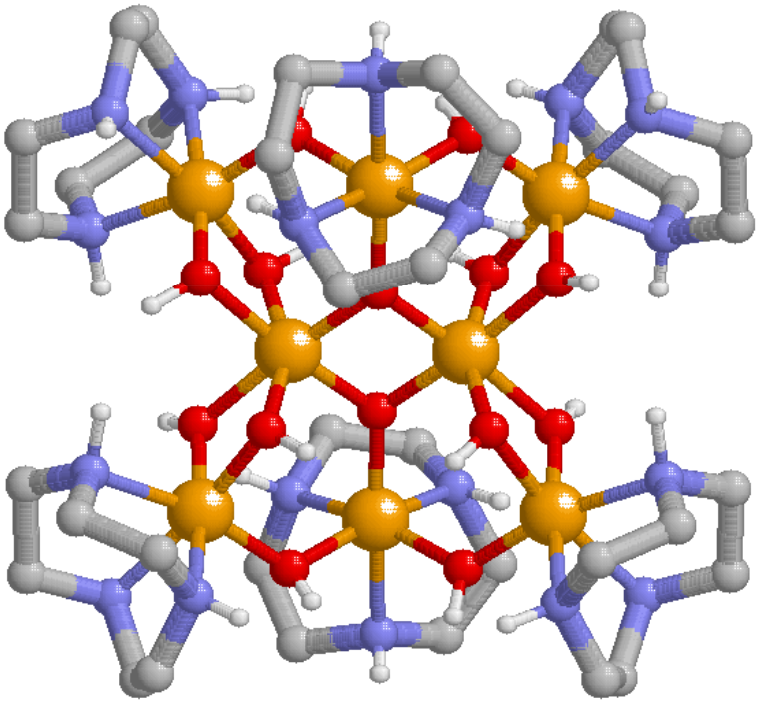
$[Fe_8O_2(OH)_{12}(tacn)_6]Br_8 \cdot 9H_20$



Fe^{3+}

S=5/2

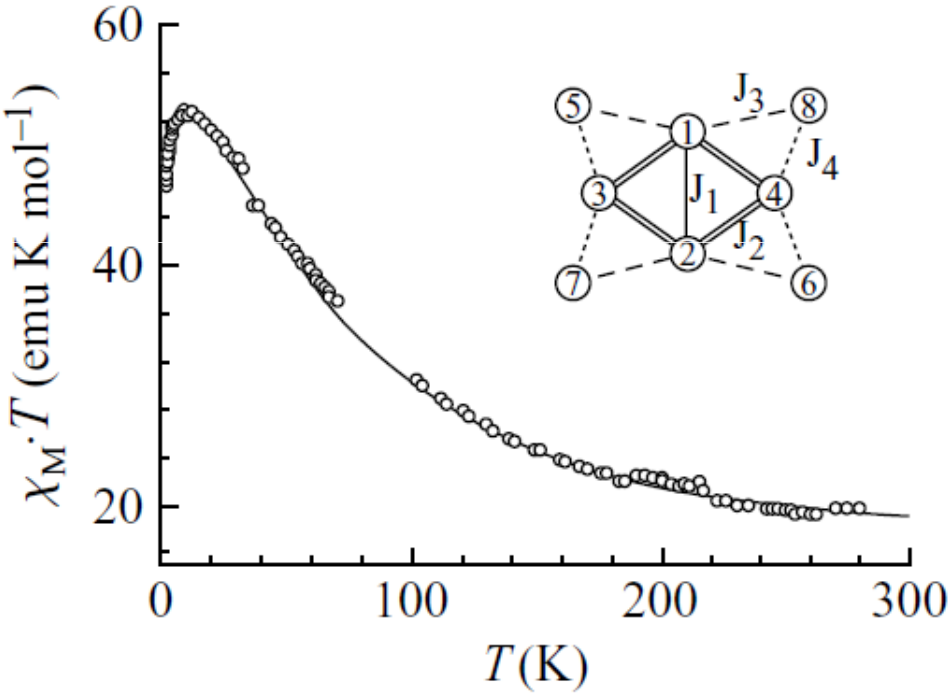
O

N

C

H

Valore dello spin nello stato fondamentale ?



Valore dello spin nello stato fondamentale ?

