xx|(0.5,0.0,0.5)\}
                                   +z+1/2,-x,+y+1/2
 \{-4^- \times 00 \mid (0.0, 0.0, 0.5)\}
                                     -x,-z,+y+1/2
  \{m_-xyz \mid (0.0,0.5,0.0)\}
                                     -z,+y+1/2,-x
 {-3^-_xxx|(0.0,0.0,0.0)}
                                       -y,-z,-x
 {-4^-_0y0|(0.5,0.0,0.0)}
                                     +z+1/2,-y,-x
 \{-4^+_0y0|(0.0,0.0,0.5)\}
                                     -z,-y,+x+1/2
\{-3^--x-xx|(0.0,0.5,0.5)\}
                                   -y, +z+1/2, +x+1/2
  \{m_xyx \mid (0.5, 0.5, 0.5)\}
                                +z+1/2,+y+1/2,+x+1/2
\{-3^-x-x-x|(0.5,0.0,0.5)\}
                                   +y+1/2,-z,+x+1/2
\{-3^--xx-x|(0.5,0.5,0.0)\}
                                   +y+1/2,+z+1/2,-x
```

space group: 223 {'Hall': '-P 4n 2 3', 'HM': 'P m -3 n'}

```
Crystal system: Cubic
+x,+y,+z
-y+1/2,+x+1/2,+z+1/2
+x,-y,-z
+z,+x,+y
```

```
Seitz
                                        Jones
    {1|(0.0,0.0,0.0)}
                                       +X,+Y,+Z
 \{4^+_00z|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,+z+1/2
  {2_x00|(0.0,0.0,0.0)}
                                       +x,-y,-z
 {3^+_xxx|(0.0,0.0,0.0)}
                                       +z,+x,+y
  {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
  \{2_{x} \times 0 \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,+x+1/2,-z+1/2
  {2_0yy|(0.5,0.5,0.5)}
                                -x+1/2, +z+1/2, +y+1/2
 \{4^-_00z|(0.5,0.5,0.5)\}
                                +y+1/2,-x+1/2,+z+1/2
  {2_0y0|(0.0,0.0,0.0)}
                                       -x,+y,-z
{3^+_x-x-x}(0.0,0.0,0.0)
                                       -z,-x,+y
                                -y+1/2,-x+1/2,-z+1/2
  \{2_x-x0|(0.5,0.5,0.5)\}
 {4^+_x00|(0.5,0.5,0.5)}
                                +x+1/2,-z+1/2,+y+1/2
{3^+_-xx-x|(0.0,0.0,0.0)}
                                       +z,-x,-y
  \{2_0y-y \mid (0.5,0.5,0.5)\}
                                -x+1/2, -z+1/2, -y+1/2
{3^+_-x^-x^+|(0.0,0.0,0.0)}
                                       -z,+x,-y
 \{4^-x00|(0.5,0.5,0.5)\}
                                +x+1/2,+z+1/2,-y+1/2
  \{2_x0x | (0.5,0.5,0.5)\}
                                +z+1/2,-y+1/2,+x+1/2
 {3^-_xxx|(0.0,0.0,0.0)}
                                       +y,+z,+x
 {4^-_0y0|(0.5,0.5,0.5)}
                                -z+1/2,+y+1/2,+x+1/2
 {4^+_0y0|(0.5,0.5,0.5)}
                                +z+1/2, +y+1/2, -x+1/2
\{3^--x-xx\mid (0.0,0.0,0.0)\}
                                       +y,-z,-x
  \{2_{-}\times 0\times | (0.5, 0.5, 0.5)\}
                                -z+1/2,-y+1/2,-x+1/2
{3^-_x-x-x|(0.0,0.0,0.0)}
                                       -y,+z,-x
\{3^--xx-x \mid (0.0,0.0,0.0)\}
                                       -y,-z,+x
    {-1|(0.0,0.0,0.0)}
                                       -x,-y,-z
 \{-4^+_00z \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,-x+1/2,-z+1/2
  {m_0yz|(0.0,0.0,0.0)}
                                       -x,+y,+z
 {-3^+_xxx|(0.0,0.0,0.0)}
                                       -z,-x,-y
  {m_xy0|(0.0,0.0,0.0)}
                                       +x,+y,-z
                                -y+1/2,-x+1/2,+z+1/2
  \{m_x-xz \mid (0.5,0.5,0.5)\}
  \{m_xy-y \mid (0.5,0.5,0.5)\}
                                +x+1/2,-z+1/2,-y+1/2
 \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                -y+1/2,+x+1/2,-z+1/2
  {m_x0z|(0.0,0.0,0.0)}
                                       +x,-y,+z
\{-3^+x^-x^-x^-|(0.0,0.0,0.0)\}
                                       +z,+x,-y
  \{m_{xxz}|(0.5,0.5,0.5)\}
                                +y+1/2,+x+1/2,+z+1/2
                                -x+1/2, +z+1/2, -y+1/2
 {-4^+_x00|(0.5,0.5,0.5)}
\{-3^+-xx-x \mid (0.0,0.0,0.0)\}
                                       -z,+x,+y
  {m_xyy|(0.5,0.5,0.5)}
                                +x+1/2,+z+1/2,+y+1/2
\{-3^+-x-x^+ \mid (0.0,0.0,0.0)\}
                                       +z,-x,+y
 \{-4^-x00|(0.5,0.5,0.5)\}
                                -x+1/2, -z+1/2, +y+1/2
  \{m_-xyz \mid (0.5, 0.5, 0.5)\}
                                -z+1/2,+y+1/2,-x+1/2
 \{-3^-xxx|(0.0,0.0,0.0)\}
                                       -y,-z,-x
 \{-4^-_0y0|(0.5,0.5,0.5)\}
                                +z+1/2,-y+1/2,-x+1/2
 \{-4^+_0y0|(0.5,0.5,0.5)\}
                                -z+1/2,-y+1/2,+x+1/2
\{-3^--x-xx|(0.0,0.0,0.0)\}
                                       -y, +z, +x
```

```
\{m_xyx | (0.5, 0.5, 0.5)\}
                                +z+1/2,+y+1/2,+x+1/2
  \{-3^-x-x-x|(0.0,0.0,0.0)\}
                                        +y,-z,+x
  \{-3^--xx-x \mid (0.0,0.0,0.0)\} \mid
                                        +y, +z, -x
*******
space group: 224:1 {'Hall': ' P 4n 2 3 -1n', 'HM': 'P n -3 m:1'}
Crystal system: Cubic
Setting: 1
+x,+y,+z
-y+1/2, +x+1/2, +z+1/2
+x,-y,-z
+Z,+X,+y
-x+1/2, -y+1/2, -z+1/2
             Seitz
                                        Jones
                                       +x,+y,+z
      {1|(0.0,0.0,0.0)}
   \{4^+_{00z}|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,+z+1/2
    {2_x00|(0.0,0.0,0.0)}
                                       +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                       +z,+x,+y
      \{-1|(0.5,0.5,0.5)\}
                                -x+1/2,-y+1/2,-z+1/2
    {2_00z|(0.0,0.0,0.0)}
                                       -x,-y,+z
    \{2_x \times 0 \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,+x+1/2,-z+1/2
    \{2_{0yy} | (0.5, 0.5, 0.5)\}
                                -x+1/2,+z+1/2,+y+1/2
   \{-4^+_00z \mid (0.0,0.0,0.0)\} \mid
                                       +y,-x,-z
   \{4^-_00z \mid (0.5, 0.5, 0.5)\}
                                +y+1/2,-x+1/2,+z+1/2
    {2_0y0|(0.0,0.0,0.0)}
                                       -x,+y,-z
  {3^+_x-x-x|(0.0,0.0,0.0)}
                                       -z,-x,+y
    \{m_xy0|(0.5,0.5,0.5)\}
                                +x+1/2,+y+1/2,-z+1/2
    \{2_x-x0|(0.5,0.5,0.5)\}
                                -y+1/2, -x+1/2, -z+1/2
   \{4^+_x00|(0.5,0.5,0.5)\}
                                +x+1/2,-z+1/2,+y+1/2
   {-4^-_00z|(0.0,0.0,0.0)}
                                       -y,+x,-z
  \{3^+-xx-x \mid (0.0,0.0,0.0)\}
                                       +z,-x,-y
    \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                -x+1/2,+y+1/2,+z+1/2
    \{2_0y-y\mid (0.5,0.5,0.5)\}
                                -x+1/2,-z+1/2,-y+1/2
    \{m_xxz \mid (0.0,0.0,0.0)\}
                                       +y,+x,+z
  {3^+-x-x}(0.0,0.0,0.0)
                                       -z,+x,-y
    \{m_x0z \mid (0.5, 0.5, 0.5)\}
                                +x+1/2,-y+1/2,+z+1/2
   \{4^-x00|(0.5,0.5,0.5)\}
                                +x+1/2,+z+1/2,-y+1/2
    \{m_x-xz \mid (0.0,0.0,0.0)\}
                                       -y,-x,+z
*******
space group: 224:2 {'Hall': '-P 4bc 2bc 3', 'HM': 'P n -3 m:2'}
Crystal system: Cubic
Setting: 2
+x,+y,+z
-y, +x+1/2, +z+1/2
+x,-y+1/2,-z+1/2
+z,+x,+y
```

······································		
Seitz	Jones	
\$\text{Seitz} \{1\(0.0,0.0,0.0\)\} \{4^+_00z\(0.0,0.5,0.5\)\} \{2_x00\(0.0,0.5,0.5\)\} \{2_x00\(0.0,0.5,0.5\)\} \{2_00z\(0.5,0.5,0.0\)\} \{2_00z\(0.5,0.5,0.0\)\} \{2_00z\(0.5,0.5,0.0\)\} \{2_00z\(0.5,0.5,0.0\)\} \{2_00z\(0.5,0.5,0.0,0.5\)\} \{4^-_00z\(0.5,0.0,0.5\)\} \{2_00y\(0.5,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.0,0.5\)\} \{2_00y\(0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0	Jones +x,+y,+z -y,+x+1/2,+z+1/2 +x,-y+1/2,-z+1/2 +z,+x,+y -x+1/2,-y+1/2,+z +y+1/2,+x+1/2,-z -x,+z+1/2,+y+1/2 +y+1/2,-x,+z+1/2 -x+1/2,-y,-z+1/2 -x+1/2,-y,-z+1/2 -z+1/2,-x+1/2,-y -y,-x,-z +x+1/2,-z,+y+1/2 +z,-x+1/2,-y+1/2 +z,-x+1/2,-y+1/2 +x+1/2,-z,+y+1/2 +x+1/2,-y,+x+1/2 +y,+z,+x -z,+y+1/2,-x+1/2 +y,+z,+x -z,+y+1/2,-x+1/2 -z,-y,-x -y+1/2,-z+1/2,-x +y,-z+1/2,-z+1/2,-x -y,-x+1/2,-z+1/2 -x,+y+1/2,-z+1/2,-z -y,-x+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-z+1/2 -x,+y+1/2,-y+1/2 -x,+y+1/2,-y+1/2 -x+1/2,-y+1/2 -y+1/2,-x+1/2,-y +x,-z+1/2,-y+1/2 -x+1/2,-z+1/2,-y -x+1/2,-z+1/2,-y -x+1/2,-z+1/2,-y -x+1/2,-z+1/2,-y	

```
space group: 225 {'Hall': '-F 4 2 3', 'HM': 'F m -3 m'}
Crystal system: Cubic
+x,+y,+z
-y,+x,+z
+x,-y,-z
+z,+x,+y
              Seitz
                                          Jones
       {1|(0.0,0.0,0.0)}
                                         +x,+y,+z
   {4^+_00z|(0.0,0.0,0.0)}
                                         -y,+x,+z
    \{2_{\times}00 \mid (0.0, 0.0, 0.0)\}
                                         +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                         +z,+x,+y
    {2_00z|(0.0,0.0,0.0)}
                                         -x,-y,+z
    {2_xx0|(0.0,0.0,0.0)}
                                         +y,+x,-z
    {2_0yy|(0.0,0.0,0.0)}
                                         -x,+z,+y
   {4^-_00z|(0.0,0.0,0.0)}
                                         +y,-x,+z
    {2_0y0|(0.0,0.0,0.0)}
                                         -x,+y,-z
  {3^+_x-x-x}(0.0,0.0,0.0)
                                         -z,-x,+y
    \{2_x-x0\mid(0.0,0.0,0.0)\}
                                         -y,-x,-z
   {4^+_x00|(0.0,0.0,0.0)}
                                         +x,-z,+y
  {3^+_-xx-x|(0.0,0.0,0.0)}
                                         +z,-x,-y
    {2_0y-y|(0.0,0.0,0.0)}
                                         -x,-z,-y
  {3^+_-x^-x^+|(0.0,0.0,0.0)}
                                         -z,+x,-y
   \{4^-x00|(0.0,0.0,0.0)\}
                                         +x,+z,-y
    \{2 \times 0 \times | (0.0, 0.0, 0.0)\}
                                         +z,-y,+x
   {3^-_xxx|(0.0,0.0,0.0)}
                                         +y,+z,+x
   {4^-_0y0|(0.0,0.0,0.0)}
                                         -z,+y,+x
   {4^+_0y0|(0.0,0.0,0.0)}
                                         +z,+y,-x
  \{3^--x-xx\mid (0.0,0.0,0.0)\}
                                         +y,-z,-x
    \{2\_-x0x \mid (0.0,0.0,0.0)\}
                                         -z,-y,-x
  {3^-_x-x-x|(0.0,0.0,0.0)}
                                         -y,+z,-x
  \{3^--xx-x \mid (0.0,0.0,0.0)\}
                                         -y,-z,+x
       \{-1 \mid (0.0, 0.0, 0.0)\}
                                         -x,-y,-z
   \{-4^+_00z \mid (0.0,0.0,0.0)\}
                                         +y,-x,-z
    \{m_0yz \mid (0.0,0.0,0.0)\}
                                         -x,+y,+z
   \{-3^+ \times \times | (0.0,0.0,0.0)\}
                                         -z,-x,-y
    \{m_xy0 | (0.0,0.0,0.0)\}
                                         +x,+y,-z
    \{m_x-xz \mid (0.0,0.0,0.0)\}
                                         -y,-x,+z
    \{m_xy-y \mid (0.0,0.0,0.0)\}
                                         +x,-z,-y
   {-4^-_00z|(0.0,0.0,0.0)}
                                         -y,+x,-z
    {m_x0z|(0.0,0.0,0.0)}
                                         +x,-y,+z
  \{-3^+x^-x^-x^-|(0.0,0.0,0.0)\}
                                         +z,+x,-y
    \{m_x \times z \mid (0.0, 0.0, 0.0)\}
                                         +y,+x,+z
   \{-4^+ \times 00 \mid (0.0, 0.0, 0.0)\}
                                         -x,+z,-y
  \{-3^+-xx-x \mid (0.0,0.0,0.0)\}
                                         -z,+x,+y
    \{m_xyy | (0.0,0.0,0.0)\}
                                         +x,+z,+y
  \{-3^+-x-xx|(0.0,0.0,0.0)\}
                                         +z,-x,+y
   \{-4^- \times 00 \mid (0.0, 0.0, 0.0)\}
                                         -x,-z,+y
    \{m_-xyz \mid (0.0,0.0,0.0)\}
                                         -z,+y,-x
   \{-3^-xxx|(0.0,0.0,0.0)\}
                                         -y,-z,-x
```

