

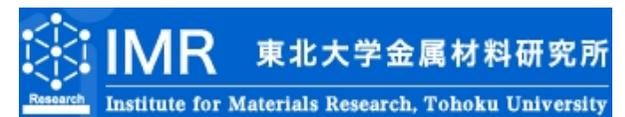
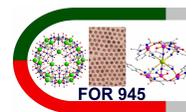
# Evaluation of anisotropic spin Hamiltonians

Jürgen Schnack

Department of Physics – University of Bielefeld – Germany

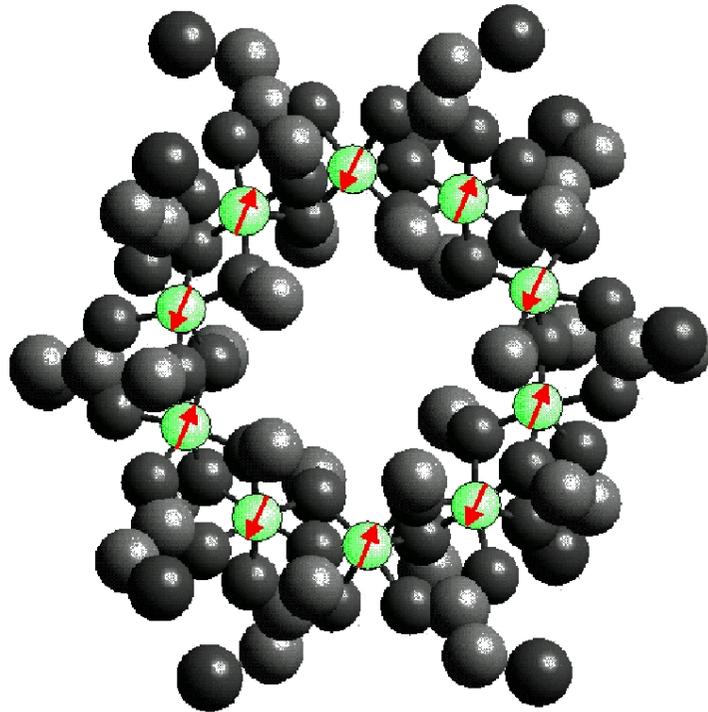
<http://obelix.physik.uni-bielefeld.de/~schnack/>

ECMM Satellite Workshop on Magnetic Anisotropy  
11-12 October 2013, KIT, Karlsruhe



# The problem

# You have got a molecule!

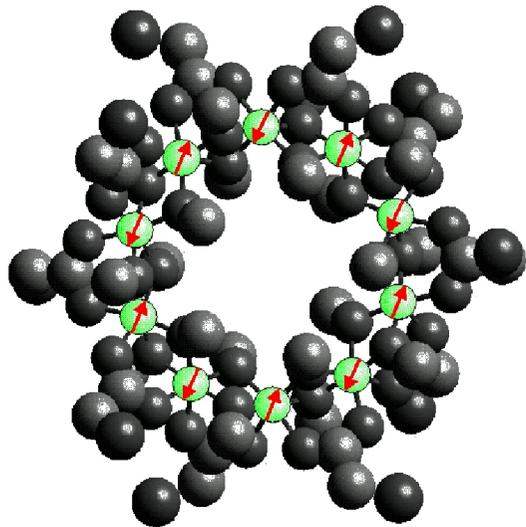


Congratulations!

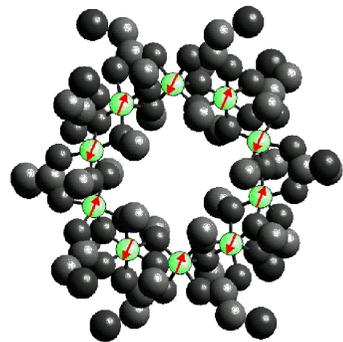
# You have got an idea about the modeling!

$$\tilde{H} = \sum_{i,j} \tilde{\mathbf{s}}(i) \cdot \mathbf{J}_{ij} \cdot \tilde{\mathbf{s}}(j) + \sum_{i,j} \vec{D}_{ij} \cdot [\tilde{\mathbf{s}}(i) \times \tilde{\mathbf{s}}(j)] + \mu_B \vec{B} \sum_i^N \mathbf{g}_i \tilde{\mathbf{s}}(i)$$

Exchange/Anisotropy
Dzyaloshinskii-Moriya
Zeeman



In the end it's always a big matrix!



