Report on Magnetic Excitations

or

Bericht über magnetische Anregungen

or

Raport o wzbudzeniach magnetycznych

By:

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Subject finding

How to find a subject?

- Go to neutron scattering school in Sardegna

Subject finding

How to find a subject?

- Listen to the lectures

Subject finding

How to find a subject?

- Eat well – empty stomach leads to empty brain!

Subject finding

How to find a subject?

- Think about the subject

Subject finding

How to find a subject?

- Drink some mirto rosso

Subject finding

How to find a subject?

- And get an inspiration from other people

Subject finding

How to find a subject?

- Go to neutron scattering school in Sardegna
- Listen to the lectures
- Discussion at the Pool
- Think about the subject
- Drink some mirtho bianco
- Get an inspiration from other people

That's all!

Now seriously!

Magnetic Anisotropy- Zero field splitting

2^{nd} order Spin – Spin Interaction Hamiltonian

$$H^{ZFS} = \vec{S} \cdot \bar{D} \cdot \vec{S} = \sum_{i=1}^{3} \sum_{j=1}^{3} \bar{D}_{ij} \, S_i \, S_j \qquad (i, j = x, y, z)$$

$\bar{D}$ is a cartesian tensor of rank 2.

Magnetic Anisotropy – Zero field splitting

Reference frame with axis parallel to the principal axis of $\tilde{D}$:

$$H^{ZFS} = \sum_{i=1}^{3} \tilde{D}_{ii}\, S_i\, S_i = \tilde{D}_{xx}\, S_x^2 + \tilde{D}_{yy}\, S_y^2 + \tilde{D}_{zz}\, S_z^2$$

We define the parameters

$$D = \frac{1}{2}\,(2\,\tilde{D}_{zz} - \tilde{D}_{xx} - \tilde{D}_{yy})$$

$$E = \frac{1}{2}\,(\tilde{D}_{xx} - \tilde{D}_{yy})$$

$$K = \frac{1}{3}\,(\tilde{D}_{xx} + \tilde{D}_{yy} + \tilde{D}_{zz})$$

Magnetic Anisotropy – Zero field splitting

$$H^{ZFS} = D\left(S_z^2 - \frac{1}{3}S(S+1)\right) + E(S_x^2 - S_y^2) + K\,S(S+1)$$

or

$$H^{ZFS} = D\left(S_z^2 - \frac{1}{3}S(S+1)\right) + \frac{1}{2}E(S_+{}^2 + S_-{}^2) + K\,S(S+1)$$

In terms of the Stevens operator equivalents

$$\hat{O}_0^0 = S(S+1) \qquad \hat{O}_2^0 = 3S_z^2 - S(S+1) \qquad \hat{O}_2^2 = S_x^2 - S_y^2$$

$$H^{ZFS} = B_0^0\,\hat{O}_0^0 + B_2^0\,\hat{O}_2^0 + B_2^2\,\hat{O}_2^2$$

Magnetic Anisotropy – Zero field splitting

$$H^{CF} = \sum_{k=0}^{\min(2l,2j)} \sum_{m=0}^{k} B_k^n \hat{O}_k^n$$

Examples of Stevens Operator Equivalents

$$\hat{O}_2^0 = 3\,S_z^2 - S\,(S+1)$$

$$\hat{O}_2^1 = \frac{1}{4}\,[S_z\,(S_+ + S_-) + (S_+ + S_-)\,S_z]$$

$$\hat{O}_2^2 = \frac{1}{2}\,[S_+^2 + S_-^2]$$

$$\hat{O}_4^0 = 35\,S_z^4 - [30\,S\,(S+1) - 25]\,S_z^2 - 6\,S\,(S+1) + 3\,S^2\,(S+1)^2$$

$$\hat{O}_4^1 = \frac{1}{4}\,\{[7\,S_z^2 - 3\,S\,(S+1) - 1]\,S_z\,(S_+ + S_-) + (S_+ + S_-)\,S_z[7\,S_z^2 - 3\,S\,(S+1) - 1]\}$$