```
\{-4^-_0y0|(0.0,0.0,0.0)\}
                                     +z,-y,-x
 {-4^+_0y0|(0.0,0.0,0.0)}
                                     -z,-y,+x
\{-3^--x-xx|(0.0,0.0,0.0)\}
                                     -y,+z,+x
  \{m_xyx | (0.0,0.0,0.0)\}
                                     +z,+y,+x
{-3^-_x-x-x|(0.0,0.0,0.0)}
{-3^-_-xx-x|(0.0,0.0,0.0)}
                                     +y,-z,+x
                                     +y,+z,-x
    \{1|(0.0,0.5,0.5)\}
                                 +x,+y+1/2,+z+1/2
 \{4^+_{00z}|(0.0,0.5,0.5)\}
                                 -y, +x+1/2, +z+1/2
  \{2_{x00}|(0.0,0.5,0.5)\}
                                 +x,-y+1/2,-z+1/2
 \{3^+ xxx | (0.0, 0.5, 0.5)\}
                                 +z,+x+1/2,+y+1/2
  {2_00z|(0.0,0.5,0.5)}
                                 -x,-y+1/2,+z+1/2
  {2_xx0|(0.0,0.5,0.5)}
                                 +y, +x+1/2, -z+1/2
  {2_0yy|(0.0,0.5,0.5)}
                                 -x, +z+1/2, +y+1/2
 {4^-_00z|(0.0,0.5,0.5)}
                                 +y,-x+1/2,+z+1/2
  {2_0y0|(0.0,0.5,0.5)}
                                 -x, +y+1/2, -z+1/2
\{3^+x^-x^-x^-\}
                                 -z, -x+1/2, +y+1/2
  \{2_x-x0|(0.0,0.5,0.5)\}
                                 -y, -x+1/2, -z+1/2
 {4^+_x00|(0.0,0.5,0.5)}
                                 +x,-z+1/2,+y+1/2
{3^+-xx-x|(0.0,0.5,0.5)}
                                 +z,-x+1/2,-y+1/2
  \{2_0y-y|(0.0,0.5,0.5)\}
                                 -x,-z+1/2,-y+1/2
\{3^+_-x^-x^-\}
                                 -z, +x+1/2, -y+1/2
 \{4^-x00|(0.0,0.5,0.5)\}
                                 +x,+z+1/2,-y+1/2
  \{2_x0x \mid (0.0,0.5,0.5)\}
                                 +z,-y+1/2,+x+1/2
 {3^-_xxx|(0.0,0.5,0.5)}
                                 +y, +z+1/2, +x+1/2
 {4^-_0y0|(0.0,0.5,0.5)}
                                 -z, +y+1/2, +x+1/2
 {4^+_0y0|(0.0,0.5,0.5)}
                                 +z,+y+1/2,-x+1/2
\{3^--x-xx\mid(0.0,0.5,0.5)\}
                                 +y,-z+1/2,-x+1/2
  \{2\_-x0x \mid (0.0,0.5,0.5)\}
                                 -z,-y+1/2,-x+1/2
{3^-_x-x-x|(0.0,0.5,0.5)}
                                 -y, +z+1/2, -x+1/2
\{3^--xx-x \mid (0.0,0.5,0.5)\}
                                 -y, -z+1/2, +x+1/2
    {-1|(0.0,0.5,0.5)}
                                 -x,-y+1/2,-z+1/2
 \{-4^+_00z \mid (0.0, 0.5, 0.5)\}
                                 +y,-x+1/2,-z+1/2
  \{m_0yz \mid (0.0,0.5,0.5)\}
                                 -x, +y+1/2, +z+1/2
 \{-3^+ \times \times | (0.0, 0.5, 0.5) \}
                                 -z, -x+1/2, -y+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                                 +x,+y+1/2,-z+1/2
  \{m_x-xz\mid(0.0,0.5,0.5)\}
                                 -y, -x+1/2, +z+1/2
  {m_xy-y|(0.0,0.5,0.5)}
                                 +x,-z+1/2,-y+1/2
 \{-4^-00z \mid (0.0,0.5,0.5)\}
                                 -y, +x+1/2, -z+1/2
  {m_x0z|(0.0,0.5,0.5)}
                                 +x,-y+1/2,+z+1/2
\{-3^+x^-x^-x^- (0.0,0.5,0.5)\}
                                 +z,+x+1/2,-y+1/2
  {m_xxz|(0.0,0.5,0.5)}
                                 +y, +x+1/2, +z+1/2
 {-4^+_x00|(0.0,0.5,0.5)}
                                 -x, +z+1/2, -y+1/2
\{-3^+-xx-x|(0.0,0.5,0.5)\}
                                 -z, +x+1/2, +y+1/2
  {m_xyy|(0.0,0.5,0.5)}
                                 +x,+z+1/2,+y+1/2
\{-3^+-x-xx|(0.0,0.5,0.5)\}
                                 +z,-x+1/2,+y+1/2
 \{-4^- \times 00 \mid (0.0, 0.5, 0.5)\}
                                 -x, -z+1/2, +y+1/2
  \{m_-xyz \mid (0.0,0.5,0.5)\}
                                 -z, +y+1/2, -x+1/2
 \{-3^-xxx|(0.0,0.5,0.5)\}
                                 -y, -z+1/2, -x+1/2
 \{-4^-_0y0|(0.0,0.5,0.5)\}
                                 +z,-y+1/2,-x+1/2
                                 -z,-y+1/2,+x+1/2
 {-4^+_0y0|(0.0,0.5,0.5)}
\{-3^--x-xx \mid (0.0,0.5,0.5)\}
                                 -y, +z+1/2, +x+1/2
  \{m_xyx | (0.0,0.5,0.5)\}
                                 +z, +y+1/2, +x+1/2
\{-3^-x-x-x|(0.0,0.5,0.5)\}
                                 +y,-z+1/2,+x+1/2
\{-3^--xx-x|(0.0,0.5,0.5)\}
                              +y,+z+1/2,-x+1/2
```

```
{1|(0.5,0.0,0.5)}
                                +x+1/2,+y,+z+1/2
 \{4^+_{00z}|(0.5,0.0,0.5)\}
                                -y+1/2,+x,+z+1/2
  \{2_{x00} | (0.5, 0.0, 0.5)\}
                                +x+1/2,-y,-z+1/2
 {3^+_xxx|(0.5,0.0,0.5)}
                                +z+1/2, +x, +y+1/2
  {2_00z|(0.5,0.0,0.5)}
                                -x+1/2,-y,+z+1/2
  \{2_x \times 0 \mid (0.5, 0.0, 0.5)\}
                                +y+1/2,+x,-z+1/2
  {2_0yy|(0.5,0.0,0.5)}
                                -x+1/2,+z,+y+1/2
 {4^-_00z|(0.5,0.0,0.5)}
                                +y+1/2,-x,+z+1/2
  {2_0y0|(0.5,0.0,0.5)}
                                -x+1/2,+y,-z+1/2
{3^+_x-x-x|(0.5,0.0,0.5)}
                                -z+1/2,-x,+y+1/2
                                -y+1/2,-x,-z+1/2
  \{2_x-x0\mid(0.5,0.0,0.5)\}
 {4^+_x00|(0.5,0.0,0.5)}
                                +x+1/2,-z,+y+1/2
\{3^+_-xx^-x \mid (0.5,0.0,0.5)\}
                                +z+1/2,-x,-y+1/2
  \{2_0y-y\mid (0.5,0.0,0.5)\}
                                -x+1/2,-z,-y+1/2
{3^+_-x^-x^-|(0.5,0.0,0.5)}
                                -z+1/2,+x,-y+1/2
 {4^-_x00|(0.5,0.0,0.5)}
                                +x+1/2,+z,-y+1/2
  \{2_x0x|(0.5,0.0,0.5)\}
                                +z+1/2,-y,+x+1/2
 {3^-_xxx|(0.5,0.0,0.5)}
                                +y+1/2,+z,+x+1/2
 {4^-_0y0|(0.5,0.0,0.5)}
                                -z+1/2,+y,+x+1/2
 {4^+_0y0|(0.5,0.0,0.5)}
                                +z+1/2, +y, -x+1/2
\{3^--x-xx\mid(0.5,0.0,0.5)\}
                                +y+1/2,-z,-x+1/2
  \{2\_-x0x \mid (0.5,0.0,0.5)\}
                                -z+1/2,-y,-x+1/2
\{3^-x-x-x|(0.5,0.0,0.5)\}
                                -y+1/2,+z,-x+1/2
     _-xx-x|(0.5,0.0,0.5)}
                                -y+1/2,-z,+x+1/2
                                -x+1/2, -y, -z+1/2
    {-1|(0.5,0.0,0.5)}
 {-4^+_00z|(0.5,0.0,0.5)}
                                +y+1/2,-x,-z+1/2
  {m_0yz|(0.5,0.0,0.5)}
                                -x+1/2,+y,+z+1/2
 \{-3^+ \times \times | (0.5, 0.0, 0.5)\}
                                -z+1/2,-x,-y+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                                +x+1/2,+y,-z+1/2
  \{m_x-xz\mid(0.5,0.0,0.5)\}
                                -y+1/2, -x, +z+1/2
  \{m_xy-y \mid (0.5,0.0,0.5)\}
                                +x+1/2,-z,-y+1/2
 \{-4^-_00z \mid (0.5,0.0,0.5)\}
                                -y+1/2,+x,-z+1/2
  {m_x0z|(0.5,0.0,0.5)}
                                +x+1/2,-y,+z+1/2
\{-3^+x^-x^-x^-|(0.5,0.0,0.5)\}
                                +z+1/2, +x, -y+1/2
  {m_xxz|(0.5,0.0,0.5)}
                                +y+1/2,+x,+z+1/2
 {-4^+_x00|(0.5,0.0,0.5)}
                                -x+1/2,+z,-y+1/2
\{-3^+-xx-x|(0.5,0.0,0.5)\}
                                -z+1/2,+x,+y+1/2
  \{m_xyy \mid (0.5,0.0,0.5)\}
                                +x+1/2,+z,+y+1/2
\{-3^+-x-xx|(0.5,0.0,0.5)\}
                                +z+1/2,-x,+y+1/2
 \{-4^-x00|(0.5,0.0,0.5)\}
                                -x+1/2,-z,+y+1/2
  \{m_-xyz \mid (0.5,0.0,0.5)\}
                                -z+1/2,+y,-x+1/2
 \{-3^-xxx|(0.5,0.0,0.5)\}
                                -y+1/2,-z,-x+1/2
 {-4^-_0y0|(0.5,0.0,0.5)}
                                +z+1/2,-y,-x+1/2
 {-4^+_0y0|(0.5,0.0,0.5)}
                                -z+1/2,-y,+x+1/2
\{-3^--x-xx|(0.5,0.0,0.5)\}
                                -y+1/2,+z,+x+1/2
  \{m_xyx | (0.5,0.0,0.5)\}
                                +z+1/2, +y, +x+1/2
\{-3^-x-x-x|(0.5,0.0,0.5)\}
                                +y+1/2,-z,+x+1/2
\{-3^--xx-x|(0.5,0.0,0.5)\}
                                +y+1/2,+z,-x+1/2
    {1|(0.5,0.5,0.0)}
                                +x+1/2,+y+1/2,+z
 \{4^+_{00z}|(0.5,0.5,0.0)\}
                                -y+1/2,+x+1/2,+z
  {2_x00|(0.5,0.5,0.0)}
                                +x+1/2,-y+1/2,-z
 {3^+_xxx|(0.5,0.5,0.0)}
                                +z+1/2,+x+1/2,+y
                                -x+1/2, -y+1/2, +z
  {2_00z|(0.5,0.5,0.0)}
  \{2_x \times 0 \mid (0.5, 0.5, 0.0)\}
                                +y+1/2,+x+1/2,-z
```

