Magnetic response of magnetic molecules with non-collinear local d-tensors

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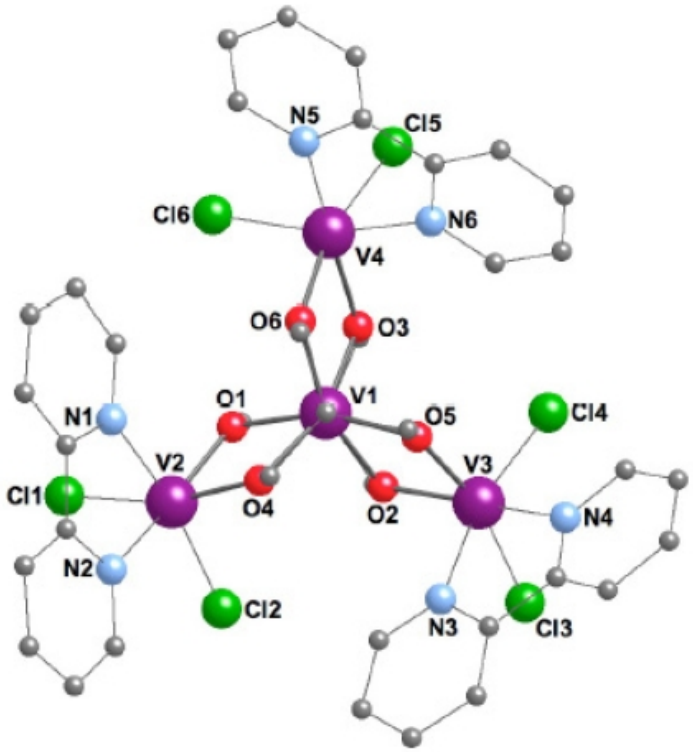
Contents for you today



V_4

1. Aim
2. The Hamiltonian
3. V_4
4. Some Systematics

Aim

Understand depenence of magnetic properties on microscopic, i.e. local d-tensors

Derive microscopic parameters from macroscopic observables

Compare to *ab initio* calculations

The Hamiltonian

Getting eigenvalues

$$\underset{\sim}{H}(\vec{B}) \;=\; -\sum_{i,j} J_{ij}\,\vec{\underset{\sim}{s}}(i)\cdot\vec{\underset{\sim}{s}}(j) \;+\sum_{i} d_i\left(\vec{e}_i\cdot\vec{\underset{\sim}{s}}(i)\right)^2+ \;\mu_B\,\vec{B}\cdot\sum_{i}^{N}\mathbf{g}_i\cdot\vec{\underset{\sim}{s}}(i)$$

- $\left[\underset{\sim}{H},\vec{\underset{\sim}{S}}^2\right]\neq 0,\ \left[\underset{\sim}{H},\vec{\underset{\sim}{S}}_z\right]\neq 0;\quad\Rightarrow$ MAGPACK does not work!
- You have to diagonalize $\underset{\sim}{H}(\vec{B})$ for every field (direction and strength)!
- Orientational average for powder samples.

$[V_4^{III}Cl_6(thme)_2(bipy)_3]$

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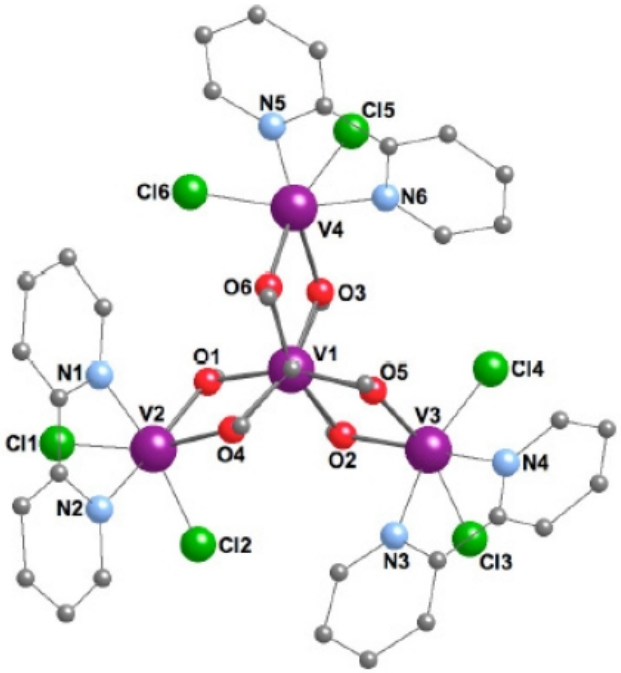
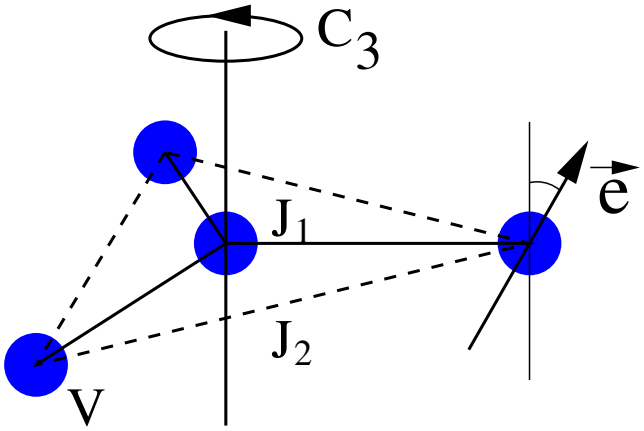