$$\hat{O}_4^2 = \frac{1}{4}\,\{[7\,S_z^2 - S\,(S+1) - 5]\,(S_+^2 + S_-^2) + (S_+^2 + S_-^2)\,[7\,S_z^2 - S\,(S+1) - 5]\}$$

$$\hat{O}_4^3 = \frac{1}{4}\,[S_z\,(S_+^3 + S_-^3) + (S_+^3 + S_-^3)\,S_z]$$

$$\hat{O}_4^4 = \frac{1}{2}\,(S_+^4 + S_-^4)$$

Cubic symmetry, quantization axis along the 4-fold axis

$$H_C^{CF} = B_4\left(\hat{O}_4^0 + 5\,\hat{O}_4^4\right) + B_6\left(\hat{O}_6^0 - 21\,\hat{O}_6^4\right)$$

Tetragonal symmetry (D_{4h})

$$H_t^{CF} = B_2^0\,\hat{O}_2^0 + B_4^0\,\hat{O}_4^0 + B_4^4\,\hat{O}_4^4 + B_6^0\,\hat{O}_6^0 + B_6^4\,\hat{O}_6^4$$

Trigonal symmetry (D_{3d}), up to fourth order

$$H_{tr}^{CF} = B_2^0\,\hat{O}_2^0 + B_4^0\,\hat{O}_4^0 - \frac{2}{3}\,B_4\left(\hat{O}_4^0 + 20\sqrt{2}\,\hat{O}_4^3\right)$$

Only axial symmetry

$$H^{CF} = D\left(S_z^2 - \frac{1}{3} S(S+1) \right) + aS_z B_z$$

Eigenvalues without Field

D = 1 K

$$H = \begin{pmatrix} 4-2aB & 0 & 0 & 0 & 0 \\ 0 & 1-aB & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1+aB & 0 \\ 0 & 0 & 0 & 0 & 4+2aB \end{pmatrix}$$

