

MS-Word Example for SINQ/SμS Experimental Reports: Magnetic Excitations in CsMn(SO₄)₂·(D₂O)₁₂

_ Use Small and Capital Letters in Title as Shown Above. TimesNewRoman 12 _

A. Muster¹, B. Mustermann², C. Example³

¹Laboratory for Neutron Scattering and Imaging, PSI, CH-5232 Villigen PSI, Switzerland

²Laboratory for Scientific Developments and Novel Materials, PSI, CH-5232 Villigen PSI, Switzerland

³Laboratory for Muon Spin Spectroscopy, PSI, CH-5232 Villigen PSI, Switzerland

Include country and do not use full given name. Include ZIP Code with international -2-letter precode.

In CsMn(SO₄)₂·(D₂O)₁₂ a co-operative Jahn–Teller effect is responsible for a cubic to orthorhombic phase transition occurring at ca. 160 K. We resolved five inelastic transitions on FOCUS with $\lambda = 5.32 \text{ \AA}$ within the 5A_g ground state of the orthorhombic phase. Both energies and intensities of these magnetic transitions were modelled successfully by an effective Spin Hamiltonian accounting for an axial and rhombic zero-field splitting. In Italic, TimesNewRoman 10.

The title compound CsMn(SO₄)₂·(D₂O)₁₂ belongs to the well known family of alums. It undergoes a cubic to orthorhombic phase transition at ca. 160 K due to a co-operative Jahn-Teller effect. The [Mn(OD₂)₆]³⁺ coordination distorts from S₆ to C_i point symmetry. Thus the ground state of Mn(III) in the low temperature phase is a zero-field split 5A_g term. The following effective Spin Hamiltonian, acting in the basis of five S=2 spin functions, describes this splitting:

$$\hat{H} = D \left[\hat{S}_z^2 - \frac{1}{3} S(S+1) \right] + E \left[\hat{S}_x^2 - \hat{S}_y^2 \right] \quad (1)$$

The parameters D and E are the axial and rhombic zero-field splitting parameters, respectively.

An inelastic neutron scattering (INS) experiment on a polycrystalline sample of the title compound was performed on the SINQ time-of-flight spectrometer FOCUS. In Figure 1 the spectra obtained at $T = 1.4, 15$ and 30 K ($\lambda = 5.32 \text{ \AA}$) are shown.

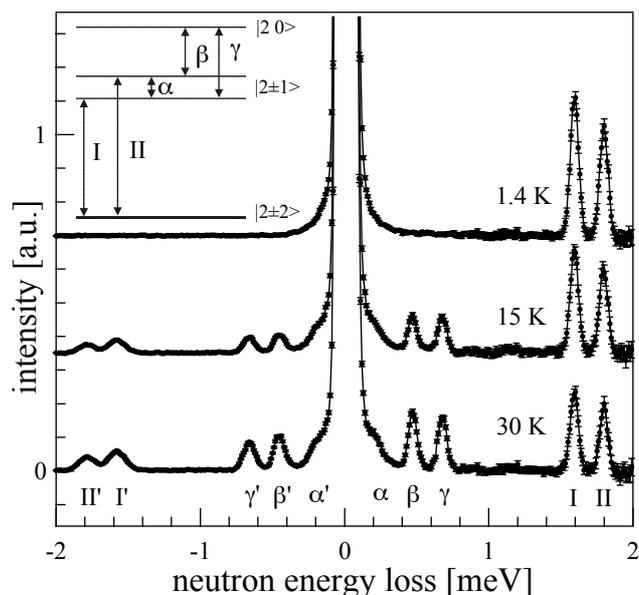


Figure 1: INS spectra of CsMn(SO₄)₂·(D₂O)₁₂ at $T = 1.4, 15$ and 30 K measured on FOCUS ($\lambda = 5.32 \text{ \AA}$). The transitions are labeled on the bottom of the Figure. **Labels inside, use jpg-files if possible.**

An increase of the temperature to 15 and 30 K is concomitant with the appearance of three hot transitions α, β and γ at 0.199(3), 0.4646(7) and 0.6717(8) meV, respectively. The corresponding transitions I', II', α', β' and γ' on the neutron energy gain side (negative energy transfer) are observed at elevated temperatures. The measured transition energies are nicely reproduced by eq. (1) as seen in table 1. The best fit parameters are $D = -0.5608(7) \text{ meV}$ and $E = 0.0339(3) \text{ meV}$.

Additionally, table 1 shows the comparison between the measured relative intensities at 30K and the ones calculated according to the dipole approximation for non-interacting ions. The agreement between experimental and calculated intensities is excellent and confirms of the model.

label	energy [meV]		normalized intensities energy loss 30 K	
	exp	calc	exp	calc
I	1.5864(7)	1.5867	0.56(2)	0.58
II	1.790(1)	1.790	0.46(4)	0.48
α	0.199(3)	0.204	0.22(1)	0.14
β	0.4646(7)	0.4651	0.39(1)	0.42
γ	0.6717(8)	0.6687	0.38(1)	0.40

Table 1: Experimentally determined energies and relative intensities with estimated errors of the various INS transitions for neutron energy loss at 30 K. The values are normalized to transition I at 1.4 K.

[1] R. Caciuffo, G. Amoretti, A. Murani, R. Sessoli, A. Caneschi and D. Gatteschi, Phys. Rev. Lett. **81**, 4744 (1998).

Work partially/fully performed at SINQ/SμS
Proposal-number: 20051234

Instruments: FOCUS/TASP/DOLLY

Put this part as low as possible into this column.