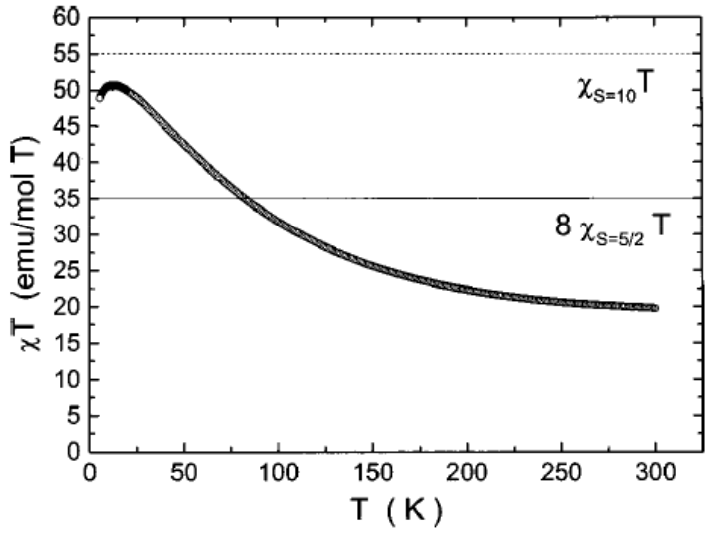
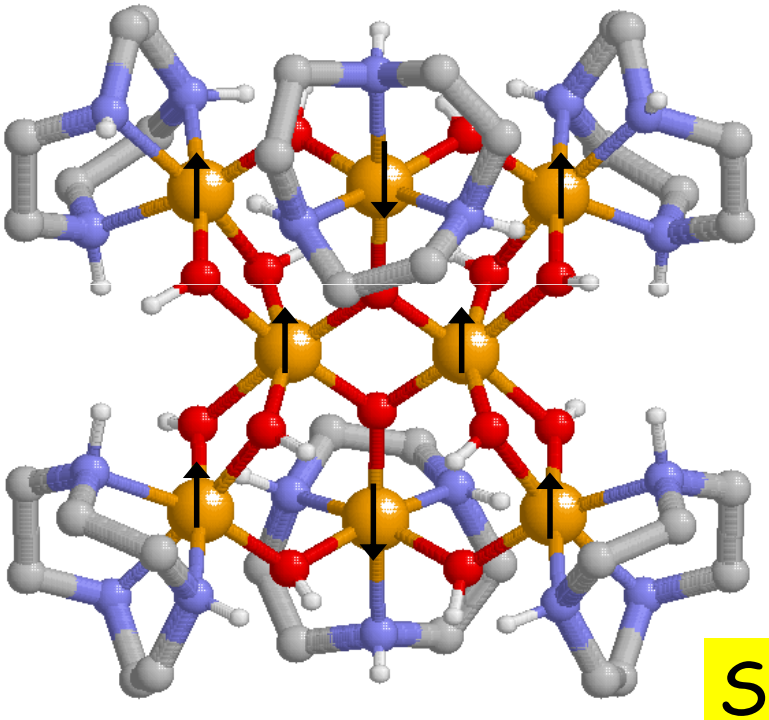


FIG. 2. Temperature dependence of the product of the susceptibility times temperature for stFe8 powders compared with the theoretical values expected for eight independent spins $S = 5/2$ and for a unique macrospin $S = 10$.