- From a physicists point of view this molecule contains 4 interesting V_4^{III} ions with $s = 1$ and very likely large anisotropy.
- The other stuff – thyme? – seems to be important for the cooking.

Ian S. Tidmarsh, Luke J. Batchelor, Emma Scales, Rebecca H. Laye, Lorenzo Sorace, Andrea Caneschi, Jürgen Schnack and Eric J.L. McInnes, Dalton Trans. (2009) 9402-9409

V_4 I

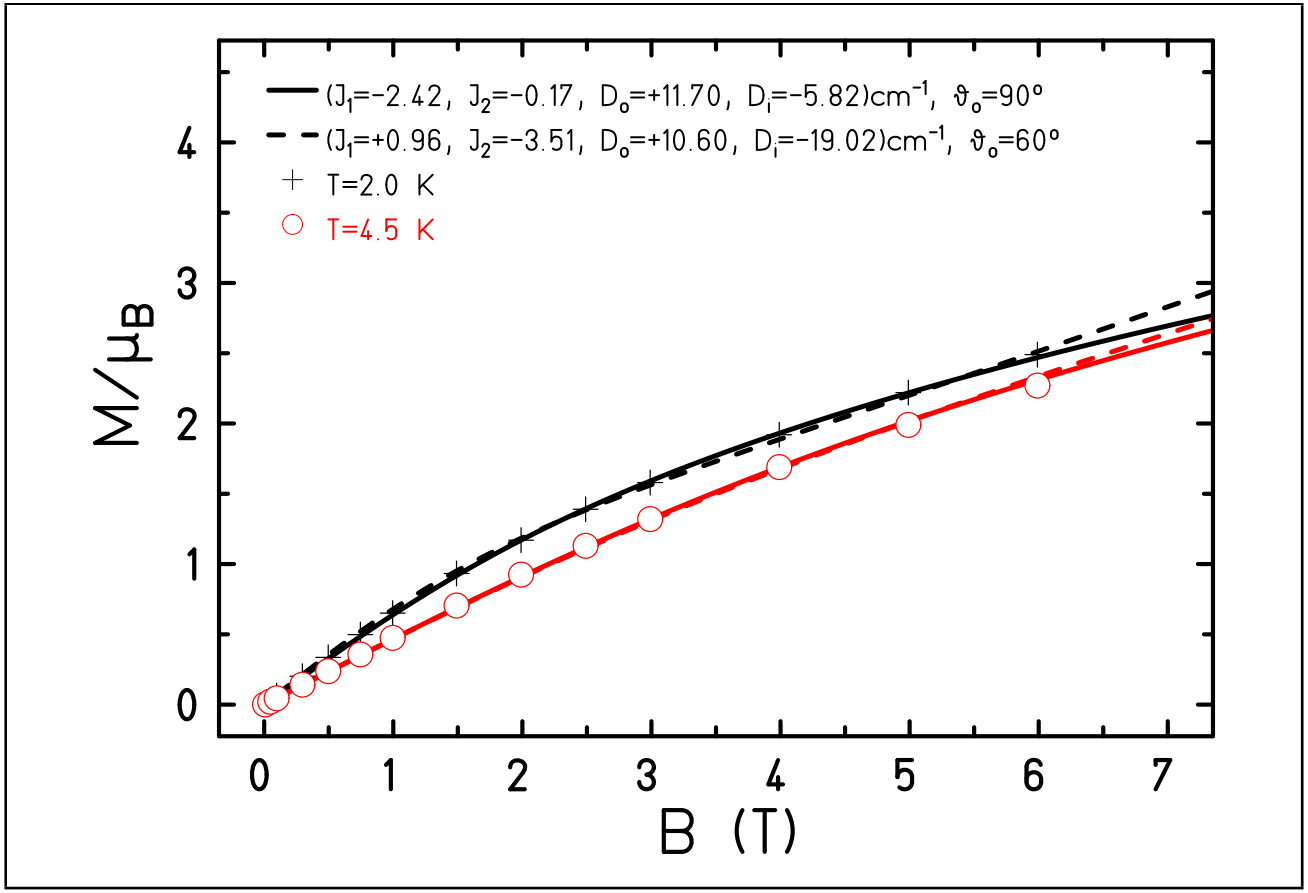