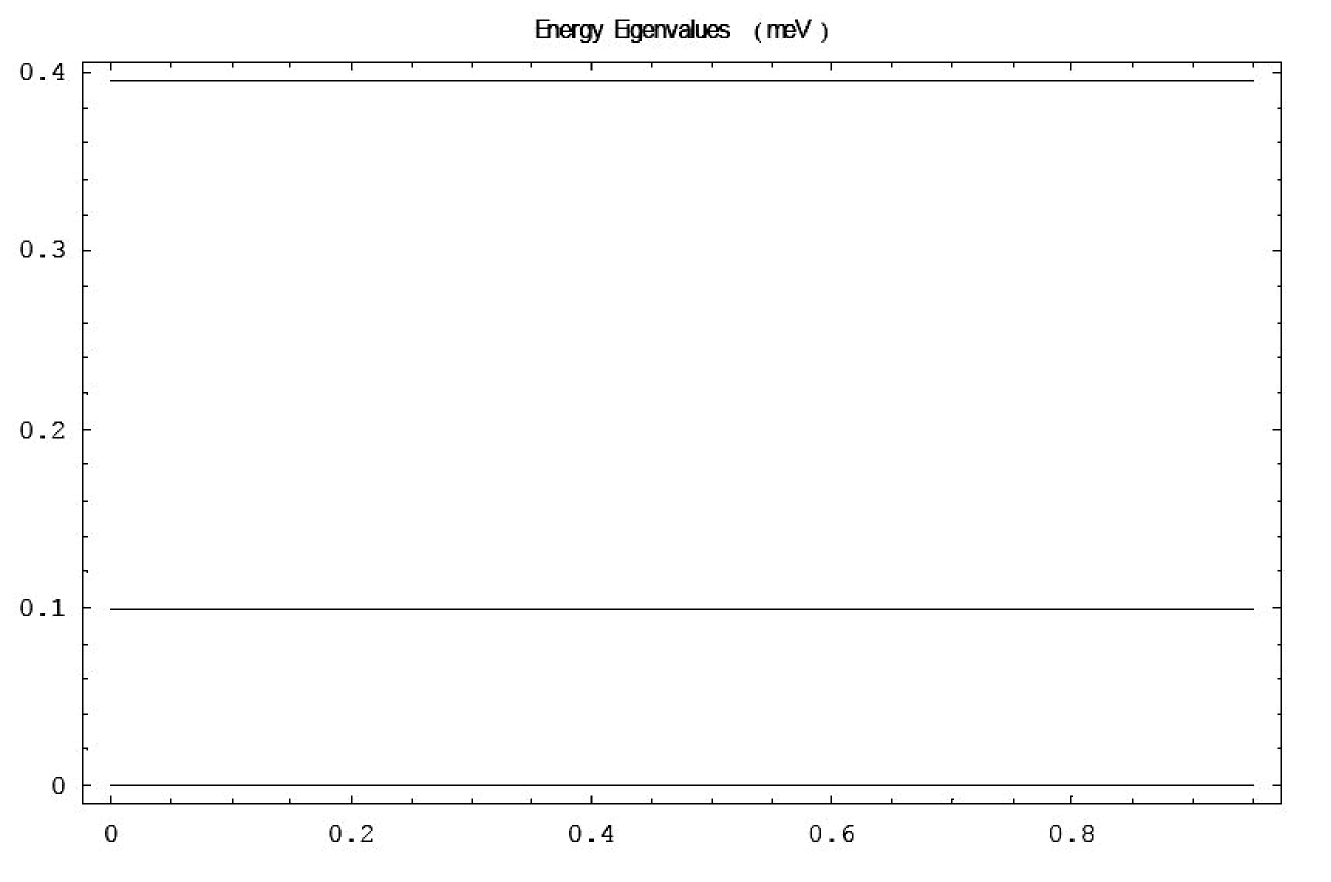
{{4 − 2.688 B, 0, 0, 0, 0}, {0, 1 − 1.344 B, 0, 0, 0},
{0, 0, 0, 0, 0}, {0, 0, 0, 1 + 1.344 B, 0}, {0, 0, 0, 0, 4 + 2.688 B}}

e = Eigenvalues[H]

{0, 4 − 2.688 B, 1 − 1.344 B, 1 + 1.344 B, 4 + 2.688 B}

Excitation energies, B=0T

E (meV)