```
{2_0yy|(0.5,0.5,0.0)}
                                  -x+1/2,+z+1/2,+y
   \{4^-_00z \mid (0.5, 0.5, 0.0)\}
                                  +y+1/2,-x+1/2,+z
    {2_0y0|(0.5,0.5,0.0)}
                                  -x+1/2,+y+1/2,-z
  {3^+_x-x-x|(0.5,0.5,0.0)}
                                  -z+1/2, -x+1/2, +y
    \{2_x-x0|(0.5,0.5,0.0)\}
                                  -y+1/2, -x+1/2, -z
   {4^+_x00|(0.5,0.5,0.0)}
                                  +x+1/2,-z+1/2,+y
  {3^+_-xx-x|(0.5,0.5,0.0)}
                                  +z+1/2,-x+1/2,-y
    \{2_0y-y\mid (0.5,0.5,0.0)\}
                                  -x+1/2,-z+1/2,-y
  \{3^+-x-x^+ \mid (0.5,0.5,0.0)\}
                                  -z+1/2,+x+1/2,-y
   \{4^- \times 00 \mid (0.5, 0.5, 0.0)\}
                                  +x+1/2,+z+1/2,-y
    \{2_{x0x} | (0.5, 0.5, 0.0)\}
                                  +z+1/2,-y+1/2,+x
   {3^-_xxx|(0.5,0.5,0.0)}
                                  +y+1/2,+z+1/2,+x
   {4^-_0y0|(0.5,0.5,0.0)}
                                  -z+1/2,+y+1/2,+x
   {4^+_0y0|(0.5,0.5,0.0)}
                                  +z+1/2, +y+1/2, -x
  \{3^--x-xx\mid(0.5,0.5,0.0)\}
                                  +y+1/2,-z+1/2,-x
    \{2_{-x0x} | (0.5, 0.5, 0.0)\}
                                  -z+1/2,-y+1/2,-x
  \{3^-x-x-x|(0.5,0.5,0.0)\}
                                  -y+1/2,+z+1/2,-x
  {3^-_xx-x|(0.5,0.5,0.0)}
                                  -y+1/2,-z+1/2,+x
      {-1|(0.5,0.5,0.0)}
                                  -x+1/2, -y+1/2, -z
                                  +y+1/2,-x+1/2,-z
   \{-4^+_00z|(0.5,0.5,0.0)\}
    \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                  -x+1/2,+y+1/2,+z
   \{-3^+ \times \times | (0.5, 0.5, 0.0)\}
                                  -z+1/2, -x+1/2, -y
    {m_xy0|(0.5,0.5,0.0)}
                                  +x+1/2,+y+1/2,-z
    \{m_x-xz\mid(0.5,0.5,0.0)\}
                                  -y+1/2,-x+1/2,+z
    {m_xy-y|(0.5,0.5,0.0)}
                                  +x+1/2,-z+1/2,-y
   {-4^-_00z|(0.5,0.5,0.0)}
                                  -y+1/2,+x+1/2,-z
    {m_x0z|(0.5,0.5,0.0)}
                                  +x+1/2,-y+1/2,+z
  \{-3^+x^-x^-x^-\}
                                  +z+1/2, +x+1/2, -y
    \{m_{xxz} | (0.5, 0.5, 0.0)\}
                                  +y+1/2,+x+1/2,+z
   {-4^+_x00|(0.5,0.5,0.0)}
                                  -x+1/2,+z+1/2,-y
  \{-3^+-xx-x|(0.5,0.5,0.0)\}
                                  -z+1/2,+x+1/2,+y
    \{m_xyy | (0.5, 0.5, 0.0)\}
                                  +x+1/2,+z+1/2,+y
  \{-3^+-x-xx\mid(0.5,0.5,0.0)\}
                                  +z+1/2,-x+1/2,+y
   \{-4^-x00|(0.5,0.5,0.0)\}
                                  -x+1/2, -z+1/2, +y
    \{m_-xyz \mid (0.5, 0.5, 0.0)\}
                                  -z+1/2,+y+1/2,-x
   {-3^-_xxx|(0.5,0.5,0.0)}
                                  -y+1/2,-z+1/2,-x
   {-4^-_0y0|(0.5,0.5,0.0)}
                                  +z+1/2,-y+1/2,-x
   \{-4^+_0y0|(0.5,0.5,0.0)\}
                                  -z+1/2,-y+1/2,+x
  \{-3^--x-xx|(0.5,0.5,0.0)\}
                                  -y+1/2,+z+1/2,+x
    \{m_xyx | (0.5, 0.5, 0.0)\}
                                  +z+1/2,+y+1/2,+x
  \{-3^-x-x-x|(0.5,0.5,0.0)\}
                                  +y+1/2,-z+1/2,+x
  \{-3^--xx-x \mid (0.5,0.5,0.0)\}
                                 +y+1/2,+z+1/2,-x
*******
space group: 226 {'Hall': '-F 4c 2 3', 'HM': 'F m -3 c'}
Crystal system: Cubic
+x,+y,+z
-y,+x,+z+1/2
+x,-y,-z
+z,+x,+y
 . . . . . . . . . . . . . . . . . . .
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Seitz	Jones
+	+x,+y,+z -y,+x,+z+1/2 +x,-y,-z +z,+x,+y -x,-y,+z +y,+x,-z+1/2 -x,+z,+y+1/2 +y,-x,+z+1/2 -x,+y,-z
{3^+_x-x-x (0.0,0.0,0.0)} {2_x-x0 (0.0,0.0,0.5)} {4^+_x00 (0.0,0.0,0.5)} {3^+xx-x (0.0,0.0,0.0)} {2_0y-y (0.0,0.0,0.5)} {3^+x-x (0.0,0.0,0.0)} {4^x00 (0.0,0.0,0.5)} {2_x0x (0.5,0.0,0.0)} {3^xxx (0.0,0.0,0.0)}	-z,-x,+y -y,-x,-z+1/2 +x,-z,+y+1/2 +z,-x,-y -x,-z,-y+1/2 -z,+x,-y +x,+z,-y+1/2 +z+1/2,-y,+x +y,+z,+x
\[\{4^0y0\ (0.5,0.0,0.0)\} \\ \{4^+_0y0\ (0.5,0.0,0.0)\} \\ \{3^x-xx\ (0.0,0.0,0.0)\} \\ \{2x0x\ (0.5,0.0,0.0)\} \\ \{3^x-x-x\ (0.0,0.0,0.0)\} \\ \{3^x-x-x\ (0.0,0.0,0.0)\} \\ \{3^xx-x\ (0.0,0.0,0.0)\} \\ \{-1\ (0.0,0.0,0.0,0.0)\} \\ \{-4^+_00z\ (0.0,0.0,0.0,0.0)\} \\ \{m_0yz\ (0.0,0.0,0.0,0.0)\}	-z+1/2,+y,+x +z+1/2,+y,-x +y,-z,-x -z+1/2,-y,-x -y,+z,-x -y,-z,+x -x,-y,-z +y,-x,-z+1/2 -x,+y,+z
<pre> {-3^+_xxx (0.0,0.0,0.0)} {m_xy0 (0.0,0.0,0.0)} {m_xy-xz (0.0,0.0,0.5)} {m_xy-y (0.0,0.0,0.5)} {-4^00z (0.0,0.0,0.5)} {m_x0z (0.0,0.0,0.0)} {-3^+_x-x-x (0.0,0.0,0.5)} {m_xxz (0.0,0.0,0.5)} {-4^+_x00 (0.0,0.0,0.5)}</pre>	-z,-x,-y +x,+y,-z -y,-x,+z+1/2 +x,-z,-y+1/2 -y,+x,-z+1/2 +x,-y,+z +z,+x,-y +y,+x,+z+1/2 -x,+z,-y+1/2
<pre> {-3^+xx-x (0.0,0.0,0.0)} {m_xyy (0.0,0.0,0.5)} {-3^+x-xx (0.0,0.0,0.0)} {-4^x00 (0.0,0.0,0.5)} {mxyz (0.5,0.0,0.0)} {-3^xxx (0.0,0.0,0.0)} {-4^0y0 (0.5,0.0,0.0)} {-4^+_0y0 (0.5,0.0,0.0)} {-3^xxx (0.0,0.0,0.0)}</pre>	-z,+x,+y +x,+z,+y+1/2 +z,-x,+y -x,-z,+y+1/2 -z+1/2,+y,-x -y,-z,-x +z+1/2,-y,-x -z+1/2,-y,+x -y,+z,+x
<pre> {m_xyx (0.5,0.0,0.0)} {-3^x-x-x (0.0,0.0,0.0)} {-3^xx-x (0.0,0.0,0.0)} {1 (0.0,0.5,0.5)} {4^+_00z (0.0,0.5,0.0)} {2_x00 (0.0,0.5,0.5)} {3^+_xxx (0.0,0.5,0.5)}</pre>	+z+1/2,+y,+x +y,-z,+x +y,+z,-x +x,+y+1/2,+z+1/2 -y,+x+1/2,+z +x,-y+1/2,-z+1/2 +z,+x+1/2,+y+1/2

```
{2_00z|(0.0,0.5,0.5)}
                                   -x,-y+1/2,+z+1/2
  \{2_x \times 0 \mid (0.0, 0.5, 0.0)\}
                                     +y,+x+1/2,-z
  {2_0yy|(0.0,0.5,0.0)}
                                     -x,+z+1/2,+y
 \{4^-_00z \mid (0.0, 0.5, 0.0)\}
                                     +y,-x+1/2,+z
  {2_0y0|(0.0,0.5,0.5)}
                                   -x,+y+1/2,-z+1/2
\{3^+x^-x^-x^-\}
                                   -z, -x+1/2, +y+1/2
  {2_x-x0|(0.0,0.5,0.0)}
                                     -y, -x+1/2, -z
 {4^+_x00|(0.0,0.5,0.0)}
                                     +x,-z+1/2,+y
\{3^+-xx-x\mid(0.0,0.5,0.5)\}
                                   +z,-x+1/2,-y+1/2
  {2_0y-y|(0.0,0.5,0.0)}
                                     -x,-z+1/2,-y
\{3^+_-x^-x^-\}
                                   -z, +x+1/2, -y+1/2
 {4^-_x00|(0.0,0.5,0.0)}
                                     +x,+z+1/2,-y
  \{2_x0x \mid (0.5, 0.5, 0.5)\}
                                +z+1/2,-y+1/2,+x+1/2
 {3^-_xxx|(0.0,0.5,0.5)}
                                   +y, +z+1/2, +x+1/2
 \{4^-_0y0|(0.5,0.5,0.5)\}
                                -z+1/2,+y+1/2,+x+1/2
 {4^+_0y0|(0.5,0.5,0.5)}
                                +z+1/2, +y+1/2, -x+1/2
\{3^--x-xx|(0.0,0.5,0.5)\}
                                   +y,-z+1/2,-x+1/2
  \{2\_-x0x \mid (0.5,0.5,0.5)\}
                                -z+1/2,-y+1/2,-x+1/2
\{3^-x-x-x|(0.0,0.5,0.5)\}
                                   -y, +z+1/2, -x+1/2
{3^-_xx-x|(0.0,0.5,0.5)}
                                   -y, -z+1/2, +x+1/2
    {-1|(0.0,0.5,0.5)}
                                   -x,-y+1/2,-z+1/2
 \{-4^+_00z \mid (0.0, 0.5, 0.0)\}
                                     +y,-x+1/2,-z
  \{m_0yz \mid (0.0,0.5,0.5)\}
                                   -x, +y+1/2, +z+1/2
 \{-3^+ xxx | (0.0, 0.5, 0.5)\}
                                   -z, -x+1/2, -y+1/2
  \{m_xy0|(0.0,0.5,0.5)\}
                                   +x,+y+1/2,-z+1/2
  \{m_x-xz\mid(0.0,0.5,0.0)\}
                                     -y, -x+1/2, +z
  \{m_xy-y \mid (0.0,0.5,0.0)\}
                                     +x,-z+1/2,-y
 \{-4^-00z \mid (0.0,0.5,0.0)\}
                                     -y, +x+1/2, -z
  {m_x0z|(0.0,0.5,0.5)}
                                   +x,-y+1/2,+z+1/2
\{-3^+x^-x^-x^-|(0.0,0.5,0.5)\}
                                   +z, +x+1/2, -y+1/2
  \{m_x \times z \mid (0.0, 0.5, 0.0)\}
                                     +y,+x+1/2,+z
 {-4^+_x00|(0.0,0.5,0.0)}
                                     -x,+z+1/2,-y
\{-3^+-xx-x|(0.0,0.5,0.5)\}
                                   -z, +x+1/2, +y+1/2
  \{m_xyy \mid (0.0, 0.5, 0.0)\}
                                     +x,+z+1/2,+y
\{-3^+-x-xx|(0.0,0.5,0.5)\}
                                   +z,-x+1/2,+y+1/2
 \{-4^- \times 00 \mid (0.0, 0.5, 0.0)\}
                                     -x,-z+1/2,+y
  {m_-xyz|(0.5,0.5,0.5)}
                                -z+1/2, +y+1/2, -x+1/2
 \{-3^-xxx|(0.0,0.5,0.5)\}
                                   -y, -z+1/2, -x+1/2
 \{-4^-_0y0|(0.5,0.5,0.5)\}
                                +z+1/2,-y+1/2,-x+1/2
 \{-4^+_0y0|(0.5,0.5,0.5)\}
                                -z+1/2,-y+1/2,+x+1/2
\{-3^--x-xx|(0.0,0.5,0.5)\}
                                   -y, +z+1/2, +x+1/2
  {m_xyx|(0.5,0.5,0.5)}
                                +z+1/2,+y+1/2,+x+1/2
\{-3^-x-x-x|(0.0,0.5,0.5)\}
                                   +y,-z+1/2,+x+1/2
\{-3^--xx-x|(0.0,0.5,0.5)\}
                                   +y, +z+1/2, -x+1/2
    \{1 \mid (0.5, 0.0, 0.5)\}
                                   +x+1/2, +y, +z+1/2
 {4^+_00z|(0.5,0.0,0.0)}
                                     -y+1/2,+x,+z
  \{2_{x00}|(0.5,0.0,0.5)\}
                                   +x+1/2,-y,-z+1/2
 {3^+_xxx|(0.5,0.0,0.5)}
                                   +z+1/2,+x,+y+1/2
  {2_00z|(0.5,0.0,0.5)}
                                   -x+1/2,-y,+z+1/2
  {2_xx0|(0.5,0.0,0.0)}
                                     +y+1/2,+x,-z
  {2_0yy|(0.5,0.0,0.0)}
                                     -x+1/2,+z,+y
 {4^-_00z|(0.5,0.0,0.0)}
                                     +y+1/2,-x,+z
  \{2_0y0|(0.5,0.0,0.5)\}
                                   -x+1/2,+y,-z+1/2
{3^+_x-x-x}(0.5,0.0,0.5)
                                   -z+1/2, -x, +y+1/2
```

```
\{2_x-x0|(0.5,0.0,0.0)\}
                                     -y+1/2,-x,-z
 {4^+_x00|(0.5,0.0,0.0)}
                                     +x+1/2,-z,+y
\{3^+-xx-x\mid(0.5,0.0,0.5)\}
                                  +z+1/2,-x,-y+1/2
  \{2_0y-y \mid (0.5,0.0,0.0)\}
                                     -x+1/2,-z,-y
{3^+_-x^-x^+|(0.5,0.0,0.5)}
                                  -z+1/2,+x,-y+1/2
 {4^-_x00|(0.5,0.0,0.0)}
                                     +x+1/2,+z,-y
  \{2_x0x | (0.0,0.0,0.5)\}
                                     +z,-y,+x+1/2
 {3^-_xxx|(0.5,0.0,0.5)}
                                  +y+1/2,+z,+x+1/2
 \{4^-_0y0|(0.0,0.0,0.5)\}
                                     -z,+y,+x+1/2
 {4^+_0y0|(0.0,0.0,0.5)}
                                     +z,+y,-x+1/2
\{3^--x-xx\mid(0.5,0.0,0.5)\}
                                  +y+1/2,-z,-x+1/2
  {2_-x0x|(0.0,0.0,0.5)}
                                     -z,-y,-x+1/2
\{3^-x-x-x|(0.5,0.0,0.5)\}
                                  -y+1/2,+z,-x+1/2
\{3^--xx-x|(0.5,0.0,0.5)\}
                                  -y+1/2,-z,+x+1/2
    \{-1 \mid (0.5, 0.0, 0.5)\}
                                  -x+1/2,-y,-z+1/2
 \{-4^+00z|(0.5,0.0,0.0)\}
                                     +y+1/2,-x,-z
  \{m_0yz \mid (0.5,0.0,0.5)\}
                                  -x+1/2,+y,+z+1/2
 \{-3^+ \times \times | (0.5, 0.0, 0.5)\}
                                  -z+1/2,-x,-y+1/2
  \{m_xy0|(0.5,0.0,0.5)\}
                                  +x+1/2, +y, -z+1/2
  \{m_x-xz \mid (0.5,0.0,0.0)\}
                                     -y+1/2,-x,+z
  \{m_xy-y \mid (0.5,0.0,0.0)\}
                                     +x+1/2,-z,-y
 {-4^-_00z|(0.5,0.0,0.0)}
                                     -y+1/2,+x,-z
  \{m_x0z \mid (0.5,0.0,0.5)\}
                                  +x+1/2,-y,+z+1/2
                                  +z+1/2,+x,-y+1/2
\{-3^+x^-x^-x^- (0.5,0.0,0.5)\}
  \{m_xxz|(0.5,0.0,0.0)\}
                                     +y+1/2,+x,+z
 {-4^+_x00|(0.5,0.0,0.0)}
                                     -x+1/2,+z,-y
\{-3^+-xx-x|(0.5,0.0,0.5)\}
                                  -z+1/2,+x,+y+1/2
  \{m_xyy \mid (0.5,0.0,0.0)\}
                                     +x+1/2,+z,+y
\{-3^+-x-xx|(0.5,0.0,0.5)\}
                                  +z+1/2,-x,+y+1/2
                                     -x+1/2,-z,+y
 \{-4^- \times 00 \mid (0.5, 0.0, 0.0)\}
                                     -z, +y, -x+1/2
  {m_-xyz|(0.0,0.0,0.5)}
 \{-3^-xxx|(0.5,0.0,0.5)\}
                                  -y+1/2,-z,-x+1/2
 \{-4^-_0y0|(0.0,0.0,0.5)\}
                                     +z,-y,-x+1/2
 \{-4^+_0y0|(0.0,0.0,0.5)\}
                                     -z,-y,+x+1/2
\{-3^--x-xx|(0.5,0.0,0.5)\}
                                  -y+1/2,+z,+x+1/2
  \{m_xyx | (0.0,0.0,0.5)\}
                                     +z,+y,+x+1/2
\{-3^-x-x-x|(0.5,0.0,0.5)\}
                                  +y+1/2,-z,+x+1/2
\{-3^--xx-x \mid (0.5,0.0,0.5)\}
                                  +y+1/2,+z,-x+1/2
    {1|(0.5,0.5,0.0)}
                                  +x+1/2, +y+1/2, +z
 {4^+_00z|(0.5,0.5,0.5)}
                                -y+1/2, +x+1/2, +z+1/2
  \{2_{x00} | (0.5, 0.5, 0.0)\}
                                  +x+1/2,-y+1/2,-z
 {3^+_xxx|(0.5,0.5,0.0)}
                                  +z+1/2,+x+1/2,+y
  {2_00z|(0.5,0.5,0.0)}
                                  -x+1/2, -y+1/2, +z
  {2_xx0|(0.5,0.5,0.5)}
                                +y+1/2,+x+1/2,-z+1/2
  \{2_{0yy} | (0.5, 0.5, 0.5)\}
                                -x+1/2,+z+1/2,+y+1/2
 {4^-_00z|(0.5,0.5,0.5)}
                                +y+1/2,-x+1/2,+z+1/2
  {2_0y0|(0.5,0.5,0.0)}
                                  -x+1/2, +y+1/2, -z
\{3^+x^-x^-x^-\}
                                  -z+1/2,-x+1/2,+y
  {2_x-x0|(0.5,0.5,0.5)}
                                -y+1/2, -x+1/2, -z+1/2
 \{4^+x00|(0.5,0.5,0.5)\}
                                +x+1/2,-z+1/2,+y+1/2
{3^+_-xx-x|(0.5,0.5,0.0)}
                                  +z+1/2,-x+1/2,-y
  \{2_0y-y\mid (0.5,0.5,0.5)\}
                                -x+1/2,-z+1/2,-y+1/2
{3^+_-x-xx|(0.5,0.5,0.0)}
                                  -z+1/2,+x+1/2,-y
 \{4^-x00|(0.5,0.5,0.5)\}
                                +x+1/2,+z+1/2,-y+1/2
```

```
\{2_x0x|(0.0,0.5,0.0)\}
                                      +z,-y+1/2,+x
   {3^-_xxx|(0.5,0.5,0.0)}
                                    +y+1/2,+z+1/2,+x
   {4^-_0y0|(0.0,0.5,0.0)}
                                      -z,+y+1/2,+x
   {4^+_0y0|(0.0,0.5,0.0)}
                                      +z, +y+1/2, -x
  \{3^--x-xx\mid(0.5,0.5,0.0)\}
                                    +y+1/2,-z+1/2,-x
    \{2\_-x0x \mid (0.0,0.5,0.0)\}
                                      -z,-y+1/2,-x
  {3^-_x-x-x|(0.5,0.5,0.0)}
                                    -y+1/2,+z+1/2,-x
  \{3^--xx-x\mid(0.5,0.5,0.0)\}
                                    -y+1/2,-z+1/2,+x
      \{-1|(0.5,0.5,0.0)\}
                                    -x+1/2, -y+1/2, -z
   \{-4^+00z|(0.5,0.5,0.5)\}
                                  +y+1/2,-x+1/2,-z+1/2
    \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                    -x+1/2,+y+1/2,+z
   {-3^+_xxx|(0.5,0.5,0.0)}
                                    -z+1/2, -x+1/2, -y
    \{m_xy0|(0.5,0.5,0.0)\}
                                    +x+1/2, +y+1/2, -z
    \{m_x-xz\mid(0.5,0.5,0.5)\}
                                  -y+1/2,-x+1/2,+z+1/2
    {m_xy-y|(0.5,0.5,0.5)}
                                  +x+1/2,-z+1/2,-y+1/2
   \{-4^-00z \mid (0.5, 0.5, 0.5)\}
                                  -y+1/2,+x+1/2,-z+1/2
    {m_x0z|(0.5,0.5,0.0)}
                                    +x+1/2,-y+1/2,+z
  \{-3^+x^-x^-x^-\}
                                    +z+1/2, +x+1/2, -y
    \{m_xxz \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,+x+1/2,+z+1/2
   {-4^+_x00|(0.5,0.5,0.5)}
                                  -x+1/2, +z+1/2, -y+1/2
  \{-3^+-xx-x|(0.5,0.5,0.0)\}
                                    -z+1/2,+x+1/2,+y
    \{m_xyy \mid (0.5, 0.5, 0.5)\}
                                  +x+1/2,+z+1/2,+y+1/2
  \{-3^+-x-xx\mid(0.5,0.5,0.0)\}
                                    +z+1/2,-x+1/2,+y
   \{-4^- \times 00 \mid (0.5, 0.5, 0.5)\}
                                  -x+1/2, -z+1/2, +y+1/2
    \{m_-xyz \mid (0.0,0.5,0.0)\}
                                      -z, +y+1/2, -x
   \{-3^-xxx|(0.5,0.5,0.0)\}
                                    -y+1/2,-z+1/2,-x
   {-4^-_0y0|(0.0,0.5,0.0)}
                                      +z,-y+1/2,-x
   \{-4^+_0y0|(0.0,0.5,0.0)\}
                                      -z, -y+1/2, +x
  \{-3^--x-xx|(0.5,0.5,0.0)\}
                                    -y+1/2,+z+1/2,+x
    \{m_xyx | (0.0,0.5,0.0)\}
                                      +z,+y+1/2,+x
  \{-3^-x-x-x|(0.5,0.5,0.0)\}
                                    +y+1/2,-z+1/2,+x
        _-xx-x|(0.5,0.5,0.0)}
                                    +y+1/2,+z+1/2,-x
*******
space group: 227:1 {'Hall': ' F 4d 2 3 -1d', 'HM': 'F d -3 m:1'}
Crystal system: Cubic
Setting: 1
+X,+Y,+Z
-y+1/4,+x+1/4,+z+1/4
+x,-y,-z
+z,+x,+y
-x+1/4,-y+1/4,-z+1/4
             Seitz
                                          Jones
      {1|(0.0,0.0,0.0)}
                                         +x,+y,+z
  \{4^+_{00z}|(0.25,0.25,0.25)\}
                                  -y+1/4, +x+1/4, +z+1/4
    \{2_{x00} | (0.0,0.0,0.0)\}
                                        +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                        +z,+x,+y
                                  -x+1/4, -y+1/4, -z+1/4
    \{-1 \mid (0.25, 0.25, 0.25)\}
```