$[V_4^{III}Cl_6(thme)_2(bipy)_3]$

- 4 V_4^{III} ions with $s = 1$; approximate C_3 symmetry;
- 2 exchange interactions;
- Central V: axial anisotropy;
- Outer Vs: local anisotropy axis with azimuthal angle ϑ.
- Powder average.

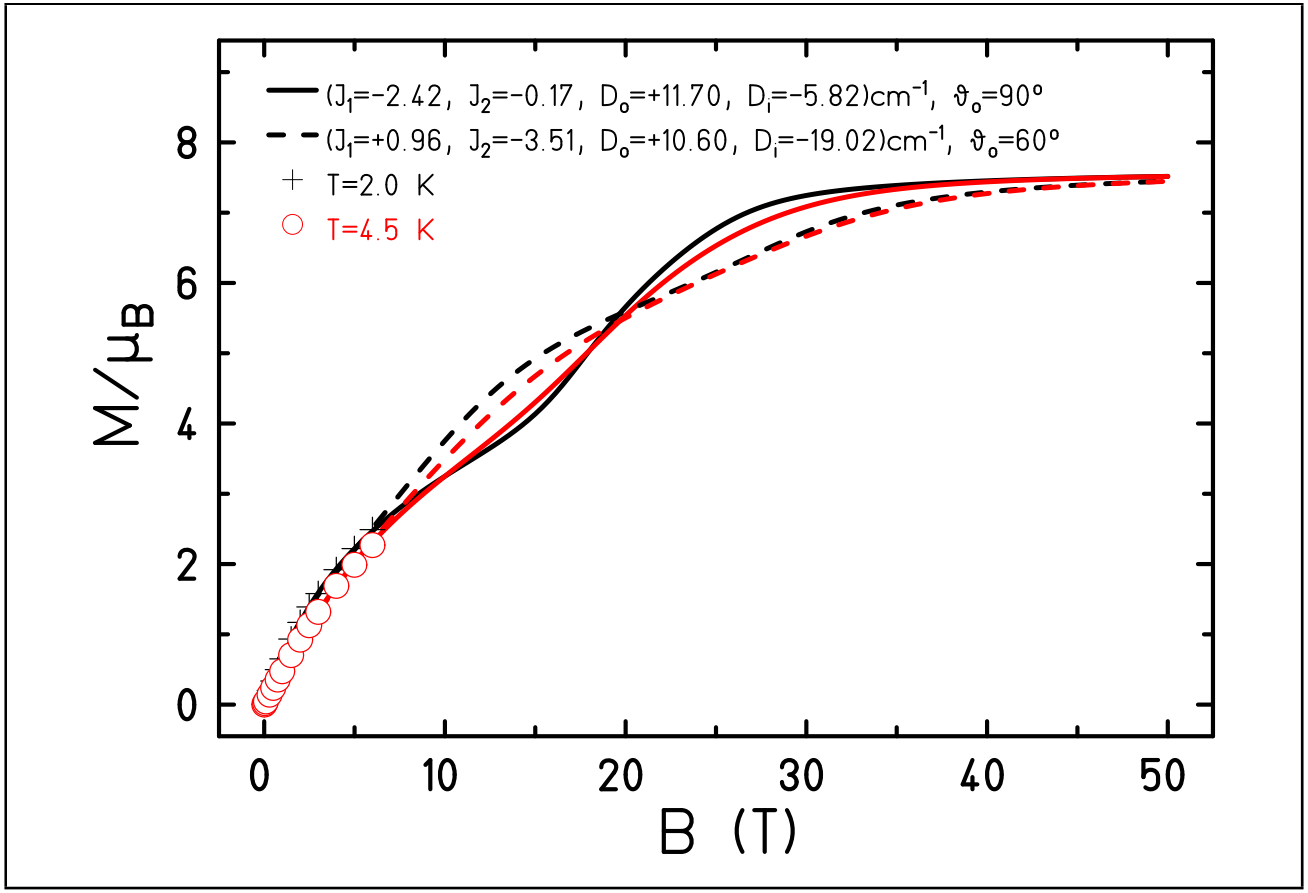
Ian S. Tidmarsh, Luke J. Batchelor, Emma Scales, Rebecca H. Laye, Lorenzo Sorace, Andrea Caneschi, Jürgen Schnack and Eric J.L. McInnes, Dalton Trans. (2009) 9402-9409