$[Fe_8O_2(OH)_{12}(tacn)_6]Br_8 \cdot 9H_20$



S=10

Fe^{3+}

S=5/2

O

N

C

H

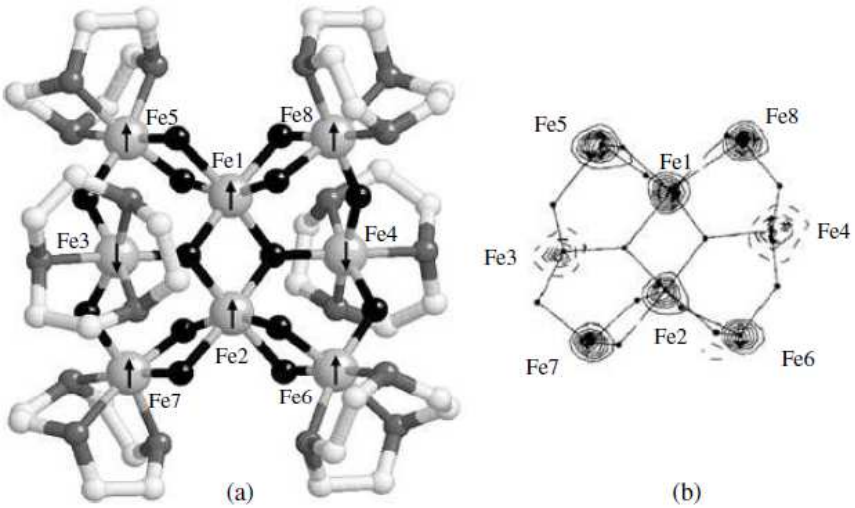
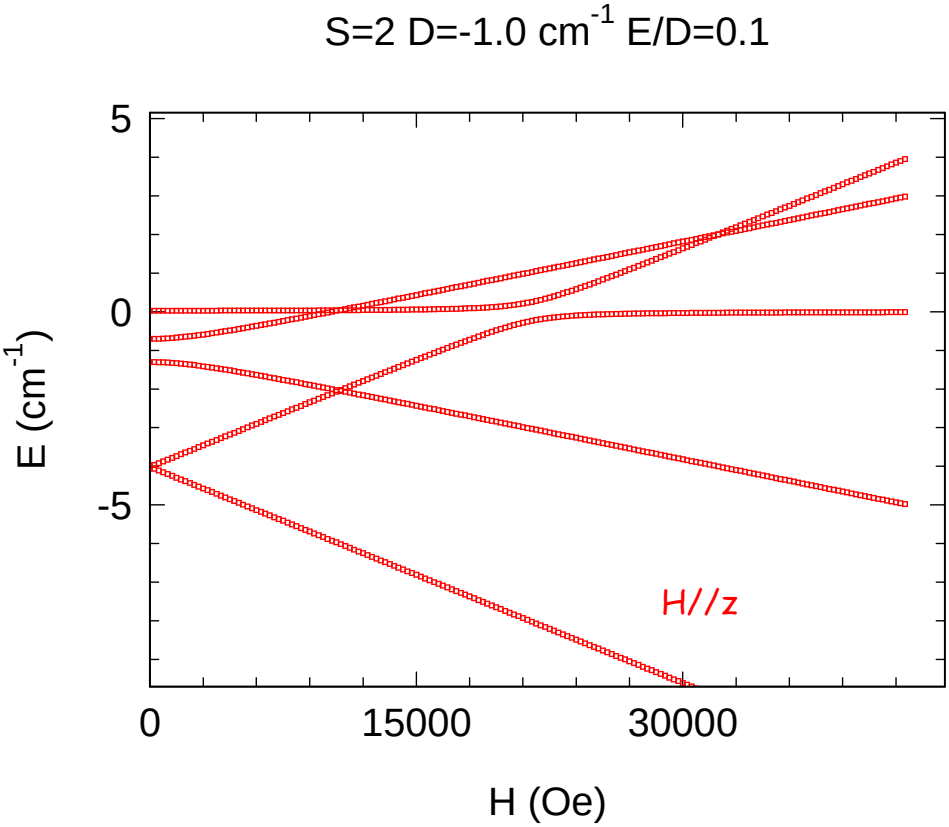
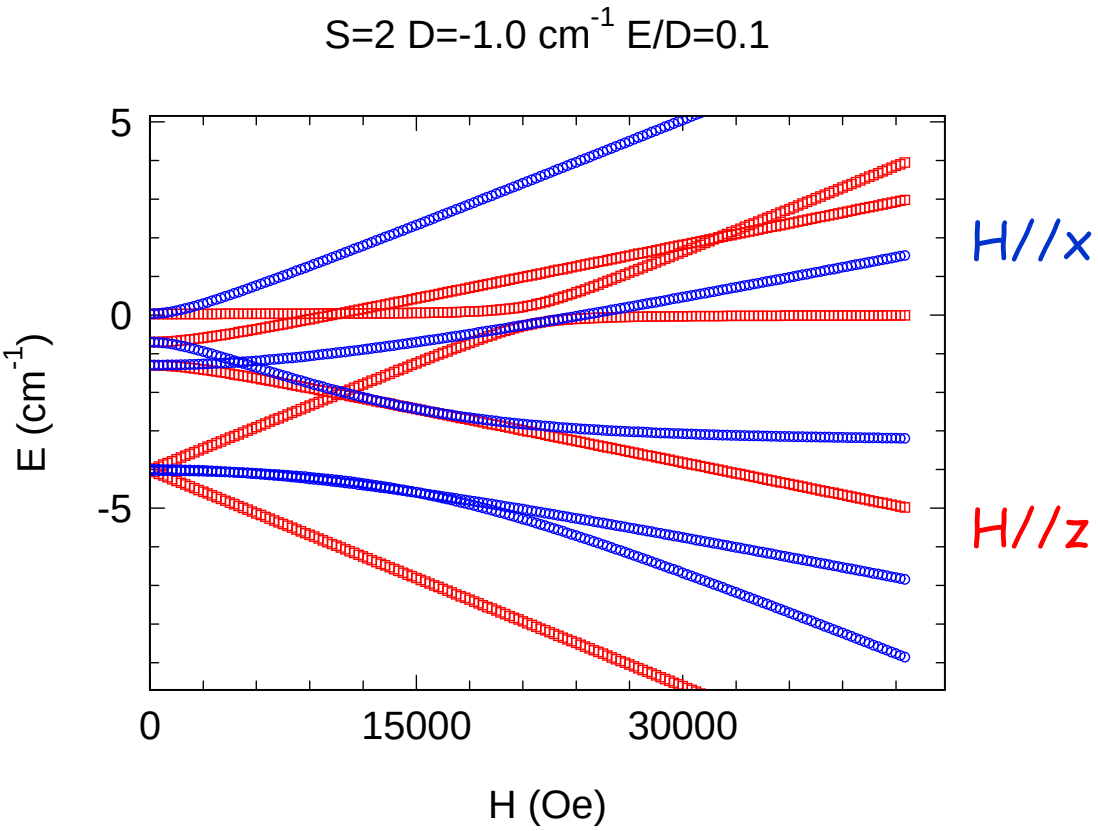