-x,-y+1/2,+z+1/2

{2_00z|(0.0,0.5,0.5)}

```
{2_xx0|(0.25,0.25,0.25)}
                                 +y+1/4, +x+1/4, -z+1/4
 {2_0yy|(0.25,0.25,0.25)}
                                 -x+1/4, +z+1/4, +y+1/4
 \{-4^+_00z \mid (0.0,0.5,0.5)\}
                                   +y,-x+1/2,-z+1/2
                                 +y+3/4,-x+1/4,+z+3/4
\{4^- 00z \mid (0.75, 0.25, 0.75)\}
  {2_0y0|(0.0,0.5,0.5)}
                                   -x,+y+1/2,-z+1/2
\{3^+x^-x^-x^-\}
                                   -z, -x+1/2, +y+1/2
                                 +x+3/4, +y+1/4, -z+3/4
 \{m_xy0|(0.75,0.25,0.75)\}
\{2_x-x0|(0.75,0.25,0.75)\}
                                 -y+3/4, -x+1/4, -z+3/4
\{4^+ \times 00 \mid (0.75, 0.25, 0.75)\}
                                 +x+3/4,-z+1/4,+y+3/4
 \{-4^-\ 00z \mid (0.0,0.0,0.0)\}
                                        -y, +x, -z
\{3^+-xx-x\mid(0.0,0.0,0.0)\}
                                       +z,-x,-y
 {m_0yz|(0.25,0.75,0.75)}
                                 -x+1/4, +y+3/4, +z+3/4
\{2_0y-y\mid (0.25,0.75,0.75)\}
                                 -x+1/4, -z+3/4, -y+3/4
  {m_xxz|(0.0,0.5,0.5)}
                                   +y, +x+1/2, +z+1/2
{3^+_-x^-x^-|(0.0,0.5,0.5)}
                                   -z, +x+1/2, -y+1/2
                                 +x+3/4,-y+3/4,+z+1/4
 \{m_x0z|(0.75,0.75,0.25)\}
\{4^-x00|(0.75,0.75,0.25)\}
                                 +x+3/4,+z+3/4,-y+1/4
  \{m_x-xz \mid (0.0,0.0,0.0)\}
                                        -y,-x,+z
    {1|(0.0,0.5,0.5)}
                                   +x,+y+1/2,+z+1/2
\{4^+_{00z}|(0.25,0.75,0.75)\}
                                 -y+1/4, +x+3/4, +z+3/4
  \{2_{x00}|(0.0,0.5,0.5)\}
                                   +x,-y+1/2,-z+1/2
 \{3^+ xxx \mid (0.0, 0.5, 0.5)\}
                                   +z, +x+1/2, +y+1/2
  \{-1 \mid (0.25, 0.75, 0.75)\}
                                 -x+1/4, -y+3/4, -z+3/4
  {2_00z|(0.0,0.0,0.0)}
                                        -x,-y,+z
                                 +y+1/4, +x+3/4, -z+3/4
 {2_xx0|(0.25,0.75,0.75)}
 {2_0yy|(0.25,0.75,0.75)}
                                 -x+1/4, +z+3/4, +y+3/4
 \{-4^+_00z \mid (0.0,0.0,0.0)\}
                                        +y,-x,-z
\{4^-_00z \mid (0.75, 0.75, 0.25)\}
                                 +y+3/4, -x+3/4, +z+1/4
  {2_0y0|(0.0,0.0,0.0)}
                                        -x,+y,-z
\{3^+_x - x - x \mid (0.0, 0.0, 0.0)\}
                                        -z,-x,+y
 {m_xy0|(0.75,0.75,0.25)}
                                 +x+3/4, +y+3/4, -z+1/4
\{2_x-x0|(0.75,0.75,0.25)\}
                                 -y+3/4, -x+3/4, -z+1/4
\{4^+_{x00}|(0.75,0.75,0.25)\}
                                 +x+3/4,-z+3/4,+y+1/4
 \{-4^-\ 00z \mid (0.0,0.5,0.5)\}
                                   -y, +x+1/2, -z+1/2
\{3^+-xx-x\mid(0.0,0.5,0.5)\}
                                   +z,-x+1/2,-y+1/2
 \{m_0yz \mid (0.25, 0.25, 0.25)\}
                                 -x+1/4, +y+1/4, +z+1/4
\{2_0y-y\mid (0.25,0.25,0.25)\}
                                 -x+1/4, -z+1/4, -y+1/4
  {m_xxz|(0.0,0.0,0.0)}
                                       +y,+x,+z
\{3^+_-x^-x^-\}
                                        -z,+x,-y
 \{m_x0z|(0.75,0.25,0.75)\}
                                 +x+3/4,-y+1/4,+z+3/4
                                 +x+3/4, +z+1/4, -y+3/4
\{4^-x00|(0.75,0.25,0.75)\}
  \{m_x-xz\mid(0.0,0.5,0.5)\}
                                   -y, -x+1/2, +z+1/2
    \{1|(0.5,0.0,0.5)\}
                                   +x+1/2, +y, +z+1/2
\{4^+_{00z}|(0.75,0.25,0.75)\}
                                 -y+3/4, +x+1/4, +z+3/4
  {2_x00|(0.5,0.0,0.5)}
                                   +x+1/2,-y,-z+1/2
 {3^+_xxx|(0.5,0.0,0.5)}
                                   +z+1/2,+x,+y+1/2
  \{-1 \mid (0.75, 0.25, 0.75)\}
                                 -x+3/4, -y+1/4, -z+3/4
  {2_00z|(0.5,0.5,0.0)}
                                   -x+1/2,-y+1/2,+z
 {2_xx0|(0.75,0.25,0.75)}
                                 +y+3/4, +x+1/4, -z+3/4
 {2_0yy|(0.75,0.25,0.75)}
                                 -x+3/4, +z+1/4, +y+3/4
 {-4^+_00z|(0.5,0.5,0.0)}
                                   +y+1/2,-x+1/2,-z
\{4^-_00z \mid (0.25, 0.25, 0.25)\}
                                 +y+1/4, -x+1/4, +z+1/4
  {2_0y0|(0.5,0.5,0.0)}
                                   -x+1/2, +y+1/2, -z
\{3^+x^-x^-x^-\}
                                   -z+1/2, -x+1/2, +y
```

```
\{2_x-x0|(0.25,0.25,0.25)\}
                                  -y+1/4, -x+1/4, -z+1/4
  \{4^+_x00|(0.25,0.25,0.25)\}
                                  +x+1/4, -z+1/4, +y+1/4
   {-4^-_00z|(0.5,0.0,0.5)}
                                     -y+1/2,+x,-z+1/2
  {3^+_-xx-x|(0.5,0.0,0.5)}
                                     +z+1/2,-x,-y+1/2
   {m_0yz|(0.75,0.75,0.25)}
                                  -x+3/4, +y+3/4, +z+1/4
                                  -x+3/4, -z+3/4, -y+1/4
  \{2_0y-y|(0.75,0.75,0.25)\}
    \{m_xxz | (0.5,0.5,0.0)\}
                                     +y+1/2,+x+1/2,+z
  \{3^+-x-x^+ \mid (0.5,0.5,0.0)\}
                                     -z+1/2,+x+1/2,-y
   \{m_x0z|(0.25,0.75,0.75)\}
                                  +x+1/4,-y+3/4,+z+3/4
  \{4^-x00|(0.25,0.75,0.75)\}
                                  +x+1/4, +z+3/4, -y+3/4
    \{m_x-xz\mid (0.5,0.0,0.5)\}
                                     -y+1/2,-x,+z+1/2
      \{1|(0.5,0.5,0.0)\}
                                     +x+1/2, +y+1/2, +z
  \{4^+_{00z}|(0.75,0.75,0.25)\}
                                  -y+3/4, +x+3/4, +z+1/4
    \{2_{x00} | (0.5, 0.5, 0.0)\}
                                     +x+1/2, -y+1/2, -z
   {3^+_xxx|(0.5,0.5,0.0)}
                                     +z+1/2,+x+1/2,+y
    \{-1 \mid (0.75, 0.75, 0.25)\}
                                  -x+3/4, -y+3/4, -z+1/4
                                     -x+1/2,-y,+z+1/2
    {2_00z|(0.5,0.0,0.5)}
   {2_xx0|(0.75,0.75,0.25)}
                                  +y+3/4, +x+3/4, -z+1/4
   {2_0yy|(0.75,0.75,0.25)}
                                  -x+3/4, +z+3/4, +y+1/4
   \{-4^+_00z \mid (0.5,0.0,0.5)\}
                                     +y+1/2,-x,-z+1/2
  \{4^-_00z \mid (0.25, 0.75, 0.75)\}
                                  +y+1/4, -x+3/4, +z+3/4
    {2_0y0|(0.5,0.0,0.5)}
                                     -x+1/2,+y,-z+1/2
  {3^+_x-x-x}(0.5,0.0,0.5)
                                     -z+1/2,-x,+y+1/2
                                  +x+1/4, +y+3/4, -z+3/4
   {m_xy0|(0.25,0.75,0.75)}
  \{2_x-x0|(0.25,0.75,0.75)\}
                                  -y+1/4, -x+3/4, -z+3/4
  \{4^+_{\times}00 \mid (0.25, 0.75, 0.75)\}
                                  +x+1/4,-z+3/4,+y+3/4
   \{-4^-00z \mid (0.5, 0.5, 0.0)\}
                                     -y+1/2,+x+1/2,-z
  \{3^+-xx-x\mid(0.5,0.5,0.0)\}
                                     +z+1/2,-x+1/2,-y
   \{m_0yz \mid (0.75, 0.25, 0.75)\}
                                  -x+3/4, +y+1/4, +z+3/4
  \{2_0y-y|(0.75,0.25,0.75)\}
                                  -x+3/4, -z+1/4, -y+3/4
    \{m_{xxz} | (0.5, 0.0, 0.5)\}
                                     +y+1/2,+x,+z+1/2
  {3^+_-x^-x^+|(0.5,0.0,0.5)}
                                     -z+1/2,+x,-y+1/2
                                  +x+1/4, -y+1/4, +z+1/4
   {m_x0z|(0.25,0.25,0.25)}
  \{4^-x00|(0.25,0.25,0.25)\}
                                  +x+1/4,+z+1/4,-y+1/4
    \{m_x-xz\mid(0.5,0.5,0.0)\}
                                     -y+1/2,-x+1/2,+z
*******
space group: 227:2 {'Hall': '-F 4vw 2vw 3', 'HM': 'F d -3 m:2'}
Crystal system: Cubic
Setting: 2
+x,+y,+z
-y, +x+1/4, +z+1/4
+x,-y+1/4,-z+1/4
+Z,+X,+y
              Seitz
                                             Jones
       \{1 \mid (0.0, 0.0, 0.0)\}
                                           +x,+y,+z
```