V_4 II



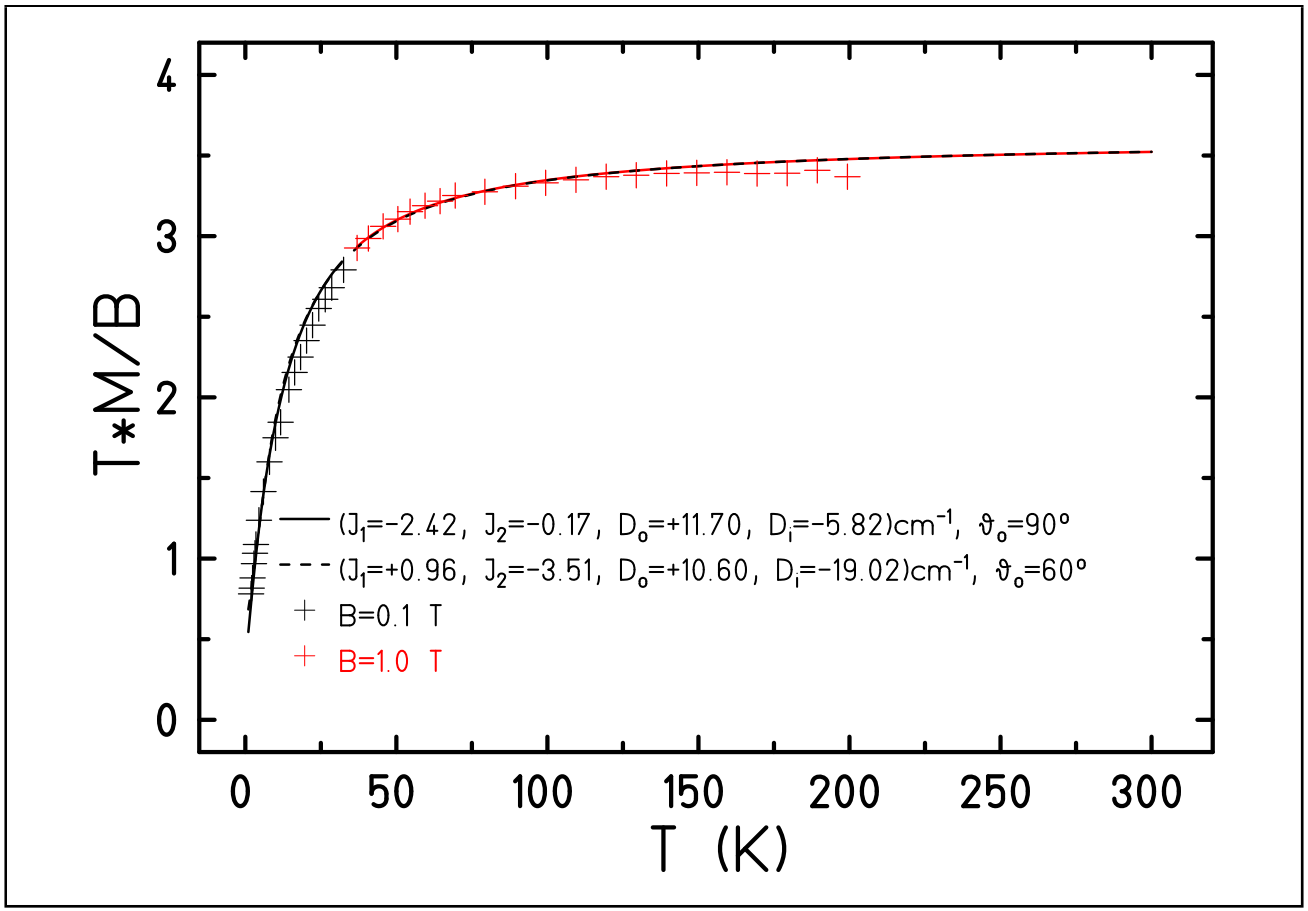
Two equally good parameter sets.