FIG. 3.36. (a) Structure of the Fe_8 cluster with the spin structure of the ground $S = 10$ state schematized by the arrows. (b) Spin density map obtained by polarized neutron diffraction experiments. Spin density contours are drawn at 0.7 $\mu_B/\text{Å}^2$. Negative spin density is represented by dashed lines. Spin density map reprinted with permission from Pontillon *et al.* (1999). Copyright (1999) American Chemical Society.

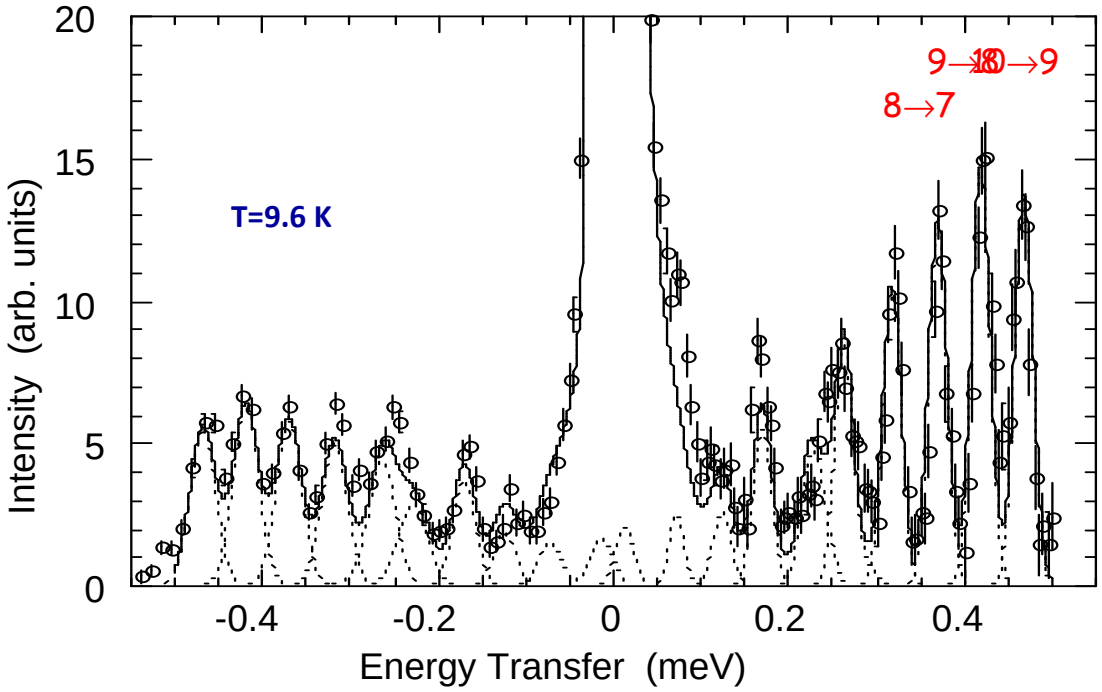




Selection rule for Inelastic Neutron Scattering

- Within the same S multiplet:
  - $\Delta m=\pm 1$
- Between different S multiplets:
  - $\Delta S=\pm 1$
  - $\Delta m=\pm 1$