-y, +x+1/4, +z+1/4

+x,-y+1/4,-z+1/4

+x+1/4, +y+1/4, -z+1/4

{m_xy0|(0.25,0.25,0.25)}

 $\{4^+_00z|(0.0,0.25,0.25)\}$

{2_x00|(0.0,0.25,0.25)}

```
{3^+_xxx|(0.0,0.0,0.0)}
                                         +z,+x,+y
  {2_00z|(0.75,0.25,0.5)}
                                   -x+3/4,-y+1/4,+z+1/2
  \{2_x \times 0 \mid (0.75, 0.25, 0.5)\}
                                   +y+3/4,+x+1/4,-z+1/2
  {2_0yy|(0.0,0.25,0.25)}
                                     -x, +z+1/4, +y+1/4
 {4^-_00z|(0.75,0.0,0.75)}
                                     +y+3/4,-x,+z+3/4
  {2_0y0|(0.75,0.0,0.75)}
                                     -x+3/4,+y,-z+3/4
{3^+_x-x-x|(0.75,0.25,0.5)}
                                   -z+3/4, -x+1/4, +y+1/2
   {2_x-x0|(0.0,0.0,0.0)}
                                          -y,-x,-z
 {4^+_x00|(0.75,0.0,0.75)}
                                     +x+3/4,-z,+y+3/4
                                     +z,-x+1/4,-y+1/4
\{3^+ -xx-x \mid (0.0,0.25,0.25)\}
   {2_0y-y|(0.0,0.0,0.0)}
                                         -x,-z,-y
{3^+-x-xx|(0.75,0.0,0.75)}
                                     -z+3/4,+x,-y+3/4
 {4^-_x00|(0.75,0.25,0.5)}
                                   +x+3/4, +z+1/4, -y+1/2
  {2_x0x|(0.25,0.0,0.25)}
                                     +z+1/4,-y,+x+1/4
  \{3^-xxx|(0.0,0.0,0.0)\}
                                         +y,+z,+x
 {4^-_0y0|(0.5,0.75,0.25)}
                                   -z+1/2,+y+3/4,+x+1/4
 {4^+_0y0|(0.75,0.75,0.0)}
                                     +z+3/4, +y+3/4, -x
\{3^--x-xx\mid(0.5,0.75,0.25)\}
                                   +y+1/2,-z+3/4,-x+1/4
   {2_-x0x|(0.0,0.0,0.0)}
                                          -z,-y,-x
{3^-_x-x-x|(0.25,0.0,0.25)}
                                     -y+1/4,+z,-x+1/4
\{3^--xx-x \mid (0.75,0.75,0.0)\}
                                     -y+3/4,-z+3/4,+x
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                         -x,-y,-z
 \{-4^+_00z|(0.0,0.25,0.25)\}
                                     +y,-x+1/4,-z+1/4
  \{m_0yz \mid (0.0, 0.25, 0.25)\}
                                     -x, +y+1/4, +z+1/4
  {-3^+_xxx|(0.0,0.0,0.0)}
                                          -z,-x,-y
  \{m_xy0|(0.75,0.25,0.5)\}
                                   +x+3/4, +y+1/4, -z+1/2
  \{m_x-xz\mid(0.75,0.25,0.5)\}
                                   -y+3/4, -x+1/4, +z+1/2
  \{m_xy-y \mid (0.0,0.25,0.25)\}
                                     +x,-z+1/4,-y+1/4
 {-4^-_00z|(0.75,0.0,0.75)}
                                     -y+3/4,+x,-z+3/4
  \{m_x0z \mid (0.75,0.0,0.75)\}
                                     +x+3/4,-y,+z+3/4
\{-3^+x^-x^-x^-\}
                                   +z+3/4,+x+1/4,-y+1/2
   {m_xxz|(0.0,0.0,0.0)}
                                         +y,+x,+z
 \{-4^+ \times 00 \mid (0.75, 0.0, 0.75)\}
                                     -x+3/4,+z,-y+3/4
\{-3^+-xx-x \mid (0.0,0.25,0.25)\}
                                     -z, +x+1/4, +y+1/4
   \{m_xyy \mid (0.0,0.0,0.0)\}
                                          +x,+z,+y
\{-3^+-x-xx|(0.75,0.0,0.75)\}
                                     +z+3/4,-x,+y+3/4
 \{-4^- \times 00 \mid (0.75, 0.25, 0.5)\}
                                   -x+3/4, -z+1/4, +y+1/2
  \{m_-xyz \mid (0.25,0.0,0.25)\}
                                     -z+1/4, +y, -x+1/4
  \{-3^-xxx|(0.0,0.0,0.0)\}
                                         -y,-z,-x
 \{-4^-_0y0|(0.5,0.75,0.25)\}
                                   +z+1/2,-y+3/4,-x+1/4
 \{-4^+_0y0|(0.75,0.75,0.0)\}
                                     -z+3/4,-y+3/4,+x
\{-3^--x-xx|(0.5,0.75,0.25)\}
                                   -y+1/2, +z+3/4, +x+1/4
   \{m_xyx | (0.0,0.0,0.0)\}
                                         +z,+y,+x
\{-3^-x-x-x|(0.25,0.0,0.25)\}
                                     +y+1/4,-z,+x+1/4
\{-3^--xx-x|(0.75,0.75,0.0)\}
                                     +y+3/4,+z+3/4,-x
     {1|(0.0,0.5,0.5)}
                                     +x, +y+1/2, +z+1/2
 \{4^+_{00z}|(0.0,0.75,0.75)\}
                                     -y, +x+3/4, +z+3/4
  \{2_{\times}00 \mid (0.0, 0.75, 0.75)\}
                                     +x,-y+3/4,-z+3/4
                                     +z,+x+1/2,+y+1/2
  \{3^+ xxx \mid (0.0, 0.5, 0.5)\}
  {2_00z|(0.75,0.75,0.0)}
                                     -x+3/4, -y+3/4, +z
  \{2_{x} \times 0 \mid (0.75, 0.75, 0.0)\}
                                     +y+3/4,+x+3/4,-z
  {2_0yy|(0.0,0.75,0.75)}
                                     -x, +z+3/4, +y+3/4
 {4^-_00z|(0.75,0.5,0.25)}
                                   +y+3/4,-x+1/2,+z+1/4
  {2_0y0|(0.75,0.5,0.25)}
                                   -x+3/4, +y+1/2, -z+1/4
```

```
{3^+_x-x-x|(0.75,0.75,0.0)}
                                     -z+3/4, -x+3/4, +y
   {2_x-x0|(0.0,0.5,0.5)}
                                     -y, -x+1/2, -z+1/2
 {4^+_x00|(0.75,0.5,0.25)}
                                   +x+3/4,-z+1/2,+y+1/4
{3^+-xx-x|(0.0,0.75,0.75)}
                                     +z,-x+3/4,-y+3/4
   {2_0y-y|(0.0,0.5,0.5)}
                                     -x,-z+1/2,-y+1/2
{3^+_-x^-x^-|(0.75,0.5,0.25)}
                                   -z+3/4,+x+1/2,-y+1/4
 {4^-_x00|(0.75,0.75,0.0)}
                                     +x+3/4,+z+3/4,-y
  \{2_x0x \mid (0.25, 0.5, 0.75)\}
                                   +z+1/4,-y+1/2,+x+3/4
  \{3^-xxx|(0.0,0.5,0.5)\}
                                     +y, +z+1/2, +x+1/2
 \{4^- 0 \lor 0 \mid (0.5, 0.25, 0.75)\}
                                   -z+1/2,+y+1/4,+x+3/4
 \{4^+_0y0|(0.75,0.25,0.5)\}
                                   +z+3/4, +y+1/4, -x+1/2
{3^-_x-xx|(0.5,0.25,0.75)}
                                   +y+1/2,-z+1/4,-x+3/4
   {2_-x0x|(0.0,0.5,0.5)}
                                     -z,-y+1/2,-x+1/2
\{3^-x-x-x|(0.25,0.5,0.75)\}
                                   -y+1/4, +z+1/2, -x+3/4
\{3^--xx-x \mid (0.75,0.25,0.5)\}
                                   -y+3/4, -z+1/4, +x+1/2
      \{-1 \mid (0.0, 0.5, 0.5)\}
                                     -x,-y+1/2,-z+1/2
 \{-4^+_00z \mid (0.0,0.75,0.75)\}
                                     +y,-x+3/4,-z+3/4
  \{m_0yz \mid (0.0,0.75,0.75)\}
                                     -x, +y+3/4, +z+3/4
  \{-3^+ \times \times | (0.0, 0.5, 0.5)\}
                                     -z, -x+1/2, -y+1/2
  \{m_xy0|(0.75,0.75,0.0)\}
                                     +x+3/4, +y+3/4, -z
  \{m_x-xz\mid(0.75,0.75,0.0)\}
                                     -y+3/4, -x+3/4, +z
  \{m_xy-y \mid (0.0,0.75,0.75)\}
                                     +x,-z+3/4,-y+3/4
 \{-4^-00z \mid (0.75, 0.5, 0.25)\}
                                   -y+3/4, +x+1/2, -z+1/4
  \{m_x0z|(0.75,0.5,0.25)\}
                                   +x+3/4,-y+1/2,+z+1/4
\{-3^+x^-x^-x^-(0.75,0.75,0.0)\}
                                     +z+3/4,+x+3/4,-y
                                     +y, +x+1/2, +z+1/2
   \{m_{xxz} | (0.0, 0.5, 0.5)\}
 {-4^+_x00|(0.75,0.5,0.25)}
                                   -x+3/4, +z+1/2, -y+1/4
\{-3^+-xx-x|(0.0,0.75,0.75)\}
                                     -z, +x+3/4, +y+3/4
   \{m_xyy | (0.0, 0.5, 0.5)\}
                                     +x, +z+1/2, +y+1/2
\{-3^+-x-xx|(0.75,0.5,0.25)\}
                                   +z+3/4,-x+1/2,+y+1/4
 \{-4^-x00|(0.75,0.75,0.0)\}
                                     -x+3/4, -z+3/4, +y
  \{m_-xyz \mid (0.25, 0.5, 0.75)\}
                                   -z+1/4,+y+1/2,-x+3/4
  \{-3^-xxx|(0.0,0.5,0.5)\}
                                     -y, -z+1/2, -x+1/2
 {-4^-_0y0|(0.5,0.25,0.75)}
                                   +z+1/2,-y+1/4,-x+3/4
 {-4^+_0y0|(0.75,0.25,0.5)}
                                   -z+3/4,-y+1/4,+x+1/2
\{-3^--x-xx|(0.5,0.25,0.75)\}
                                   -y+1/2, +z+1/4, +x+3/4
   \{m_xyx | (0.0,0.5,0.5)\}
                                     +z,+y+1/2,+x+1/2
{-3^-_x-x-x|(0.25,0.5,0.75)}
                                   +y+1/4,-z+1/2,+x+3/4
      _-xx-x|(0.75,0.25,0.5)}
                                   +y+3/4,+z+1/4,-x+1/2
     \{1|(0.5,0.0,0.5)\}
                                     +x+1/2,+y,+z+1/2
 \{4^+_{00z}|(0.5,0.25,0.75)\}
                                   -y+1/2,+x+1/4,+z+3/4
                                   +x+1/2,-y+1/4,-z+3/4
  \{2_{x00}|(0.5,0.25,0.75)\}
  \{3^+ xxx \mid (0.5, 0.0, 0.5)\}
                                     +z+1/2,+x,+y+1/2
  {2_00z|(0.25,0.25,0.0)}
                                     -x+1/4, -y+1/4, +z
  \{2_{x} \times 0 \mid (0.25, 0.25, 0.0)\}
                                     +y+1/4, +x+1/4, -z
  {2_0yy|(0.5,0.25,0.75)}
                                   -x+1/2, +z+1/4, +y+3/4
 \{4^-_00z \mid (0.25,0.0,0.25)\}
                                     +y+1/4,-x,+z+1/4
  {2_0y0|(0.25,0.0,0.25)}
                                     -x+1/4,+y,-z+1/4
{3^+_x-x-x|(0.25,0.25,0.0)}
                                     -z+1/4, -x+1/4, +y
   {2_x-x0|(0.5,0.0,0.5)}
                                     -y+1/2,-x,-z+1/2
 {4^+_x00|(0.25,0.0,0.25)}
                                     +x+1/4,-z,+y+1/4
{3^+-xx-x|(0.5,0.25,0.75)}
                                   +z+1/2,-x+1/4,-y+3/4
   \{2_0y-y \mid (0.5,0.0,0.5)\}
                                     -x+1/2,-z,-y+1/2
\{3^+_-x^-x^+ | (0.25,0.0,0.25)\}
                                     -z+1/4,+x,-y+1/4
```

```
{4^-_x00|(0.25,0.25,0.0)}
                                    +x+1/4,+z+1/4,-y
  \{2_x0x|(0.75,0.0,0.75)\}
                                    +z+3/4,-y,+x+3/4
                                    +y+1/2,+z,+x+1/2
  \{3^-xxx|(0.5,0.0,0.5)\}
 {4^-_0y0|(0.0,0.75,0.75)}
                                    -z, +y+3/4, +x+3/4
 {4^+_0y0|(0.25,0.75,0.5)}
                                  +z+1/4, +y+3/4, -x+1/2
\{3^--x-xx\mid(0.0,0.75,0.75)\}
                                    +y,-z+3/4,-x+3/4
   \{2\_-x0x | (0.5,0.0,0.5)\}
                                    -z+1/2,-y,-x+1/2
\{3^-x-x-x|(0.75,0.0,0.75)\}
                                    -y+3/4,+z,-x+3/4
\{3^--xx-x \mid (0.25,0.75,0.5)\}
                                  -y+1/4, -z+3/4, +x+1/2
     \{-1 \mid (0.5, 0.0, 0.5)\}
                                    -x+1/2,-y,-z+1/2
 \{-4^+_00z \mid (0.5, 0.25, 0.75)\}
                                  +y+1/2,-x+1/4,-z+3/4
                                  -x+1/2,+y+1/4,+z+3/4
  {m_0yz|(0.5,0.25,0.75)}
  \{-3^+ \times \times | (0.5, 0.0, 0.5)\}
                                    -z+1/2, -x, -y+1/2
  \{m_xy0|(0.25,0.25,0.0)\}
                                    +x+1/4, +y+1/4, -z
  \{m_x-xz \mid (0.25,0.25,0.0)\}
                                    -y+1/4, -x+1/4, +z
  \{m_xy-y \mid (0.5,0.25,0.75)\}
                                  +x+1/2,-z+1/4,-y+3/4
 \{-4^-_00z \mid (0.25,0.0,0.25)\}
                                    -y+1/4,+x,-z+1/4
  {m_x0z|(0.25,0.0,0.25)}
                                    +x+1/4,-y,+z+1/4
\{-3^+x^-x^-x^-\}
                                    +z+1/4, +x+1/4, -y
   \{m_{xxz}|(0.5,0.0,0.5)\}
                                    +y+1/2,+x,+z+1/2
 {-4^+_x00|(0.25,0.0,0.25)}
                                    -x+1/4,+z,-y+1/4
\{-3^+-xx-x \mid (0.5,0.25,0.75)\}
                                  -z+1/2,+x+1/4,+y+3/4
   {m_xyy|(0.5,0.0,0.5)}
                                    +x+1/2,+z,+y+1/2
\{-3^+-x-xx|(0.25,0.0,0.25)\}
                                    +z+1/4,-x,+y+1/4
 \{-4^- \times 00 \mid (0.25, 0.25, 0.0)\}
                                    -x+1/4, -z+1/4, +y
                                    -z+3/4,+y,-x+3/4
  \{m_-xyz \mid (0.75,0.0,0.75)\}
  \{-3^-xxx|(0.5,0.0,0.5)\}
                                    -y+1/2,-z,-x+1/2
                                    +z,-y+3/4,-x+3/4
 \{-4^-_0y0|(0.0,0.75,0.75)\}
 {-4^+_0y0|(0.25,0.75,0.5)}
                                  -z+1/4,-y+3/4,+x+1/2
\{-3^--x-xx|(0.0,0.75,0.75)\}
                                    -y, +z+3/4, +x+3/4
   {m_xyx|(0.5,0.0,0.5)}
                                    +z+1/2, +y, +x+1/2
\{-3^-x-x-x|(0.75,0.0,0.75)\}
                                    +y+3/4,-z,+x+3/4
\{-3^--xx-x|(0.25,0.75,0.5)\}
                                  +y+1/4, +z+3/4, -x+1/2
     {1|(0.5,0.5,0.0)}
                                    +x+1/2, +y+1/2, +z
 {4^+_00z|(0.5,0.75,0.25)}
                                  -y+1/2,+x+3/4,+z+1/4
                                  +x+1/2,-y+3/4,-z+1/4
  {2_x00|(0.5,0.75,0.25)}
  {3^+_xxx|(0.5,0.5,0.0)}
                                    +z+1/2,+x+1/2,+y
  \{2_{00z} | (0.25, 0.75, 0.5)\}
                                  -x+1/4,-y+3/4,+z+1/2
  {2_xx0|(0.25,0.75,0.5)}
                                  +y+1/4,+x+3/4,-z+1/2
  {2_0yy|(0.5,0.75,0.25)}
                                  -x+1/2,+z+3/4,+y+1/4
 {4^-_00z|(0.25,0.5,0.75)}
                                  +y+1/4,-x+1/2,+z+3/4
  {2_0y0|(0.25,0.5,0.75)}
                                  -x+1/4, +y+1/2, -z+3/4
\{3^+x^-x^-x^-\}
                                  -z+1/4, -x+3/4, +y+1/2
   \{2_x-x0|(0.5,0.5,0.0)\}
                                    -y+1/2,-x+1/2,-z
 {4^+_x00|(0.25,0.5,0.75)}
                                  +x+1/4,-z+1/2,+y+3/4
\{3^+-xx-x\mid(0.5,0.75,0.25)\}
                                  +z+1/2,-x+3/4,-y+1/4
   \{2_0y-y|(0.5,0.5,0.0)\}
                                    -x+1/2,-z+1/2,-y
\{3^+-x-xx\mid(0.25,0.5,0.75)\}
                                  -z+1/4, +x+1/2, -y+3/4
 \{4^-x00|(0.25,0.75,0.5)\}
                                  +x+1/4,+z+3/4,-y+1/2
  \{2_x0x|(0.75,0.5,0.25)\}
                                  +z+3/4,-y+1/2,+x+1/4
  \{3^-xxx|(0.5,0.5,0.0)\}
                                    +y+1/2,+z+1/2,+x
 {4^-_0y0|(0.0,0.25,0.25)}
                                    -z, +y+1/4, +x+1/4
 {4^+_0y0|(0.25,0.25,0.0)}
                                    +z+1/4, +y+1/4, -x
\{3^--x-xx\mid(0.0,0.25,0.25)\}
                                    +y,-z+1/4,-x+1/4
```

```
\{2\_-x0x|(0.5,0.5,0.0)\}
                                      -z+1/2,-y+1/2,-x
\{3^-x-x-x|(0.75,0.5,0.25)\}
                                   -y+3/4, +z+1/2, -x+1/4
\{3^--xx-x\mid(0.25,0.25,0.0)\}
                                      -y+1/4, -z+1/4, +x
      {-1|(0.5,0.5,0.0)}
                                      -x+1/2, -y+1/2, -z
 \{-4^+_00z|(0.5,0.75,0.25)\}
                                   +y+1/2,-x+3/4,-z+1/4
  \{m_0yz \mid (0.5, 0.75, 0.25)\}
                                   -x+1/2,+y+3/4,+z+1/4
  \{-3^+ xxx | (0.5, 0.5, 0.0)\}
                                      -z+1/2,-x+1/2,-y
  \{m_xy0|(0.25,0.75,0.5)\}
                                   +x+1/4, +y+3/4, -z+1/2
  \{m_x-xz \mid (0.25,0.75,0.5)\}
                                    -y+1/4, -x+3/4, +z+1/2
  \{m_xy-y \mid (0.5,0.75,0.25)\}
                                    +x+1/2,-z+3/4,-y+1/4
 \{-4^-_00z \mid (0.25, 0.5, 0.75)\}
                                    -y+1/4,+x+1/2,-z+3/4
                                    +x+1/4,-y+1/2,+z+3/4
  {m_x0z|(0.25,0.5,0.75)}
\{-3^+x^-x^-x^- (0.25, 0.75, 0.5)\}
                                   +z+1/4, +x+3/4, -y+1/2
   \{m_{xxz} | (0.5, 0.5, 0.0)\}
                                      +y+1/2,+x+1/2,+z
 \{-4^+ \times 00 \mid (0.25, 0.5, 0.75)\}
                                   -x+1/4, +z+1/2, -y+3/4
\{-3^+-xx-x \mid (0.5,0.75,0.25)\}
                                   -z+1/2,+x+3/4,+y+1/4
   \{m_xyy \mid (0.5, 0.5, 0.0)\}
                                      +x+1/2,+z+1/2,+y
\{-3^+-x-xx|(0.25,0.5,0.75)\}
                                    +z+1/4, -x+1/2, +y+3/4
 \{-4^- \times 00 \mid (0.25, 0.75, 0.5)\}
                                   -x+1/4, -z+3/4, +y+1/2
  \{m_-xyz \mid (0.75,0.5,0.25)\}
                                   -z+3/4,+y+1/2,-x+1/4
  \{-3^-xxx|(0.5,0.5,0.0)\}
                                      -y+1/2,-z+1/2,-x
 \{-4^-_0y0|(0.0,0.25,0.25)\}
                                      +z,-y+1/4,-x+1/4
 \{-4^+_0y0|(0.25,0.25,0.0)\}
                                      -z+1/4, -y+1/4, +x
\{-3^--x-xx|(0.0,0.25,0.25)\}
                                      -y, +z+1/4, +x+1/4
   \{m_xyx | (0.5, 0.5, 0.0)\}
                                      +z+1/2, +y+1/2, +x
\{-3^-x-x-x|(0.75,0.5,0.25)\}
                                    +y+3/4,-z+1/2,+x+1/4
\{-3^--xx-x \mid (0.25,0.25,0.0)\}
                                      +y+1/4,+z+1/4,-x
```

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```
space group: 228:1 {'Hall': ' F 4d 2 3 -1cd', 'HM': 'F d -3 c:1'}
Crystal system: Cubic
Setting: 1
+x.+v.+z
```

+x,+y,+z -y+1/4,+x+1/4,+z+1/4

y · 1/ ¬ 1 · X · 1/ ¬ 1 · 2 · 1/ ¬

+x,-y,-z +z,+x,+y

-x+1/4, -y+1/4, -z+3/4

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+	
•	Jones
{1 (0.0,0.0,0.0)} {4^+_00z (0.25,0.25,0.25)} {2_x00 (0.0,0.0,0.0)} {3^+_xxx (0.0,0.0,0.0)} {-1 (0.25,0.25,0.75)} {2_00z (0.0,0.5,0.5)} {2_xx0 (0.25,0.25,0.25)} {2_0yy (0.25,0.25,0.25)} {-4^+_00z (0.0,0.5,0.0)} {4^00z (0.75,0.25,0.75)} {2_0y0 (0.0,0.5,0.5)}	+x,+y,+z -y+1/4,+x+1/4,+z+1/4 +x,-y,-z +z,+x,+y -x+1/4,-y+1/4,-z+3/4 -x,-y+1/2,+z+1/2 +y+1/4,+x+1/4,-z+1/4 -x+1/4,+z+1/4,+y+1/4 +y,-x+1/2,-z +y+3/4,-x+1/4,+z+3/4 -x,+y+1/2,-z+1/2