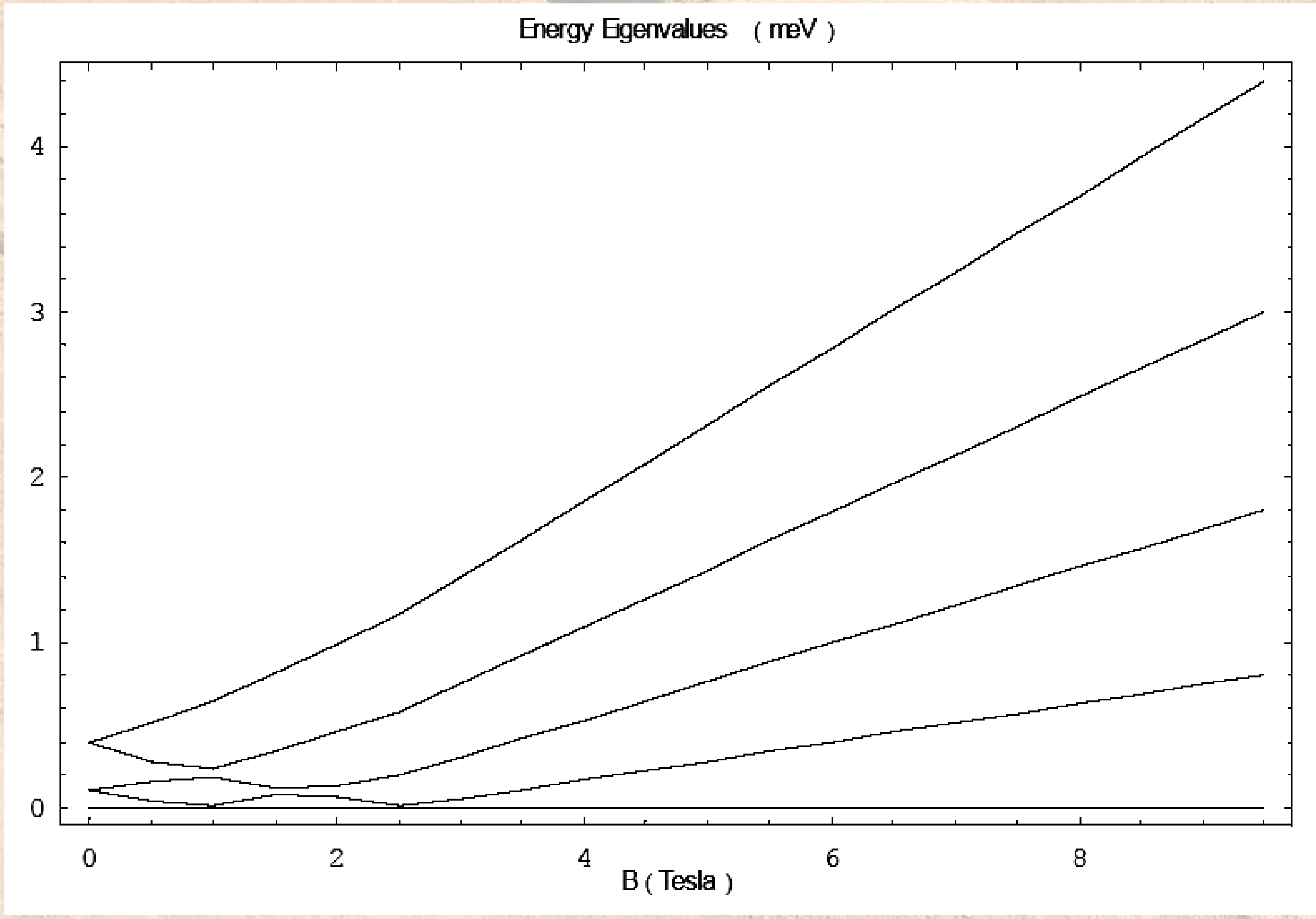


Eigenvalues

	ENERGY (meV)	$\|2,-2\rangle$	$\|2,-1\rangle$	$\|2,0\rangle$	$\|2,1\rangle$	$\|2,2\rangle$
E1	0.000	0.000	0.000	1.000	0.000	0.000
E2	0.099	0.000	1.000	0.000	0.000	0.000
E3	0.099	0.000	0.000	0.000	1.000	0.000
E4	0.396	1.000	0.000	0.000	0.000	0.000
E5	0.396	0.000	0.000	0.000	0.000	1.000

Excitation energies, B=0…10T

E (meV)



Now the thermodynamics is computable !!!