Inelastic Neutron Scattering



R. Caciuffo et al. *Phys. Rev. Lett.* **1998**, *81*, 4744.

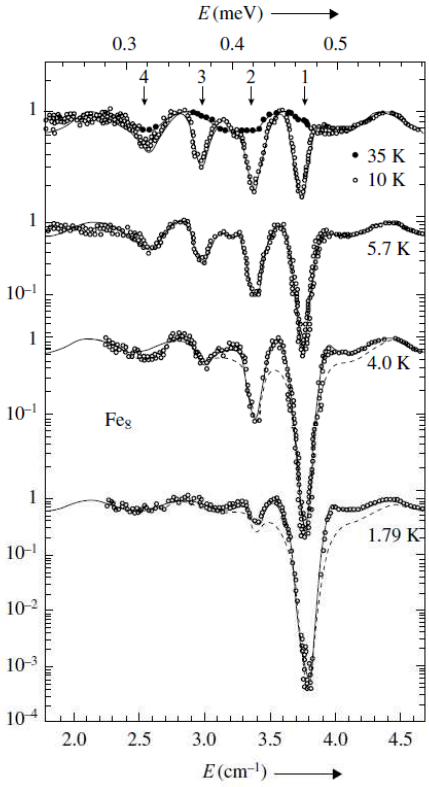
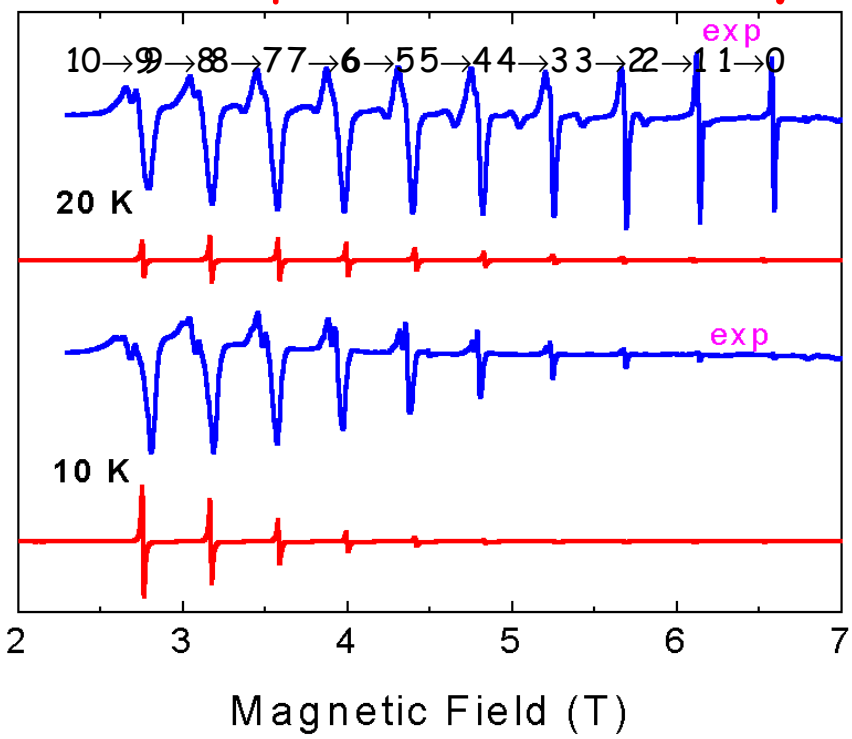


FIG. 4.29. Far-infrared spectra in zero field of Fe_8 at different temperatures. The peaks labelled as 1, 2, 3 and 4 correspond to the $m \rightarrow m'$ transitions, $\pm 10 \rightarrow \pm 9$, $\pm 9 \rightarrow \pm 8$, $\pm 8 \rightarrow \pm 7$, $\pm 7 \rightarrow \pm 6$, respectively. From Mukhin *et al.* (2001). Copyright (2001) American Physical Society.

Single crystal HFEPR @190 GHz

magnetic field parallel to the **easy** axis



Dalla separazione delle righe EPR

$\Delta Hres \sim 0.45T = 2|D|/g\mu_B$

$|D| = 0.45\ T * g * \mu_B / 2 = 0.45\ T * 9.27x10\text{-}24\ J\ T^{-1}$

$|D| = 4.1X10^{-24}\ J$

Dallo spettro di scattering inelastico di neutroni
o EPR in campo nullo

$E(m=9)-E(m=10) = 100|D| - 81|D| = 19|D| = 0.47meV =$
$= 0.47 * 1.60x10^{-22}\ J = 0.75x10^{-22}\ J$

$|D| = 4.0x10^{-24}\ J$

S=3, D<0