```
\{3^+x^-x^-x^-\}
                                    -z, -x+1/2, +y+1/2
 \{m_xy0|(0.75,0.25,0.25)\}
                                 +x+3/4, +y+1/4, -z+1/4
\{2_x-x0|(0.75,0.25,0.75)\}
                                 -y+3/4, -x+1/4, -z+3/4
\{4^+ \times 00 \mid (0.75, 0.25, 0.75)\}
                                 +x+3/4,-z+1/4,+y+3/4
 {-4^-_00z|(0.0,0.0,0.5)}
                                      -y,+x,-z+1/2
\{3^+-xx-x \mid (0.0,0.0,0.0)\}
                                         +z,-x,-y
 \{m_0yz \mid (0.25, 0.75, 0.25)\}
                                 -x+1/4, +y+3/4, +z+1/4
\{2_0y-y\mid (0.25,0.75,0.75)\}
                                 -x+1/4, -z+3/4, -y+3/4
  \{m_xxz \mid (0.0,0.5,0.0)\}
                                      +y, +x+1/2, +z
\{3^+ -x -xx \mid (0.0, 0.5, 0.5)\}
                                    -z,+x+1/2,-y+1/2
                                 +x+3/4, -y+3/4, +z+1/4
 {m_x0z|(0.75,0.75,0.25)}
{4^-_x00|(0.75,0.75,0.25)}
                                 +x+3/4, +z+3/4, -y+1/4
  \{m_x-xz\mid(0.0,0.0,0.5)\}
                                      -y,-x,+z+1/2
    \{1 \mid (0.0, 0.5, 0.5)\}
                                    +x,+y+1/2,+z+1/2
\{4^+_{00z} | (0.25, 0.75, 0.75)\}
                                 -y+1/4, +x+3/4, +z+3/4
  \{2_{x00}|(0.0,0.5,0.5)\}
                                    +x,-y+1/2,-z+1/2
 \{3^+ xxx \mid (0.0, 0.5, 0.5)\}
                                    +z, +x+1/2, +y+1/2
  \{-1 \mid (0.25, 0.75, 0.25)\}
                                 -x+1/4,-y+3/4,-z+1/4
  {2_00z|(0.0,0.0,0.0)}
                                         -x,-y,+z
 {2_xx0|(0.25,0.75,0.75)}
                                 +y+1/4, +x+3/4, -z+3/4
 {2_0yy|(0.25,0.75,0.75)}
                                 -x+1/4, +z+3/4, +y+3/4
 \{-4^+_00z \mid (0.0,0.0,0.5)\}
                                      +y,-x,-z+1/2
\{4^-_00z \mid (0.75, 0.75, 0.25)\}
                                 +y+3/4,-x+3/4,+z+1/4
  {2_0y0|(0.0,0.0,0.0)}
                                         -x, +y, -z
{3^+_x-x-x|(0.0,0.0,0.0)}
                                         -z,-x,+y
                                 +x+3/4, +y+3/4, -z+3/4
 {m_xy0|(0.75,0.75,0.75)}
                                 -y+3/4, -x+3/4, -z+1/4
\{2_x-x0|(0.75,0.75,0.25)\}
\{4^+ \times 00 \mid (0.75, 0.75, 0.25)\}
                                 +x+3/4,-z+3/4,+y+1/4
 \{-4^-\ 00z \mid (0.0,0.5,0.0)\}
                                      -y, +x+1/2, -z
\{3^+-xx-x\mid(0.0,0.5,0.5)\}
                                    +z,-x+1/2,-y+1/2
                                 -x+1/4, +y+1/4, +z+3/4
 \{m_0yz \mid (0.25, 0.25, 0.75)\}
\{2_0y-y\mid (0.25,0.25,0.25)\}
                                 -x+1/4, -z+1/4, -y+1/4
  \{m_xxz | (0.0,0.0,0.5)\}
                                      +y,+x,+z+1/2
{3^+_-x^-x^+|(0.0,0.0,0.0)}
                                         -z,+x,-y
 {m_x0z|(0.75,0.25,0.25)}
                                 +x+3/4,-y+1/4,+z+1/4
\{4^-x00|(0.75,0.25,0.75)\}
                                 +x+3/4,+z+1/4,-y+3/4
  \{m_x-xz \mid (0.0,0.5,0.0)\}
                                      -y, -x+1/2, +z
     {1|(0.5,0.0,0.5)}
                                    +x+1/2, +y, +z+1/2
\{4^+_{00z}|(0.75,0.25,0.75)\}
                                 -y+3/4, +x+1/4, +z+3/4
  \{2_{x00}|(0.5,0.0,0.5)\}
                                    +x+1/2,-y,-z+1/2
 \{3^+ xxx \mid (0.5, 0.0, 0.5)\}
                                    +z+1/2,+x,+y+1/2
                                 -x+3/4, -y+1/4, -z+1/4
  \{-1 \mid (0.75, 0.25, 0.25)\}
  {2_00z|(0.5,0.5,0.0)}
                                    -x+1/2,-y+1/2,+z
 {2_xx0|(0.75,0.25,0.75)}
                                 +y+3/4, +x+1/4, -z+3/4
 {2_0yy|(0.75,0.25,0.75)}
                                 -x+3/4, +z+1/4, +y+3/4
 {-4^+_00z|(0.5,0.5,0.5)}
                                 +y+1/2,-x+1/2,-z+1/2
\{4^-00z \mid (0.25, 0.25, 0.25)\}
                                 +y+1/4, -x+1/4, +z+1/4
  {2_0y0|(0.5,0.5,0.0)}
                                    -x+1/2,+y+1/2,-z
{3^+_x-x-x|(0.5,0.5,0.0)}
                                    -z+1/2, -x+1/2, +y
 {m_xy0|(0.25,0.25,0.75)}
                                 +x+1/4, +y+1/4, -z+3/4
\{2_x-x0|(0.25,0.25,0.25)\}
                                 -y+1/4, -x+1/4, -z+1/4
\{4^+ \times 00 \mid (0.25, 0.25, 0.25)\}
                                 +x+1/4, -z+1/4, +y+1/4
 \{-4^-_00z \mid (0.5,0.0,0.0)\}
                                      -y+1/2,+x,-z
\{3^+-xx-x\mid(0.5,0.0,0.5)\}
                                    +z+1/2,-x,-y+1/2
```

```
{m_0yz|(0.75,0.75,0.75)}
                                  -x+3/4, +y+3/4, +z+3/4
  \{2_0y-y|(0.75,0.75,0.25)\}
                                  -x+3/4, -z+3/4, -y+1/4
    \{m_{xxz} | (0.5, 0.5, 0.5)\}
                                  +y+1/2,+x+1/2,+z+1/2
  {3^+_-x^-x^+|(0.5,0.5,0.0)}
                                    -z+1/2,+x+1/2,-y
   \{m_x0z|(0.25,0.75,0.25)\}
                                  +x+1/4,-y+3/4,+z+1/4
  {4^-_x00|(0.25,0.75,0.75)}
                                  +x+1/4,+z+3/4,-y+3/4
    \{m_x-xz\mid(0.5,0.0,0.0)\}
                                      -y+1/2,-x,+z
      {1|(0.5,0.5,0.0)}
                                    +x+1/2,+y+1/2,+z
  \{4^+_{00z} | (0.75, 0.75, 0.25)\}
                                  -y+3/4, +x+3/4, +z+1/4
    \{2 \times 00 \mid (0.5, 0.5, 0.0)\}
                                    +x+1/2,-y+1/2,-z
   {3^+_xxx|(0.5,0.5,0.0)}
                                    +z+1/2,+x+1/2,+y
    \{-1 \mid (0.75, 0.75, 0.75)\}
                                  -x+3/4, -y+3/4, -z+3/4
    {2_00z|(0.5,0.0,0.5)}
                                    -x+1/2, -y, +z+1/2
   {2_xx0|(0.75,0.75,0.25)}
                                  +y+3/4,+x+3/4,-z+1/4
   {2_0yy|(0.75,0.75,0.25)}
                                  -x+3/4, +z+3/4, +y+1/4
   \{-4^+_00z \mid (0.5,0.0,0.0)\}
                                      +y+1/2,-x,-z
  {4^-_00z|(0.25,0.75,0.75)}
                                  +y+1/4,-x+3/4,+z+3/4
                                    -x+1/2,+y,-z+1/2
    {2_0y0|(0.5,0.0,0.5)}
  \{3^+x^-x^-x^-\}
                                    -z+1/2, -x, +y+1/2
   {m_xy0|(0.25,0.75,0.25)}
                                  +x+1/4, +y+3/4, -z+1/4
                                  -y+1/4, -x+3/4, -z+3/4
  \{2_x-x0|(0.25,0.75,0.75)\}
  \{4^+ \times 00 \mid (0.25, 0.75, 0.75)\}
                                  +x+1/4,-z+3/4,+y+3/4
   {-4^-_00z|(0.5,0.5,0.5)}
                                  -y+1/2,+x+1/2,-z+1/2
  {3^+_-xx-x|(0.5,0.5,0.0)}
                                    +z+1/2,-x+1/2,-y
   {m_0yz|(0.75,0.25,0.25)}
                                  -x+3/4, +y+1/4, +z+1/4
                                  -x+3/4,-z+1/4,-y+3/4
  \{2_0y-y|(0.75,0.25,0.75)\}
    {m_xxz|(0.5,0.0,0.0)}
                                      +y+1/2,+x,+z
  {3^+-x-xx|(0.5,0.0,0.5)}
                                    -z+1/2,+x,-y+1/2
   {m_x0z|(0.25,0.25,0.25)}
                                  +x+1/4,-y+1/4,+z+1/4
  \{4^-x00|(0.25,0.25,0.25)\}
                                  +x+1/4, +z+1/4, -y+1/4
    \{m_x-xz\mid(0.5,0.5,0.5)\}
                                  -y+1/2,-x+1/2,+z+1/2
*******
space group: 228:2 {'Hall': '-F 4cvw 2vw 3', 'HM': 'F d -3 c:2'}
Crystal system: Cubic
Setting: 2
+x,+y,+z
-y, +x+1/4, +z+3/4
+x,-y+1/4,-z+1/4
+Z,+X,+y
              Seitz
                                            Jones
       {1|(0.0,0.0,0.0)}
                                           +x,+y,+z
   \{4^+_{00z}|(0.0,0.25,0.75)\}
                                      -y, +x+1/4, +z+3/4
                                      +x,-y+1/4,-z+1/4
    \{2_{x00}|(0.0,0.25,0.25)\}
    {3^+_xxx|(0.0,0.0,0.0)}
                                          +z,+x,+y
    {2_00z|(0.75,0.25,0.5)}
                                    -x+3/4,-y+1/4,+z+1/2
    \{2_x \times 0 \mid (0.75, 0.25, 0.0)\}
                                      +y+3/4, +x+1/4, -z
```

-x, +z+1/4, +y+3/4

+y+3/4,-x,+z+1/4

 $\{2_{0yy} | (0.0, 0.25, 0.75)\}$

{4^-_00z|(0.75,0.0,0.25)}

```
{2_0y0|(0.75,0.0,0.75)}
                                     -x+3/4,+y,-z+3/4
\{3^+x^-x^-x^-\}(0.75,0.25,0.5)\}
                                  -z+3/4, -x+1/4, +y+1/2
   \{2_x-x0|(0.0,0.0,0.5)\}
                                       -y,-x,-z+1/2
 \{4^+ \times 00 \mid (0.75, 0.0, 0.25)\}
                                     +x+3/4,-z,+y+1/4
{3^+-xx-x|(0.0,0.25,0.25)}
                                     +z,-x+1/4,-y+1/4
   \{2_0y-y|(0.0,0.0,0.5)\}
                                       -x,-z,-y+1/2
                                     -z+3/4,+x,-y+1/4
{3^+_-x^-x^-|(0.75,0.0,0.25)}
 {4^-_x00|(0.75,0.25,0.0)}
                                     +x+3/4,+z+1/4,-y
  \{2_x0x \mid (0.75,0.0,0.25)\}
                                     +z+3/4,-y,+x+1/4
  {3^-_xxx|(0.0,0.0,0.0)}
                                         +y, +z, +x
 {4^-_0y0|(0.0,0.75,0.25)}
                                     -z, +y+3/4, +x+1/4
 {4^+_0y0|(0.25,0.75,0.0)}
                                     +z+1/4, +y+3/4, -x
\{3^--x-xx\mid(0.5,0.75,0.25)\}
                                  +y+1/2,-z+3/4,-x+1/4
   \{2\_-x0x|(0.5,0.0,0.0)\}
                                       -z+1/2,-y,-x
{3^-_x-x-x|(0.25,0.0,0.25)}
                                     -y+1/4,+z,-x+1/4
\{3^--xx-x\mid(0.25,0.75,0.0)\}
                                     -y+1/4,-z+3/4,+x
     {-1|(0.0,0.0,0.0)}
                                         -x,-y,-z
 \{-4^+_00z|(0.0,0.25,0.75)\}
                                     +y,-x+1/4,-z+3/4
  {m_0yz|(0.0,0.25,0.25)}
                                     -x, +y+1/4, +z+1/4
  \{-3^+ xxx | (0.0,0.0,0.0)\}
                                         -z,-x,-y
  \{m_xy0|(0.75,0.25,0.5)\}
                                  +x+3/4, +y+1/4, -z+1/2
  \{m_x-xz \mid (0.75,0.25,0.0)\}
                                     -y+3/4, -x+1/4, +z
  \{m_xy-y \mid (0.0,0.25,0.75)\}
                                     +x,-z+1/4,-y+3/4
                                     -y+3/4,+x,-z+1/4
 {-4^-_00z|(0.75,0.0,0.25)}
  {m_x0z|(0.75,0.0,0.75)}
                                     +x+3/4,-y,+z+3/4
                                  +z+3/4,+x+1/4,-y+1/2
\{-3^+x^-x^-x^-(0.75,0.25,0.5)\}
   \{m_{xxz} | (0.0,0.0,0.5)\}
                                       +y,+x,+z+1/2
 {-4^+_x00|(0.75,0.0,0.25)}
                                     -x+3/4,+z,-y+1/4
\{-3^+-xx-x|(0.0,0.25,0.25)\}
                                     -z, +x+1/4, +y+1/4
   \{m_xyy \mid (0.0,0.0,0.5)\}
                                       +x,+z,+y+1/2
\{-3^+-x-xx|(0.75,0.0,0.25)\}
                                     +z+3/4,-x,+y+1/4
 \{-4^- \times 00 \mid (0.75, 0.25, 0.0)\}
                                     -x+3/4, -z+1/4, +y
  \{m_-xyz \mid (0.75,0.0,0.25)\}
                                     -z+3/4,+y,-x+1/4
  \{-3^-xxx \mid (0.0,0.0,0.0)\}
                                         -y,-z,-x
 \{-4^{-}_{0}00|(0.0,0.75,0.25)\}
                                     +z,-y+3/4,-x+1/4
 {-4^+_0y0|(0.25,0.75,0.0)}
                                     -z+1/4, -y+3/4, +x
\{-3^--x-xx|(0.5,0.75,0.25)\}
                                  -y+1/2,+z+3/4,+x+1/4
   \{m_xyx | (0.5,0.0,0.0)\}
                                       +z+1/2,+y,+x
\{-3^-x-x-x|(0.25,0.0,0.25)\}
                                     +y+1/4,-z,+x+1/4
\{-3^--xx-x|(0.25,0.75,0.0)\}
                                     +y+1/4,+z+3/4,-x
     {1|(0.0,0.5,0.5)}
                                     +x,+y+1/2,+z+1/2
 {4^+_00z|(0.0,0.75,0.25)}
                                     -y, +x+3/4, +z+1/4
  \{2_{\times}00 \mid (0.0, 0.75, 0.75)\}
                                     +x,-y+3/4,-z+3/4
  {3^+_xxx|(0.0,0.5,0.5)}
                                     +z,+x+1/2,+y+1/2
  {2_00z|(0.75,0.75,0.0)}
                                     -x+3/4, -y+3/4, +z
  \{2_x \times 0 \mid (0.75, 0.75, 0.5)\}
                                   +y+3/4,+x+3/4,-z+1/2
  {2_0yy|(0.0,0.75,0.25)}
                                     -x, +z+3/4, +y+1/4
 {4^-_00z|(0.75,0.5,0.75)}
                                   +y+3/4,-x+1/2,+z+3/4
                                   -x+3/4,+y+1/2,-z+1/4
  {2_0y0|(0.75,0.5,0.25)}
{3^+_x-x-x|(0.75,0.75,0.0)}
                                     -z+3/4,-x+3/4,+y
                                       -y, -x+1/2, -z
   {2_x-x0|(0.0,0.5,0.0)}
 {4^+_x00|(0.75,0.5,0.75)}
                                  +x+3/4,-z+1/2,+y+3/4
{3^+-xx-x|(0.0,0.75,0.75)}
                                     +z,-x+3/4,-y+3/4
   \{2_0y-y \mid (0.0,0.5,0.0)\}
                                       -x,-z+1/2,-y
```