Magnetization

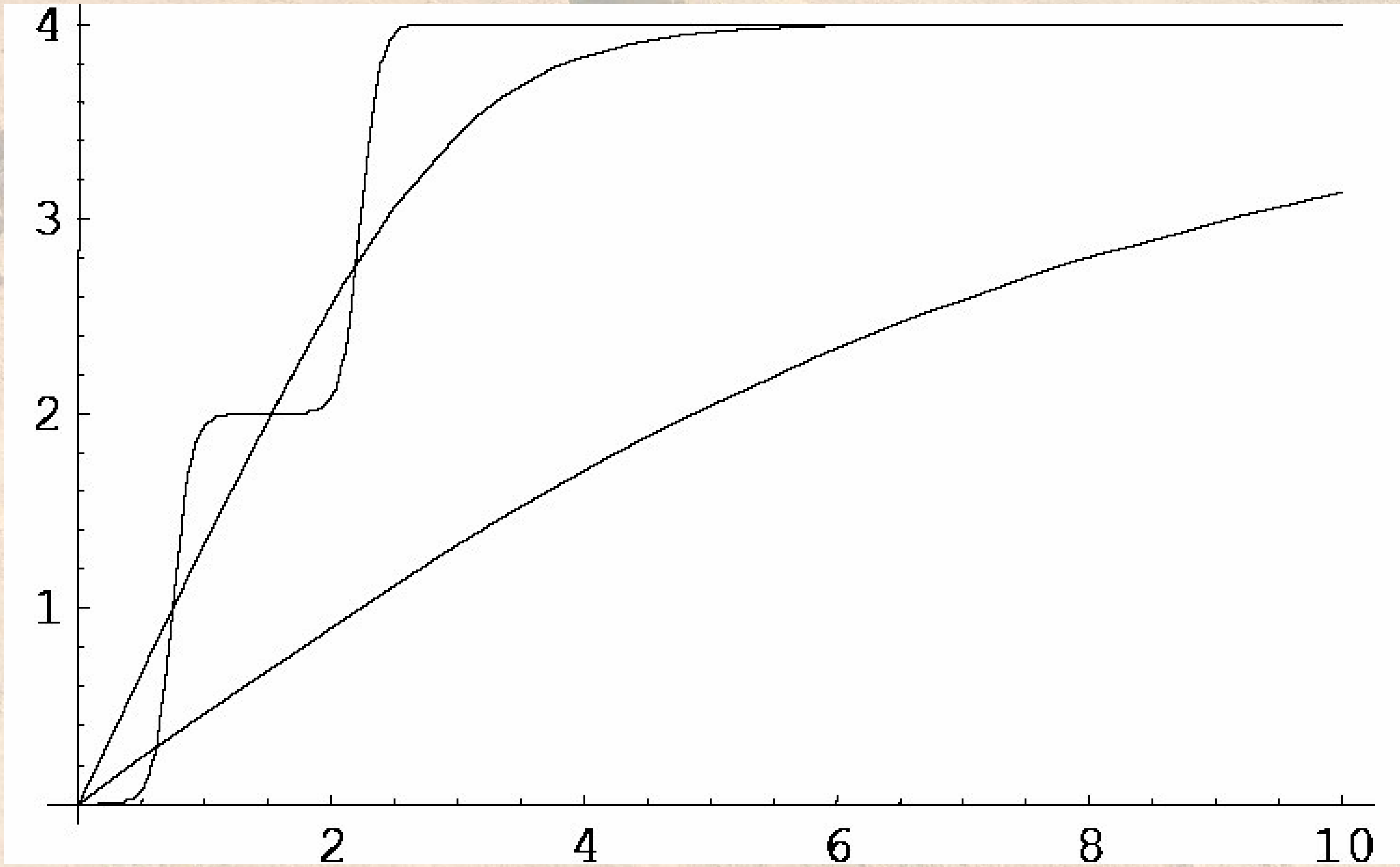
$$Z = \sum_{i=1}^{5} \mathrm{Exp}\left[-\frac{e[i]}{k_B T}\right]$$

$$Z = \mathrm{Exp}\left[-\frac{0}{T}\right] + \mathrm{Exp}\left[-\frac{4 - 2.688\,B}{T}\right] + \mathrm{Exp}\left[-\frac{1 - 1.344\,B}{T}\right] + \mathrm{Exp}\left[-\frac{1 + 1.344\,B}{T}\right] + \mathrm{Exp}\left[-\frac{4 + 2.688\,B}{T}\right]$$