V_4 III



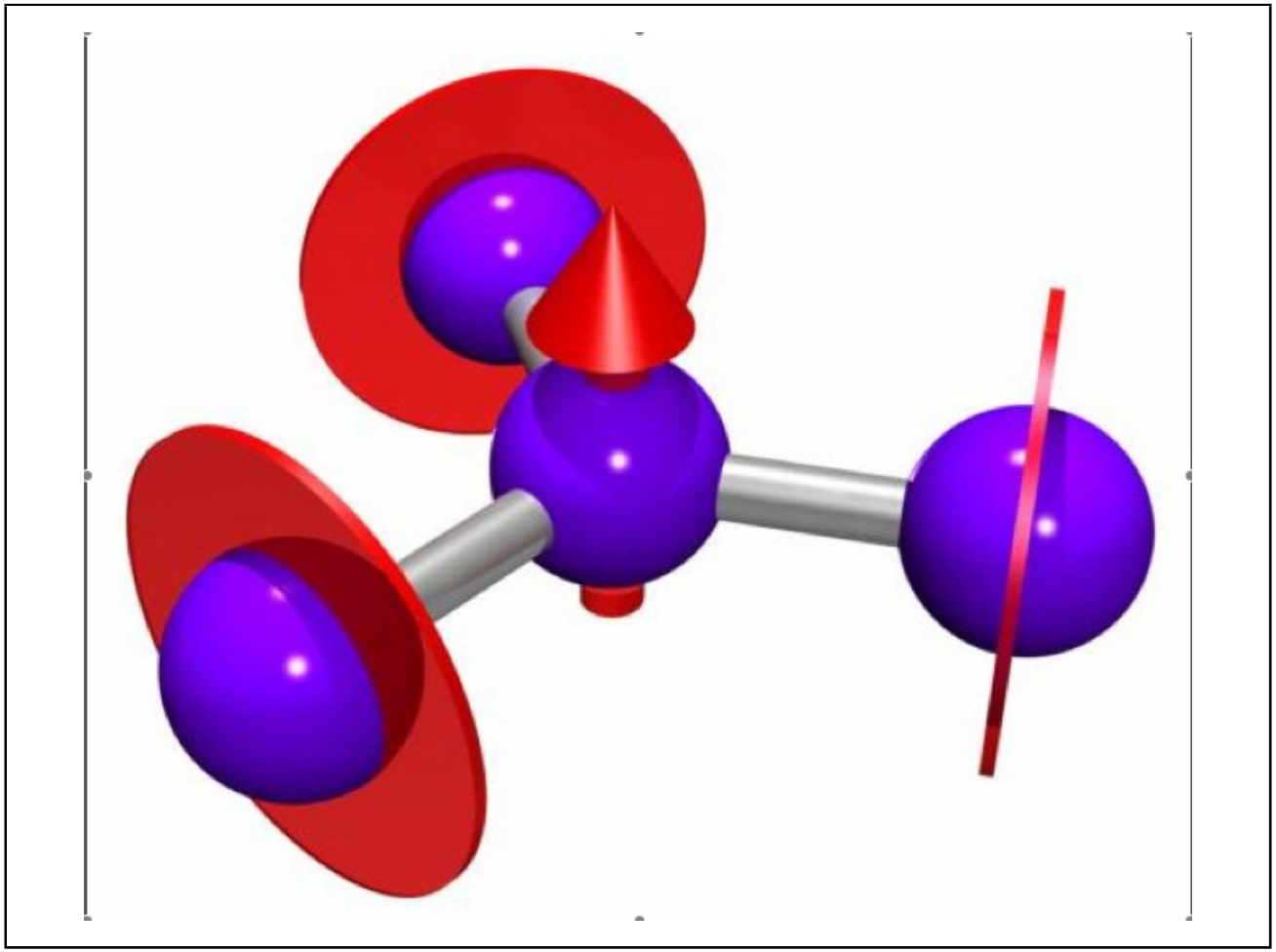
High fields could distinguish.

V_4 IV



Accuracy of measurement limits modeling.