```
\{3^+-x-xx\mid(0.75,0.5,0.25)\}
                                   -z+3/4, +x+1/2, -y+1/4
 {4^-_x00|(0.75,0.75,0.5)}
                                   +x+3/4, +z+3/4, -y+1/2
  \{2_x0x \mid (0.75, 0.5, 0.75)\}
                                   +z+3/4,-y+1/2,+x+3/4
  \{3^-xxx|(0.0,0.5,0.5)\}
                                     +y, +z+1/2, +x+1/2
 {4^-_0y0|(0.0,0.25,0.75)}
                                     -z, +y+1/4, +x+3/4
 {4^+_0y0|(0.25,0.25,0.5)}
                                   +z+1/4, +y+1/4, -x+1/2
{3^-_x-xx|(0.5,0.25,0.75)}
                                   +y+1/2,-z+1/4,-x+3/4
   \{2\_-x0x \mid (0.5,0.5,0.5)\}
                                   -z+1/2,-y+1/2,-x+1/2
\{3^-x-x-x|(0.25,0.5,0.75)\}
                                   -y+1/4, +z+1/2, -x+3/4
\{3^--xx-x|(0.25,0.25,0.5)\}
                                   -y+1/4, -z+1/4, +x+1/2
      {-1|(0.0,0.5,0.5)}
                                     -x,-y+1/2,-z+1/2
 \{-4^+_00z|(0.0,0.75,0.25)\}
                                     +y,-x+3/4,-z+1/4
  \{m_0yz \mid (0.0,0.75,0.75)\}
                                     -x, +y+3/4, +z+3/4
  {-3^+_xxx|(0.0,0.5,0.5)}
                                     -z, -x+1/2, -y+1/2
  \{m_xy0|(0.75,0.75,0.0)\}
                                     +x+3/4, +y+3/4, -z
  \{m_x-xz\mid(0.75,0.75,0.5)\}
                                   -y+3/4, -x+3/4, +z+1/2
  \{m_xy-y \mid (0.0,0.75,0.25)\}
                                     +x,-z+3/4,-y+1/4
 {-4^-_00z|(0.75,0.5,0.75)}
                                   -y+3/4, +x+1/2, -z+3/4
  {m_x0z|(0.75,0.5,0.25)}
                                   +x+3/4, -y+1/2, +z+1/4
\{-3^+x^-x^-x^-(0.75,0.75,0.0)\}
                                     +z+3/4, +x+3/4, -y
   \{m_x \times z \mid (0.0, 0.5, 0.0)\}
                                        +y, +x+1/2, +z
 \{-4^+ \times 00 \mid (0.75, 0.5, 0.75)\}
                                   -x+3/4, +z+1/2, -y+3/4
\{-3^+-xx-x|(0.0,0.75,0.75)\}
                                     -z, +x+3/4, +y+3/4
   \{m_xyy \mid (0.0,0.5,0.0)\}
                                        +x,+z+1/2,+y
\{-3^+-x-xx|(0.75,0.5,0.25)\}
                                   +z+3/4,-x+1/2,+y+1/4
                                   -x+3/4, -z+3/4, +y+1/2
 \{-4^- \times 00 \mid (0.75, 0.75, 0.5)\}
  \{m_-xyz \mid (0.75,0.5,0.75)\}
                                   -z+3/4,+y+1/2,-x+3/4
  \{-3^-xxx|(0.0,0.5,0.5)\}
                                     -y, -z+1/2, -x+1/2
 {-4^-_0y0|(0.0,0.25,0.75)}
                                     +z,-y+1/4,-x+3/4
 \{-4^+_0y0|(0.25,0.25,0.5)\}
                                   -z+1/4,-y+1/4,+x+1/2
\{-3^--x-xx|(0.5,0.25,0.75)\}
                                   -y+1/2,+z+1/4,+x+3/4
   \{m_xyx | (0.5, 0.5, 0.5)\}
                                   +z+1/2, +y+1/2, +x+1/2
\{-3^-x-x-x|(0.25,0.5,0.75)\}
                                   +y+1/4,-z+1/2,+x+3/4
\{-3^--xx-x \mid (0.25,0.25,0.5)\}
                                   +y+1/4, +z+1/4, -x+1/2
      {1|(0.5,0.0,0.5)}
                                     +x+1/2,+y,+z+1/2
 \{4^+_{00z}|(0.5,0.25,0.25)\}
                                   -y+1/2,+x+1/4,+z+1/4
  {2_x00|(0.5,0.25,0.75)}
                                   +x+1/2,-y+1/4,-z+3/4
  \{3^+ xxx \mid (0.5, 0.0, 0.5)\}
                                     +z+1/2,+x,+y+1/2
  {2_00z|(0.25,0.25,0.0)}
                                     -x+1/4, -y+1/4, +z
  \{2_x \times 0 \mid (0.25, 0.25, 0.5)\}
                                   +y+1/4, +x+1/4, -z+1/2
  {2_0yy|(0.5,0.25,0.25)}
                                   -x+1/2, +z+1/4, +y+1/4
 {4^-_00z|(0.25,0.0,0.75)}
                                     +y+1/4,-x,+z+3/4
  {2_0y0|(0.25,0.0,0.25)}
                                     -x+1/4, +y, -z+1/4
{3^+_x-x-x|(0.25,0.25,0.0)}
                                     -z+1/4, -x+1/4, +y
   \{2_x-x0|(0.5,0.0,0.0)\}
                                        -y+1/2,-x,-z
 {4^+_x00|(0.25,0.0,0.75)}
                                     +x+1/4,-z,+y+3/4
\{3^+-xx-x \mid (0.5,0.25,0.75)\}
                                   +z+1/2,-x+1/4,-y+3/4
   \{2_0y-y\mid (0.5,0.0,0.0)\}
                                       -x+1/2,-z,-y
{3^+-x-xx|(0.25,0.0,0.25)}
                                     -z+1/4,+x,-y+1/4
 {4^-_x00|(0.25,0.25,0.5)}
                                   +x+1/4, +z+1/4, -y+1/2
  \{2_x0x|(0.25,0.0,0.75)\}
                                     +z+1/4,-y,+x+3/4
  \{3^-xxx|(0.5,0.0,0.5)\}
                                     +y+1/2,+z,+x+1/2
 {4^-_0y0|(0.5,0.75,0.75)}
                                   -z+1/2,+y+3/4,+x+3/4
 {4^+_0y0|(0.75,0.75,0.5)}
                                   +z+3/4, +y+3/4, -x+1/2
```

```
{3^-_x}
                                     +y,-z+3/4,-x+3/4
   \{2\_-x0x \mid (0.0,0.0,0.5)\}
                                       -z, -y, -x+1/2
\{3^-x-x-x|(0.75,0.0,0.75)\}
                                     -y+3/4,+z,-x+3/4
\{3^--xx-x \mid (0.25,0.75,0.5)\}
                                   -y+1/4, -z+3/4, +x+1/2
      {-1|(0.5,0.0,0.5)}
                                     -x+1/2, -y, -z+1/2
 \{-4^+_00z \mid (0.5, 0.25, 0.25)\}
                                   +y+1/2,-x+1/4,-z+1/4
  \{m_0yz \mid (0.5, 0.25, 0.75)\}
                                   -x+1/2,+y+1/4,+z+3/4
                                     -z+1/2,-x,-y+1/2
  \{-3^+ \times \times | (0.5, 0.0, 0.5)\}
  \{m_xy0|(0.25,0.25,0.0)\}
                                     +x+1/4, +y+1/4, -z
  \{m \times -xz \mid (0.25, 0.25, 0.5)\}
                                   -y+1/4,-x+1/4,+z+1/2
                                   +x+1/2,-z+1/4,-y+1/4
  \{m_xy-y \mid (0.5,0.25,0.25)\}
 \{-4^-_00z \mid (0.25,0.0,0.75)\}
                                     -y+1/4,+x,-z+3/4
  {m_x0z|(0.25,0.0,0.25)}
                                     +x+1/4,-y,+z+1/4
\{-3^+x^-x^-x^-(0.25,0.25,0.0)\}
                                     +z+1/4,+x+1/4,-y
   \{m_{xxz} | (0.5, 0.0, 0.0)\}
                                       +y+1/2,+x,+z
 {-4^+_x00|(0.25,0.0,0.75)}
                                     -x+1/4,+z,-y+3/4
\{-3^+-xx-x|(0.5,0.25,0.75)\}
                                   -z+1/2,+x+1/4,+y+3/4
   {m_xyy|(0.5,0.0,0.0)}
                                       +x+1/2,+z,+y
\{-3^+-x-xx\mid(0.25,0.0,0.25)\}
                                     +z+1/4, -x, +y+1/4
 \{-4^- \times 00 \mid (0.25, 0.25, 0.5)\}
                                   -x+1/4, -z+1/4, +y+1/2
  \{m_-xyz \mid (0.25,0.0,0.75)\}
                                     -z+1/4,+y,-x+3/4
  \{-3^-xxx|(0.5,0.0,0.5)\}
                                     -y+1/2,-z,-x+1/2
 \{-4^{-}_{0}00|(0.5,0.75,0.75)\}
                                   +z+1/2,-y+3/4,-x+3/4
 {-4^+_0y0|(0.75,0.75,0.5)}
                                   -z+3/4,-y+3/4,+x+1/2
\{-3^--x-xx|(0.0,0.75,0.75)\}
                                     -y, +z+3/4, +x+3/4
   {m_xyx|(0.0,0.0,0.5)}
                                       +z,+y,+x+1/2
\{-3^-x-x-x|(0.75,0.0,0.75)\}
                                     +y+3/4,-z,+x+3/4
\{-3^--xx-x|(0.25,0.75,0.5)\}
                                   +y+1/4, +z+3/4, -x+1/2
      {1|(0.5,0.5,0.0)}
                                     +x+1/2, +y+1/2, +z
 {4^+_00z|(0.5,0.75,0.75)}
                                   -y+1/2,+x+3/4,+z+3/4
  {2_x00|(0.5,0.75,0.25)}
                                   +x+1/2,-y+3/4,-z+1/4
  \{3^+ xxx \mid (0.5, 0.5, 0.0)\}
                                     +z+1/2,+x+1/2,+y
  \{2_{00z} | (0.25, 0.75, 0.5)\}
                                   -x+1/4, -y+3/4, +z+1/2
                                     +y+1/4,+x+3/4,-z
  {2_xx0|(0.25,0.75,0.0)}
  {2_0yy|(0.5,0.75,0.75)}
                                   -x+1/2,+z+3/4,+y+3/4
 {4^-_00z|(0.25,0.5,0.25)}
                                   +y+1/4,-x+1/2,+z+1/4
  {2_0y0|(0.25,0.5,0.75)}
                                   -x+1/4, +y+1/2, -z+3/4
\{3^+x^-x^-x^-\}(0.25,0.75,0.5)\}
                                   -z+1/4, -x+3/4, +y+1/2
   \{2_x-x0|(0.5,0.5,0.5)\}
                                   -y+1/2,-x+1/2,-z+1/2
 {4^+_x00|(0.25,0.5,0.25)}
                                   +x+1/4,-z+1/2,+y+1/4
                                   +z+1/2,-x+3/4,-y+1/4
\{3^+-xx-x\mid(0.5,0.75,0.25)\}
   {2_0y-y|(0.5,0.5,0.5)}
                                   -x+1/2, -z+1/2, -y+1/2
{3^+-x-xx|(0.25,0.5,0.25)}
                                   -z+1/4,+x+1/2,-y+1/4
 {4^-_x00|(0.25,0.75,0.0)}
                                     +x+1/4,+z+3/4,-y
  \{2_x0x | (0.25, 0.5, 0.25)\}
                                   +z+1/4,-y+1/2,+x+1/4
  \{3^-xxx|(0.5,0.5,0.0)\}
                                     +y+1/2,+z+1/2,+x
 {4^-_0y0|(0.5,0.25,0.25)}
                                   -z+1/2, +y+1/4, +x+1/4
 {4^+_0y0|(0.75,0.25,0.0)}
                                     +z+3/4,+y+1/4,-x
                                     +y,-z+1/4,-x+1/4
\{3^--x-xx\mid(0.0,0.25,0.25)\}
   {2_-x0x|(0.0,0.5,0.0)}
                                       -z,-y+1/2,-x
{3^-_x-x-x|(0.75,0.5,0.25)}
                                   -y+3/4, +z+1/2, -x+1/4
\{3^--xx-x \mid (0.25,0.25,0.0)\}
                                     -y+1/4, -z+1/4, +x
      \{-1 \mid (0.5, 0.5, 0.0)\}
                                     -x+1/2, -y+1/2, -z
 \{-4^+_00z \mid (0.5, 0.75, 0.75)\}
                                  +y+1/2,-x+3/4,-z+3/4
```

```
\{m_0yz \mid (0.5, 0.75, 0.25)\}
                                     -x+1/2,+y+3/4,+z+1/4
    \{-3^+ \times \times | (0.5, 0.5, 0.0)\}
                                       -z+1/2,-x+1/2,-y
    \{m_xy0|(0.25,0.75,0.5)\}
                                     +x+1/4, +y+3/4, -z+1/2
    \{m_x-xz\mid(0.25,0.75,0.0)\}
                                       -y+1/4, -x+3/4, +z
    \{m_xy-y \mid (0.5,0.75,0.75)\}
                                     +x+1/2,-z+3/4,-y+3/4
   \{-4^-00z \mid (0.25, 0.5, 0.25)\}
                                    -y+1/4, +x+1/2, -z+1/4
    \{m_x0z \mid (0.25, 0.5, 0.75)\}
                                     +x+1/4,-y+1/2,+z+3/4
  \{-3^+x^-x^-x^-\}
                                     +z+1/4, +x+3/4, -y+1/2
     \{m_xxz | (0.5, 0.5, 0.5)\}
                                     +y+1/2,+x+1/2,+z+1/2
   \{-4^+ \times 00 \mid (0.25, 0.5, 0.25)\}
                                     -x+1/4, +z+1/2, -y+1/4
  \{-3^+-xx-x \mid (0.5,0.75,0.25)\}
                                     -z+1/2,+x+3/4,+y+1/4
     {m_xyy|(0.5,0.5,0.5)}
                                     +x+1/2, +z+1/2, +y+1/2
  \{-3^+-x-xx\mid(0.25,0.5,0.25)\}
                                    +z+1/4,-x+1/2,+y+1/4
   \{-4^-x00|(0.25,0.75,0.0)\}
                                       -x+1/4, -z+3/4, +y
    \{m_-xyz \mid (0.25, 0.5, 0.25)\}
                                    -z+1/4, +y+1/2, -x+1/4
    \{-3^-xxx|(0.5,0.5,0.0)\}
                                       -y+1/2,-z+1/2,-x
   \{-4^-_0y0|(0.5,0.25,0.25)\}
                                    +z+1/2,-y+1/4,-x+1/4
   \{-4^+_0y0|(0.75,0.25,0.0)\}
                                       -z+3/4,-y+1/4,+x
  \{-3^--x-xx|(0.0,0.25,0.25)\}
                                       -y, +z+1/4, +x+1/4
     \{m_xyx | (0.0,0.5,0.0)\}
                                         +z,+y+1/2,+x
  \{-3^-x-x-x|(0.75,0.5,0.25)\}
                                    +y+3/4,-z+1/2,+x+1/4
  \{-3^--xx-x \mid (0.25,0.25,0.0)\}
                                       +y+1/4,+z+1/4,-x
*******
space group: 229 {'Hall': '-I 4 2 3', 'HM': 'I m -3 m'}
Crystal system: Cubic
+x,+y,+z
-y,+x,+z
+x,-y,-z
+z,+x,+y
             Seitz
                                          Jones
      {1|(0.0,0.0,0.0)}
                                         +x,+y,+z
   {4^+_00z|(0.0,0.0,0.0)}
                                         -y,+x,+z
    \{2_{\times}00 \mid (0.0,0.0,0.0)\}
                                         +x,-y,-z
   {3^+_xxx|(0.0,0.0,0.0)}
                                         +Z,+X,+y
    {2_00z|(0.0,0.0,0.0)}
                                         -x,-y,+z
    {2_xx0|(0.0,0.0,0.0)}
                                         +y,+x,-z
    {2_0yy|(0.0,0.0,0.0)}
                                         -x,+z,+y
   {4^-_00z|(0.0,0.0,0.0)}
                                         +y,-x,+z
    {2_0y0|(0.0,0.0,0.0)}
                                         -x,+y,-z
```

-z,-x,+y

-y,-x,-z

+x,-z,+y

+z,-x,-y

-x,-z,-y

-z,+x,-y

+x,+z,-y

+z,-y,+x

+y,+z,+x

 $\{3^+x^-x^-x^-\}$

 $\{2_x-x0|(0.0,0.0,0.0)\}$

{4^+_x00|(0.0,0.0,0.0)}

 ${3^+_-xx-x|(0.0,0.0,0.0)}$

 ${3^+_-x^-x^-|(0.0,0.0,0.0)}$

{4^-_x00|(0.0,0.0,0.0)}

 $\{2_x0x | (0.0,0.0,0.0)\}$

{3^-_xxx|(0.0,0.0,0.0)}

 $\{2_0y-y \mid (0.0,0.0,0.0)\}$