$$M = N_A k_B T \left(\frac{\partial \mathrm{Ln} Z}{\partial B}\right)_T =$$

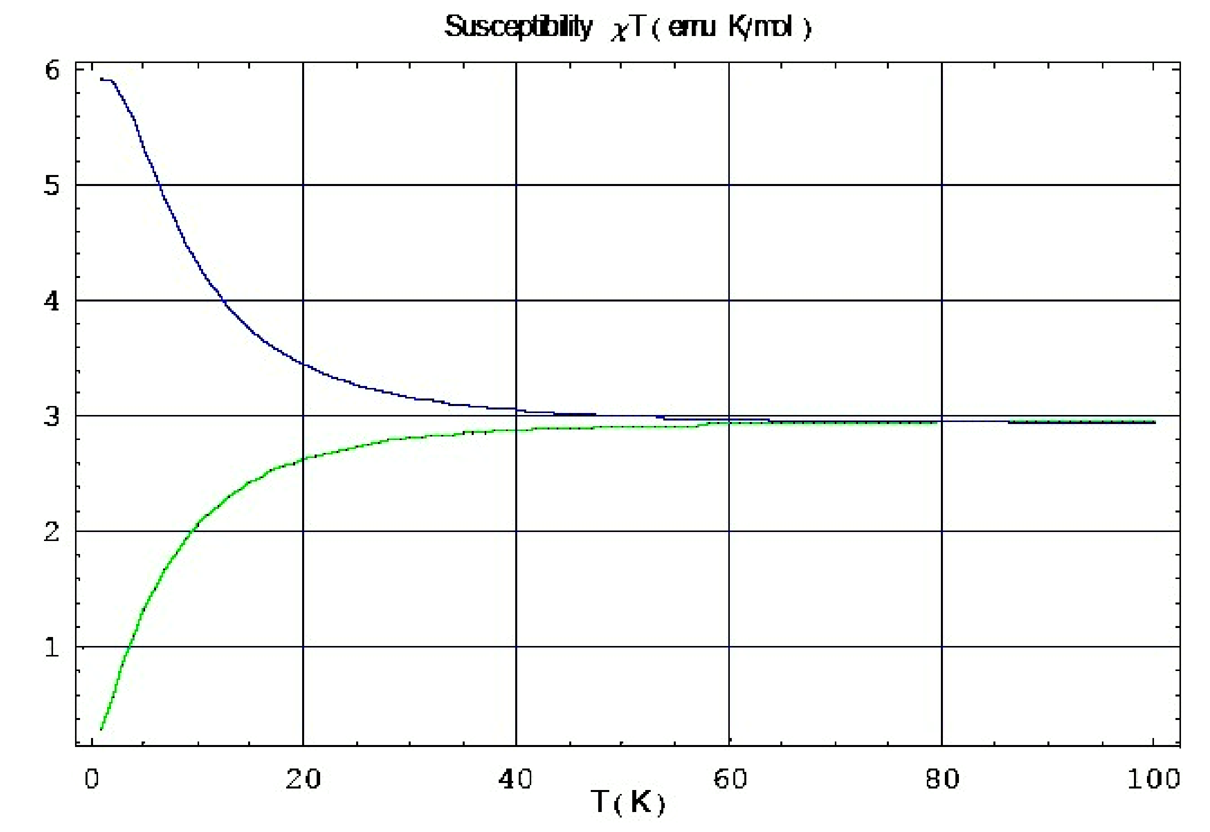
$$\frac{N_A g_z \mu_B}{Z}\left(-\mathrm{Exp}\left[-\frac{1 + 1.344\,B}{T}\right] + \mathrm{Exp}\left[-\frac{1 - 1.344\,B}{T}\right] - 2\,\mathrm{Exp}\left[-\frac{4 + 2.688\,B}{T}\right] + 2\,\mathrm{Exp}\left[-\frac{4 - 2.688\,B}{T}\right]\right)$$