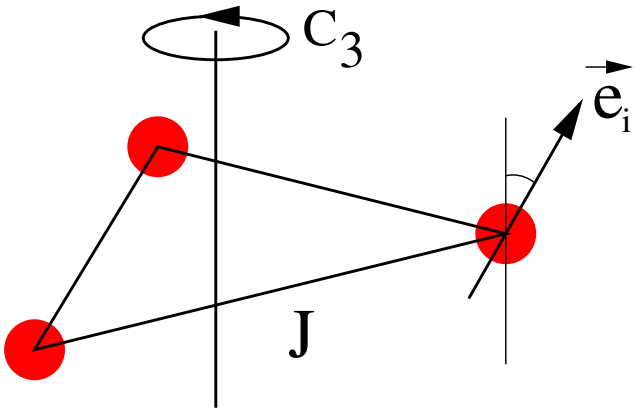
V_4 – Anisotropy tensors



Cartoon of anisotropy tensors.

Any Systematics?

Systematic study of a trimer

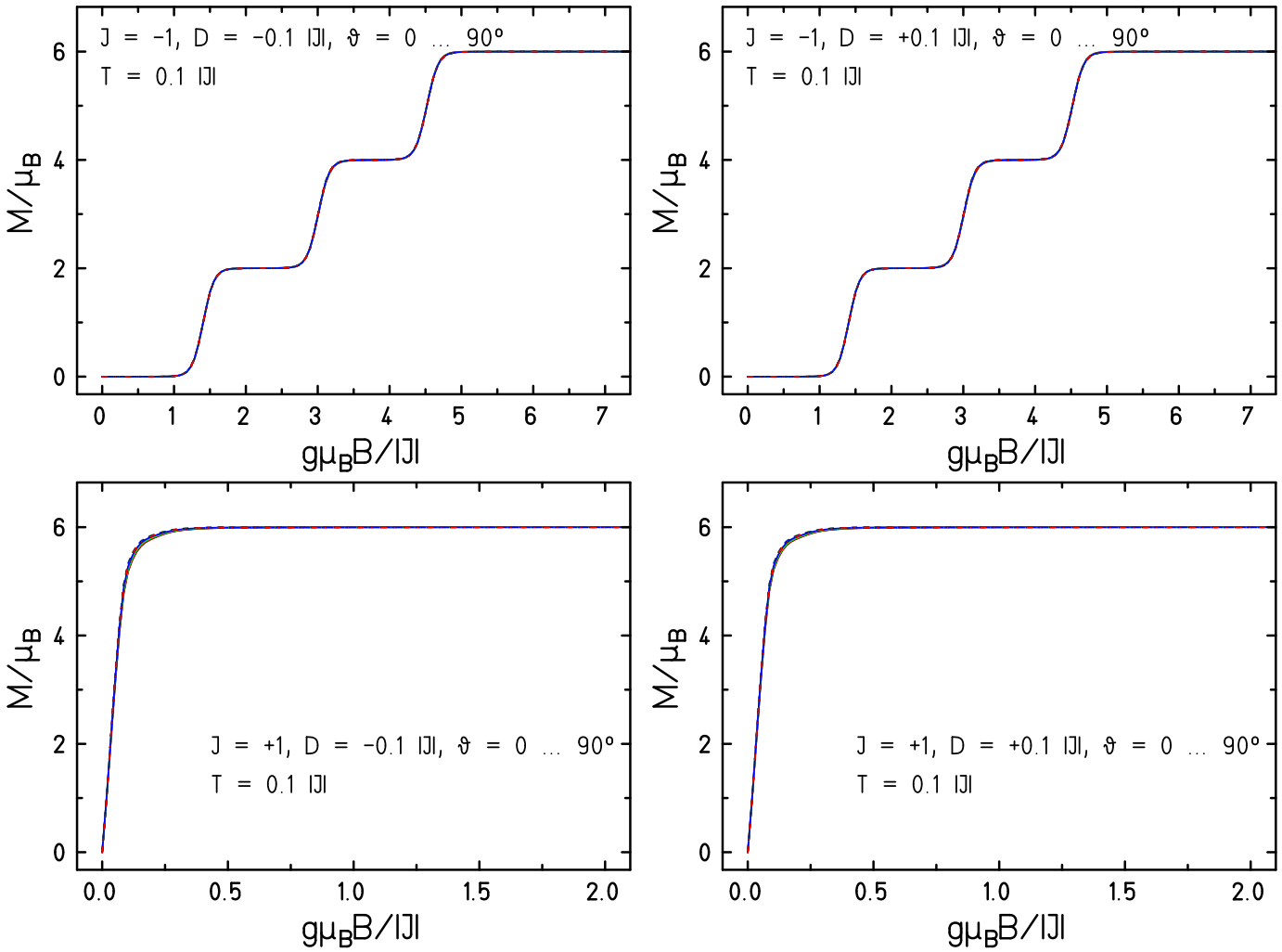