```
{4^-_0y0|(0.0,0.0,0.0)}
                                       -z,+y,+x
 {4^+_0y0|(0.0,0.0,0.0)}
                                       +z,+y,-x
\{3^--x-xx\mid (0.0,0.0,0.0)\}
                                       +y,-z,-x
  \{2\_-x0x \mid (0.0,0.0,0.0)\}
                                       -z,-y,-x
{3^-_x-x-x|(0.0,0.0,0.0)}
                                       -y, +z, -x
\{3^--xx-x \mid (0.0,0.0,0.0)\}
                                       -y,-z,+x
    {-1|(0.0,0.0,0.0)}
                                       -x,-y,-z
 \{-4^+_00z \mid (0.0,0.0,0.0)\}
                                       +y,-x,-z
  \{m_0yz \mid (0.0,0.0,0.0)\}
                                       -x,+y,+z
 \{-3^+ \times \times | (0.0,0.0,0.0)\}
                                       -z,-x,-y
  {m_xy0|(0.0,0.0,0.0)}
                                       +x,+y,-z
  \{m_x-xz \mid (0.0,0.0,0.0)\}
                                       -y,-x,+z
  \{m_xy-y \mid (0.0,0.0,0.0)\}
                                       +x,-z,-y
 {-4^-_00z|(0.0,0.0,0.0)}
                                       -y,+x,-z
  {m_x0z|(0.0,0.0,0.0)}
                                       +x,-y,+z
\{-3^+x^-x^-x^- | (0.0,0.0,0.0) \}
                                       +z,+x,-y
  {m_xxz|(0.0,0.0,0.0)}
                                       +y,+x,+z
 {-4^+_x00|(0.0,0.0,0.0)}
                                       -x,+z,-y
\{-3^+-xx-x \mid (0.0,0.0,0.0)\}
                                       -z,+x,+y
  {m_xyy|(0.0,0.0,0.0)}
                                       +x,+z,+y
\{-3^+-x-xx|(0.0,0.0,0.0)\}
                                       +z,-x,+y
 \{-4^- \times 00 \mid (0.0, 0.0, 0.0)\}
                                       -x,-z,+y
  \{m_-xyz \mid (0.0,0.0,0.0)\}
                                       -z,+y,-x
 \{-3^-xxx|(0.0,0.0,0.0)\}
                                       -y,-z,-x
 {-4^-_0y0|(0.0,0.0,0.0)}
                                       +z,-y,-x
 {-4^+_0y0|(0.0,0.0,0.0)}
                                       -z,-y,+x
\{-3^--x-xx|(0.0,0.0,0.0)\}
                                       -y,+z,+x
  \{m_xyx | (0.0,0.0,0.0)\}
                                       +z,+y,+x
{-3^-_x-x-x|(0.0,0.0,0.0)}
                                       +y,-z,+x
\{-3^--xx-x \mid (0.0,0.0,0.0)\}
                                       +y, +z, -x
    {1|(0.5,0.5,0.5)}
                                +x+1/2,+y+1/2,+z+1/2
 \{4^+_{00z}|(0.5,0.5,0.5)\}
                                -y+1/2,+x+1/2,+z+1/2
  \{2_{x00}|(0.5,0.5,0.5)\}
                                +x+1/2,-y+1/2,-z+1/2
 {3^+_xxx|(0.5,0.5,0.5)}
                                +z+1/2,+x+1/2,+y+1/2
  \{2\_00z \mid (0.5, 0.5, 0.5)\}
                                -x+1/2, -y+1/2, +z+1/2
  {2_xx0|(0.5,0.5,0.5)}
                                +y+1/2,+x+1/2,-z+1/2
  {2_0yy|(0.5,0.5,0.5)}
                                -x+1/2,+z+1/2,+y+1/2
 {4^-_00z|(0.5,0.5,0.5)}
                                +y+1/2,-x+1/2,+z+1/2
  {2_0y0|(0.5,0.5,0.5)}
                                -x+1/2,+y+1/2,-z+1/2
{3^+_x-x-x|(0.5,0.5,0.5)}
                                -z+1/2,-x+1/2,+y+1/2
  \{2_x-x0|(0.5,0.5,0.5)\}
                                -y+1/2,-x+1/2,-z+1/2
 {4^+_x00|(0.5,0.5,0.5)}
                                +x+1/2,-z+1/2,+y+1/2
\{3^+-xx-x\mid(0.5,0.5,0.5)\}
                                +z+1/2,-x+1/2,-y+1/2
  \{2_0y-y|(0.5,0.5,0.5)\}
                                -x+1/2, -z+1/2, -y+1/2
\{3^+_-x^-x^-\}
                                -z+1/2,+x+1/2,-y+1/2
 \{4^-x00|(0.5,0.5,0.5)\}
                                +x+1/2,+z+1/2,-y+1/2
  \{2_x0x|(0.5,0.5,0.5)\}
                                +z+1/2,-y+1/2,+x+1/2
 {3^-_xxx|(0.5,0.5,0.5)}
                                +y+1/2,+z+1/2,+x+1/2
 {4^-_0y0|(0.5,0.5,0.5)}
                                -z+1/2,+y+1/2,+x+1/2
 {4^+_0y0|(0.5,0.5,0.5)}
                                +z+1/2, +y+1/2, -x+1/2
\{3^--x-xx|(0.5,0.5,0.5)\}
                                +y+1/2,-z+1/2,-x+1/2
  \{2_{-}\times 0\times | (0.5, 0.5, 0.5)\}
                                -z+1/2,-y+1/2,-x+1/2
\{3^-x-x-x|(0.5,0.5,0.5)\}
                                -y+1/2,+z+1/2,-x+1/2
\{3^--xx-x \mid (0.5,0.5,0.5)\}
                                -y+1/2,-z+1/2,+x+1/2
```

```
\{-1|(0.5,0.5,0.5)\}
                                  -x+1/2,-y+1/2,-z+1/2
   \{-4^+_00z \mid (0.5, 0.5, 0.5)\}
                                  +y+1/2,-x+1/2,-z+1/2
    \{m_0yz \mid (0.5, 0.5, 0.5)\}
                                  -x+1/2,+y+1/2,+z+1/2
   \{-3^+ \times \times | (0.5, 0.5, 0.5)\}
                                  -z+1/2, -x+1/2, -y+1/2
    \{m_xy0|(0.5,0.5,0.5)\}
                                  +x+1/2, +y+1/2, -z+1/2
    \{m_x-xz\mid(0.5,0.5,0.5)\}
                                  -y+1/2, -x+1/2, +z+1/2
    \{m_xy-y \mid (0.5,0.5,0.5)\}
                                  +x+1/2,-z+1/2,-y+1/2
   \{-4^-00z|(0.5,0.5,0.5)\}
                                  -y+1/2,+x+1/2,-z+1/2
    \{m_x0z \mid (0.5,0.5,0.5)\}
                                  +x+1/2,-y+1/2,+z+1/2
  \{-3^+ x-x-x|(0.5,0.5,0.5)\}
                                  +z+1/2,+x+1/2,-y+1/2
    \{m_xxz | (0.5, 0.5, 0.5)\}
                                  +y+1/2,+x+1/2,+z+1/2
                                  -x+1/2, +z+1/2, -y+1/2
   {-4^+_x00|(0.5,0.5,0.5)}
  \{-3^+-xx-x|(0.5,0.5,0.5)\}
                                  -z+1/2,+x+1/2,+y+1/2
    \{m_xyy | (0.5, 0.5, 0.5)\}
                                  +x+1/2,+z+1/2,+y+1/2
  \{-3^+-x-xx\mid(0.5,0.5,0.5)\}
                                  +z+1/2, -x+1/2, +y+1/2
   \{-4^- \times 00 \mid (0.5, 0.5, 0.5)\}
                                  -x+1/2,-z+1/2,+y+1/2
    \{m_-xyz \mid (0.5, 0.5, 0.5)\}
                                  -z+1/2,+y+1/2,-x+1/2
   \{-3^-xxx|(0.5,0.5,0.5)\}
                                  -y+1/2,-z+1/2,-x+1/2
   {-4^-_0y0|(0.5,0.5,0.5)}
                                  +z+1/2,-y+1/2,-x+1/2
                                  -z+1/2,-y+1/2,+x+1/2
   {-4^+_0y0|(0.5,0.5,0.5)}
  \{-3^--x-xx|(0.5,0.5,0.5)\}
                                  -y+1/2,+z+1/2,+x+1/2
    \{m_xyx | (0.5, 0.5, 0.5)\}
                                  +z+1/2, +y+1/2, +x+1/2
  \{-3^-x-x-x|(0.5,0.5,0.5)\}
                                  +y+1/2,-z+1/2,+x+1/2
  \{-3^--xx-x|(0.5,0.5,0.5)\}
                                  +y+1/2,+z+1/2,-x+1/2
*******
space group: 230 {'Hall': '-I 4bd 2c 3', 'HM': 'I a -3 d'}
Crystal system: Cubic
+X,+Y,+Z
-y+1/4, +x+3/4, +z+1/4
+x,-y,-z+1/2
+Z,+X,+y
              Seitz
                                           Jones
        {1|(0.0,0.0,0.0)}
                                          +x,+y,+z
   \{4^+_{00z} | (0.25, 0.75, 0.25)\}
                                   -y+1/4, +x+3/4, +z+1/4
     {2_x00|(0.0,0.0,0.5)}
                                        +x,-y,-z+1/2
    {3^+_xxx|(0.0,0.0,0.0)}
                                          +Z,+X,+y
     {2_00z|(0.5,0.0,0.5)}
                                      -x+1/2, -y, +z+1/2
    {2_xx0|(0.25,0.75,0.75)}
                                   +y+1/4, +x+3/4, -z+3/4
    \{2_{0yy} | (0.25, 0.75, 0.25)\}
                                   -x+1/4, +z+3/4, +y+1/4
   {4^-_00z|(0.25,0.25,0.75)}
                                   +y+1/4,-x+1/4,+z+3/4
     {2_0y0|(0.5,0.0,0.0)}
                                        -x+1/2,+y,-z
   {3^+_x-x-x|(0.5,0.0,0.5)}
                                      -z+1/2,-x,+y+1/2
   \{2_x-x0\mid(0.25,0.25,0.25)\}
                                   -y+1/4, -x+1/4, -z+1/4
   {4^+_x00|(0.25,0.25,0.75)}
                                   +x+1/4,-z+1/4,+y+3/4
   {3^+_-xx-x|(0.0,0.0,0.5)}
                                        +z,-x,-y+1/2
   \{2_0y-y \mid (0.25,0.25,0.25)\}
                                   -x+1/4, -z+1/4, -y+1/4
   {3^+_-x^-x^-|(0.5,0.0,0.0)}
                                        -z+1/2,+x,-y
```

+x+1/4,+z+3/4,-y+3/4

 $\{4^-x00|(0.25,0.75,0.75)\}$

```
\{2_x0x \mid (0.25, 0.25, 0.75)\}
                                 +z+1/4,-y+1/4,+x+3/4
  \{3^-xxx|(0.0,0.0,0.0)\}
                                        +y,+z,+x
 {4^-_0y0|(0.75,0.25,0.75)}
                                 -z+3/4,+y+1/4,+x+3/4
 \{4^+_0y0|(0.75,0.25,0.25)\}
                                 +z+3/4, +y+1/4, -x+1/4
 {3^-_x-x}(0.5,0.5,0.0)
                                    +y+1/2,-z+1/2,-x
 \{2_-x0x \mid (0.25, 0.25, 0.25)\}
                                 -z+1/4, -y+1/4, -x+1/4
 {3^-_x-x-x|(0.5,0.0,0.0)}
                                      -y+1/2,+z,-x
 \{3^--xx-x\mid (0.0,0.5,0.0)\}
                                      -y,-z+1/2,+x
     \{-1 \mid (0.0, 0.0, 0.0)\}
                                         -x,-y,-z
\{-4^+_00z \mid (0.25, 0.75, 0.25)\}
                                 +y+1/4,-x+3/4,-z+1/4
   \{m_0yz \mid (0.0,0.0,0.5)\}
                                      -x,+y,+z+1/2
  \{-3^+ \times \times | (0.0, 0.0, 0.0) \}
                                         -z,-x,-y
   {m_xy0|(0.5,0.0,0.5)}
                                    +x+1/2, +y, -z+1/2
 {m_x-xz|(0.25,0.75,0.75)}
                                 -y+1/4, -x+3/4, +z+3/4
 \{m_xy-y \mid (0.25,0.75,0.25)\}
                                 +x+1/4,-z+3/4,-y+1/4
\{-4^-00z \mid (0.25,0.25,0.75)\}
                                 -y+1/4, +x+1/4, -z+3/4
   {m_x0z|(0.5,0.0,0.0)}
                                      +x+1/2,-y,+z
 \{-3^+x^-x^-x^-\}
                                    +z+1/2,+x,-y+1/2
                                 +y+1/4, +x+1/4, +z+1/4
  {m_xxz|(0.25,0.25,0.25)}
\{-4^+ \times 00 \mid (0.25, 0.25, 0.75)\}
                                 -x+1/4, +z+1/4, -y+3/4
 \{-3^+-xx-x \mid (0.0,0.0,0.5)\}
                                      -z, +x, +y+1/2
  \{m_xyy \mid (0.25, 0.25, 0.25)\}
                                 +x+1/4, +z+1/4, +y+1/4
 \{-3^+-x-xx \mid (0.5,0.0,0.0)\}
                                      +z+1/2,-x,+y
\{-4^-x00|(0.25,0.75,0.75)\}
                                 -x+1/4, -z+3/4, +y+3/4
 \{m_-xyz \mid (0.25,0.25,0.75)\}
                                 -z+1/4, +y+1/4, -x+3/4
  {-3^-_xxx|(0.0,0.0,0.0)}
                                         -y,-z,-x
\{-4^-_0y0|(0.75,0.25,0.75)\}
                                 +z+3/4,-y+1/4,-x+3/4
\{-4^+_0y0|(0.75,0.25,0.25)\}
                                 -z+3/4,-y+1/4,+x+1/4
 \{-3^--x-xx|(0.5,0.5,0.0)\}
                                    -y+1/2,+z+1/2,+x
  \{m_xyx \mid (0.25, 0.25, 0.25)\}
                                 +z+1/4, +y+1/4, +x+1/4
 \{-3^-x-x-x|(0.5,0.0,0.0)\}
                                      +y+1/2,-z,+x
 \{-3^--xx-x|(0.0,0.5,0.0)\}
                                      +y,+z+1/2,-x
     \{1|(0.5,0.5,0.5)\}
                                 +x+1/2, +y+1/2, +z+1/2
                                 -y+3/4,+x+1/4,+z+3/4
 \{4^+ 00z \mid (0.75, 0.25, 0.75)\}
   \{2_{x00} | (0.5, 0.5, 0.0)\}
                                    +x+1/2,-y+1/2,-z
                                 +z+1/2,+x+1/2,+y+1/2
  {3^+_xxx|(0.5,0.5,0.5)}
   {2_00z|(0.0,0.5,0.0)}
                                      -x,-y+1/2,+z
  {2_xx0|(0.75,0.25,0.25)}
                                 +y+3/4,+x+1/4,-z+1/4
  {2_0yy|(0.75,0.25,0.75)}
                                 -x+3/4, +z+1/4, +y+3/4
 \{4^-_00z \mid (0.75, 0.75, 0.25)\}
                                  +y+3/4,-x+3/4,+z+1/4
                                    -x,+y+1/2,-z+1/2
   {2_0y0|(0.0,0.5,0.5)}
 {3^+_x-x-x|(0.0,0.5,0.0)}
                                      -z, -x+1/2, +y
                                 -y+3/4, -x+3/4, -z+3/4
 {2_x-x0|(0.75,0.75,0.75)}
 {4^+_x00|(0.75,0.75,0.25)}
                                 +x+3/4,-z+3/4,+y+1/4
 {3^+_-xx-x|(0.5,0.5,0.0)}
                                    +z+1/2,-x+1/2,-y
 {2_0y-y|(0.75,0.75,0.75)}
                                 -x+3/4, -z+3/4, -y+3/4
 \{3^+_-x^-x^-\}
                                    -z, +x+1/2, -y+1/2
 \{4^-x00|(0.75,0.25,0.25)\}
                                  +x+3/4, +z+1/4, -y+1/4
  \{2_x0x \mid (0.75, 0.75, 0.25)\}
                                 +z+3/4,-y+3/4,+x+1/4
  {3^-_xxx|(0.5,0.5,0.5)}
                                 +y+1/2,+z+1/2,+x+1/2
 {4^-_0y0|(0.25,0.75,0.25)}
                                 -z+1/4, +y+3/4, +x+1/4
 {4^+_0y0|(0.25,0.75,0.75)}
                                 +z+1/4, +y+3/4, -x+3/4
 \{3^--x-xx\mid (0.0,0.0,0.5)\}
                                      +y,-z,-x+1/2
 \{2\_-x0x \mid (0.75, 0.75, 0.75)\}
                                 -z+3/4, -y+3/4, -x+3/4
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-y, +z+1/2, -x+1/2
 \{3^-x-x-x|(0.0,0.5,0.5)\}
 \{3^--xx-x|(0.5,0.0,0.5)\}
                                    -y+1/2,-z,+x+1/2
     \{-1 \mid (0.5, 0.5, 0.5)\}
                                  -x+1/2, -y+1/2, -z+1/2
\{-4^+_00z \mid (0.75, 0.25, 0.75)\}
                                  +y+3/4,-x+1/4,-z+3/4
   \{m_0yz \mid (0.5, 0.5, 0.0)\}
                                    -x+1/2,+y+1/2,+z
  \{-3^+ \times \times | (0.5, 0.5, 0.5) \}
                                  -z+1/2, -x+1/2, -y+1/2
   \{m_xy0|(0.0,0.5,0.0)\}
                                      +x,+y+1/2,-z
 {m_x-xz|(0.75,0.25,0.25)}
                                  -y+3/4, -x+1/4, +z+1/4
 \{m_xy-y \mid (0.75,0.25,0.75)\}
                                  +x+3/4,-z+1/4,-y+3/4
\{-4^-00z \mid (0.75, 0.75, 0.25)\}
                                  -y+3/4,+x+3/4,-z+1/4
   {m_x0z|(0.0,0.5,0.5)}
                                    +x,-y+1/2,+z+1/2
 \{-3^+x^-x^-x^-\}
                                      +z,+x+1/2,-y
  {m_xxz|(0.75,0.75,0.75)}
                                  +y+3/4, +x+3/4, +z+3/4
                                  -x+3/4, +z+3/4, -y+1/4
{-4^+_x00|(0.75,0.75,0.25)}
 \{-3^+-xx-x \mid (0.5,0.5,0.0)\}
                                    -z+1/2,+x+1/2,+y
  \{m_xyy \mid (0.75, 0.75, 0.75)\}
                                  +x+3/4, +z+3/4, +y+3/4
 \{-3^+-x-xx|(0.0,0.5,0.5)\}
                                    +z,-x+1/2,+y+1/2
\{-4^-x00|(0.75,0.25,0.25)\}
                                  -x+3/4, -z+1/4, +y+1/4
                                  -z+3/4,+y+3/4,-x+1/4
 \{m_-xyz \mid (0.75, 0.75, 0.25)\}
  \{-3^-xxx|(0.5,0.5,0.5)\}
                                  -y+1/2,-z+1/2,-x+1/2
\{-4^-_0y0|(0.25,0.75,0.25)\}
                                  +z+1/4, -y+3/4, -x+1/4
\{-4^+_0y0|(0.25,0.75,0.75)\}
                                  -z+1/4,-y+3/4,+x+3/4
 \{-3^--x-xx|(0.0,0.0,0.5)\}
                                      -y, +z, +x+1/2
  \{m_xyx \mid (0.75, 0.75, 0.75)\}
                                  +z+3/4, +y+3/4, +x+3/4
 \{-3^-x-x-x|(0.0,0.5,0.5)\}
                                    +y,-z+1/2,+x+1/2
 \{-3^--xx-x|(0.5,0.0,0.5)\}
                                    +y+1/2,+z,-x+1/2
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