Magnetization =0.1, 1, 10 K

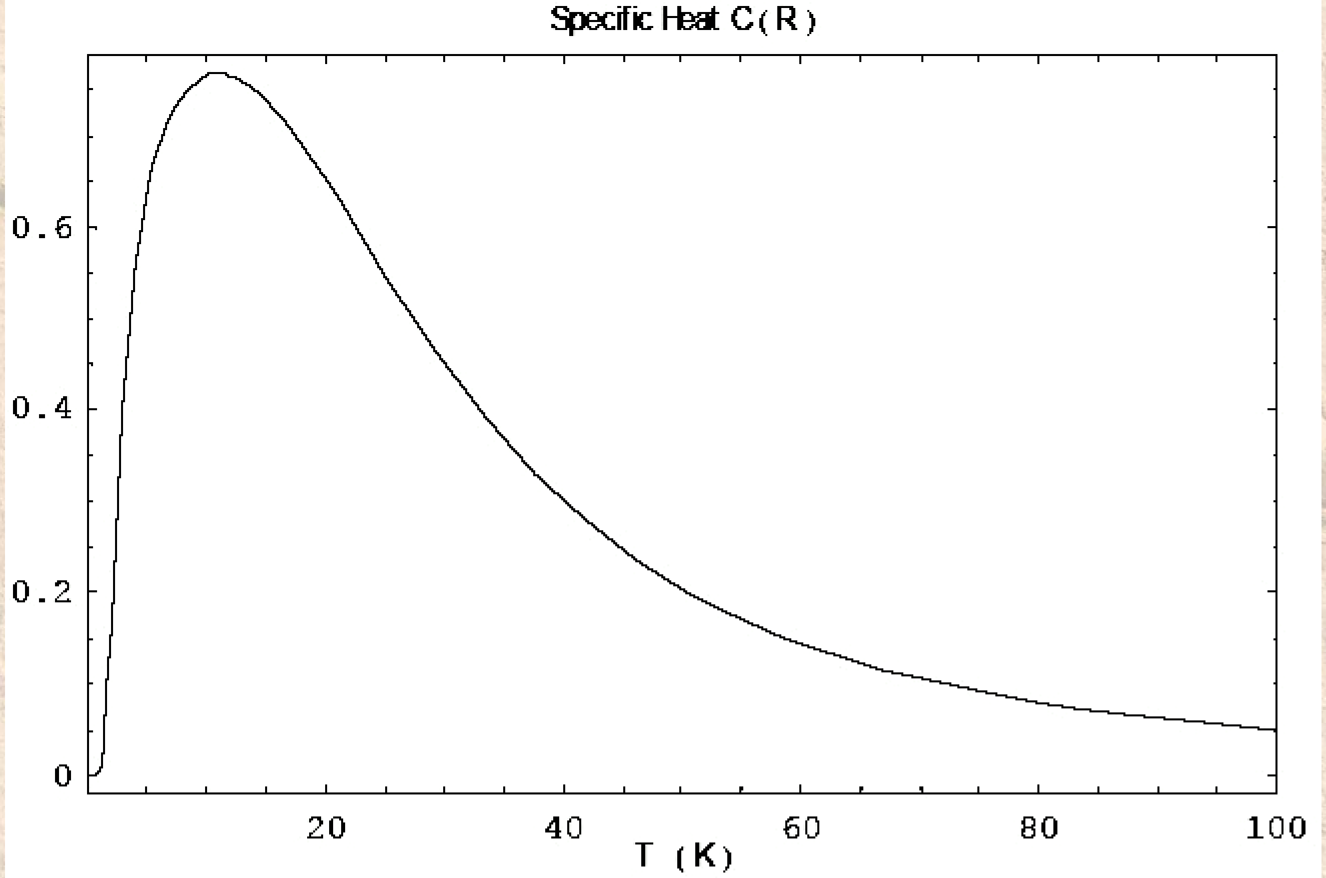


Susceptibility

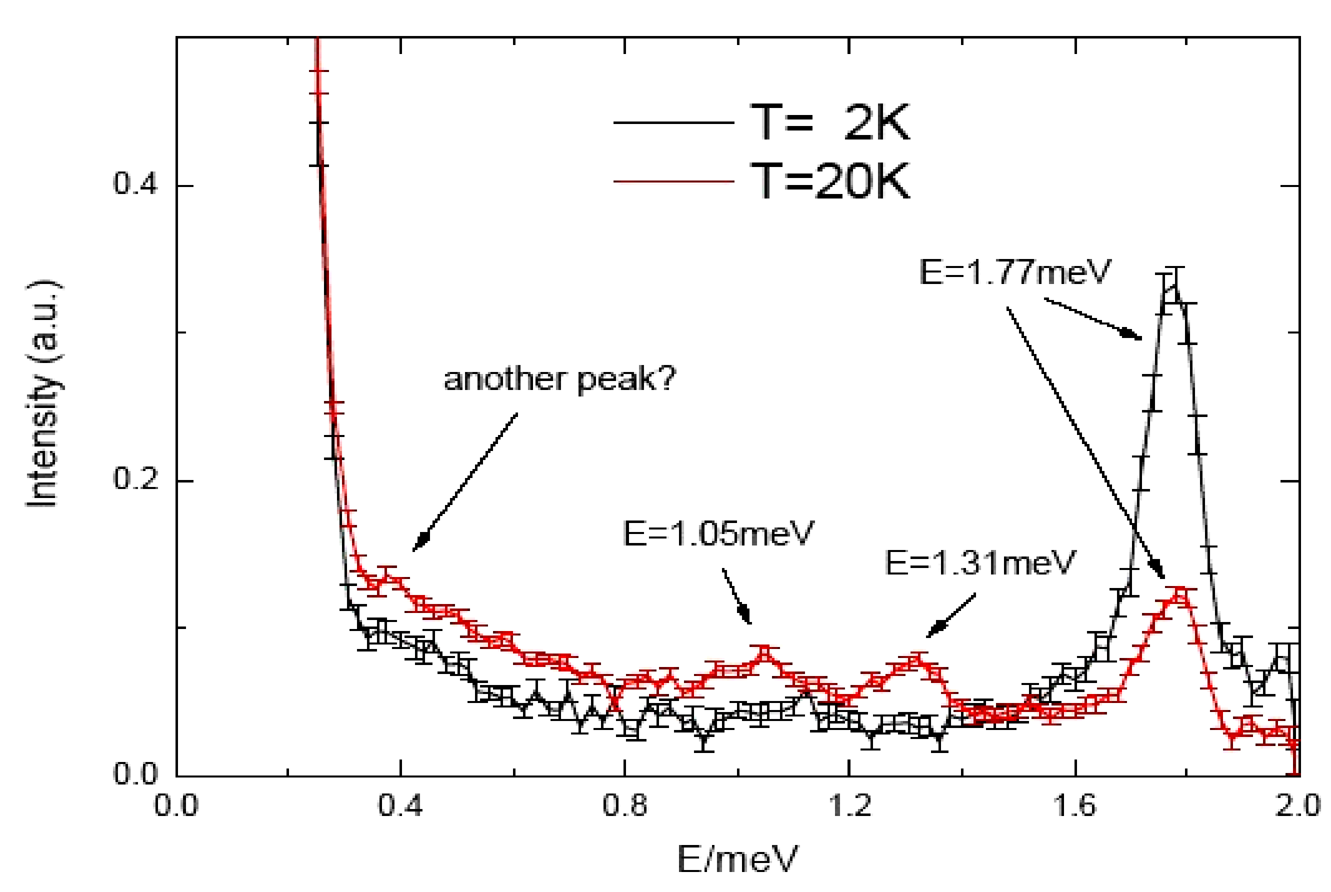
$$\chi = \mu_0 \frac{\partial M}{\partial B} = \frac{4.714 * 10^{-6} g_z^{\,2}}{T} \frac{(Z X_2 - X_1^{\,2})}{Z^2} \; m^3 / mol$$



Specific Heat



SMM - Mn_6 cluster



J. Van Slagern, O. Pieper, B. Lake, A. Schnegg, BENSC HMI experimental report 2006

Thank you
for your attention!