Anisotropic trimer

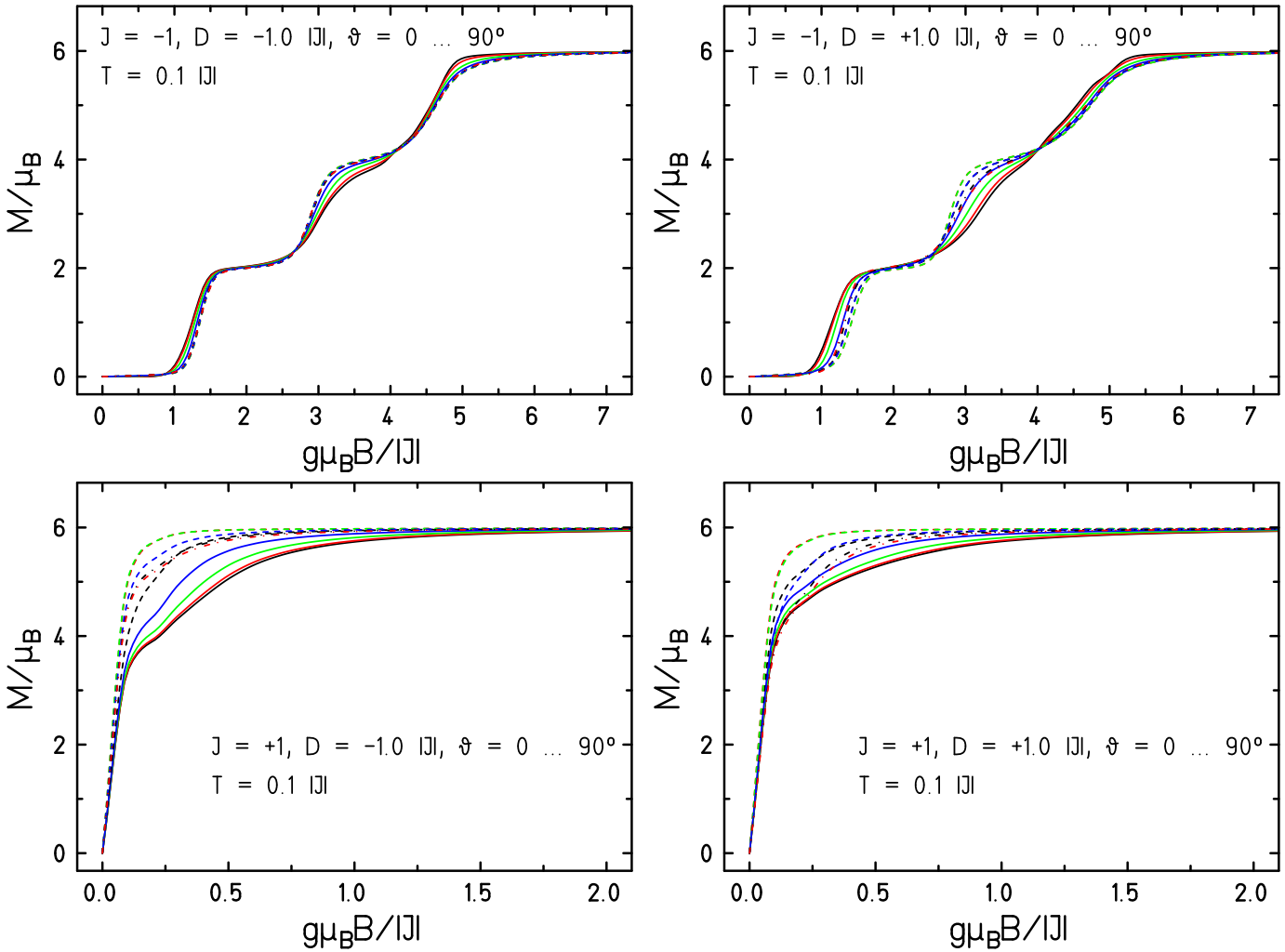
- Ions with $s = 1$; C_3 symmetry;
- 1 exchange interaction;
- Local anisotropy axis with azimuthal angle ϑ.
- Powder average.

J. Schnack, Condens. Matter Phys. **12** (2009) 323-330

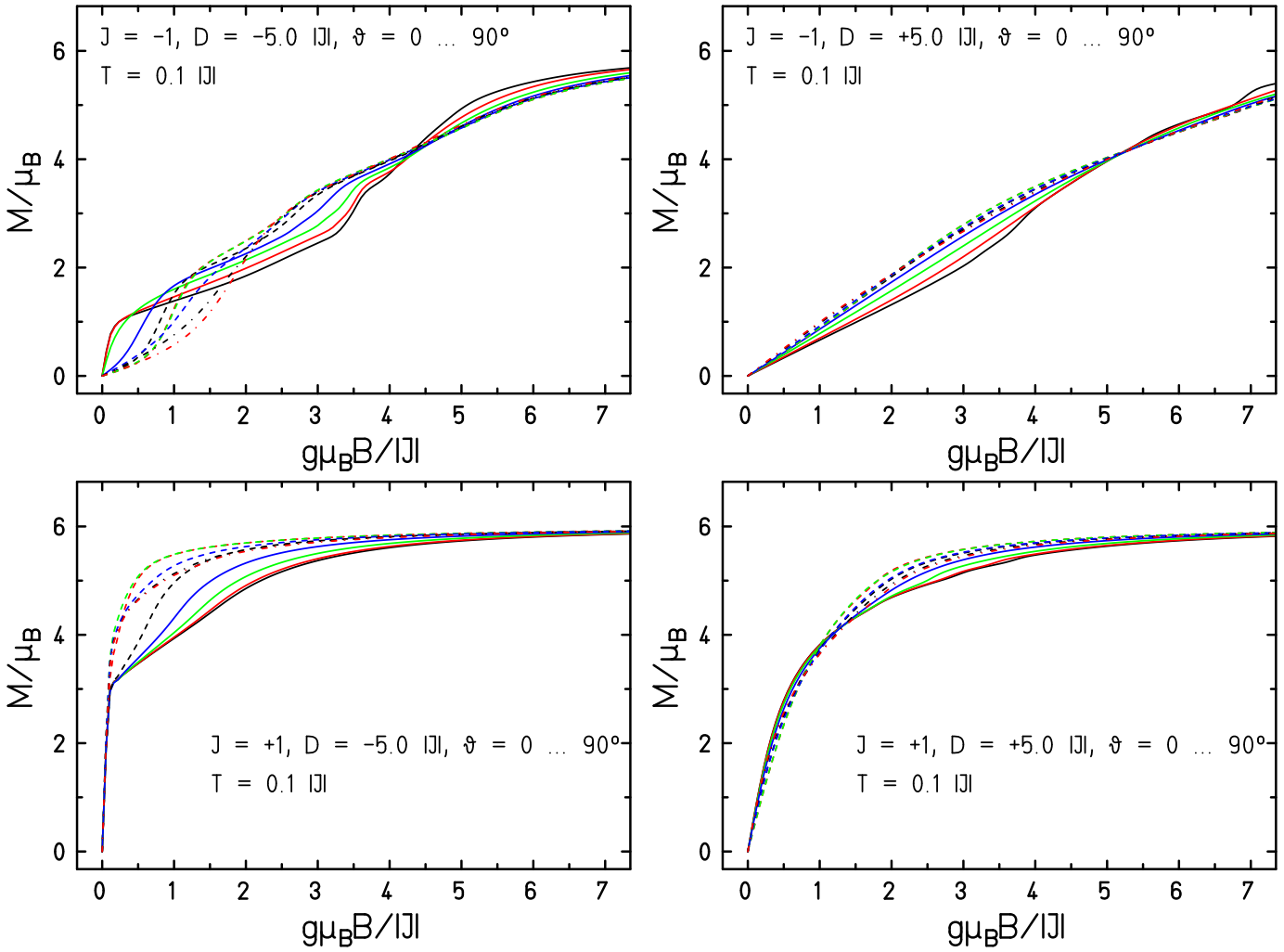
Strong coupling



Intermediate coupling



Weak coupling



Conclusion

Understand depenence of magnetic properties on microscopic, i.e. local d-tensors √

Derive microscopic parameters from macroscopic observables √

Compare to *ab initio* calculations !!!

Thank you very much for your attention.

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