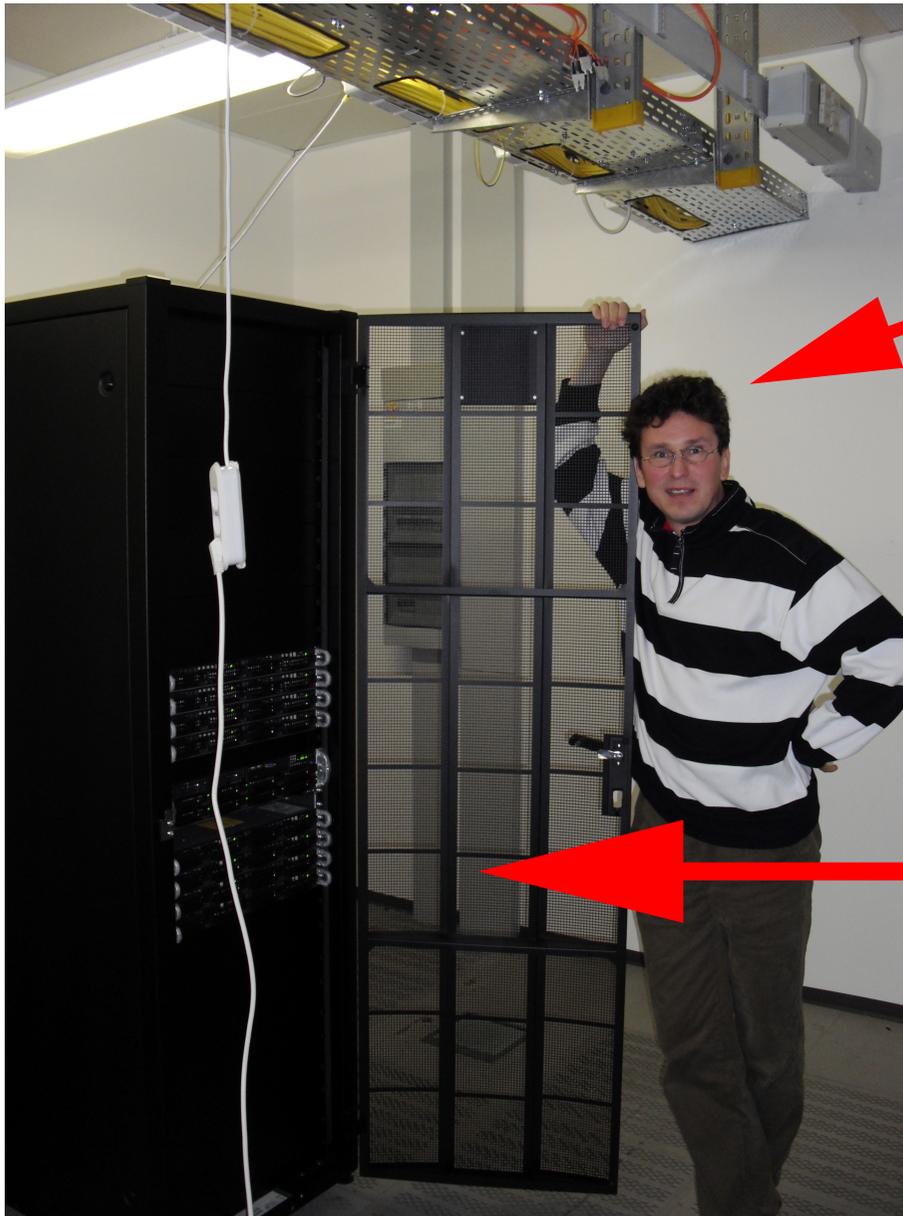
$$\Rightarrow \begin{pmatrix} -27.8 & 3.46 & 0.18 & \dots \\ 3.46 & -2.35 & -1.7 & \dots \\ 0.18 & -1.7 & 5.64 & \dots \\ \vdots & \vdots & \vdots & \dots \end{pmatrix} \Rightarrow$$



$$\text{Fe}_{10}^{\text{III}}: N = 10, s = 5/2$$

Dimension=**60,466,176**. Maybe **too** big?

# Thank God, we have computers

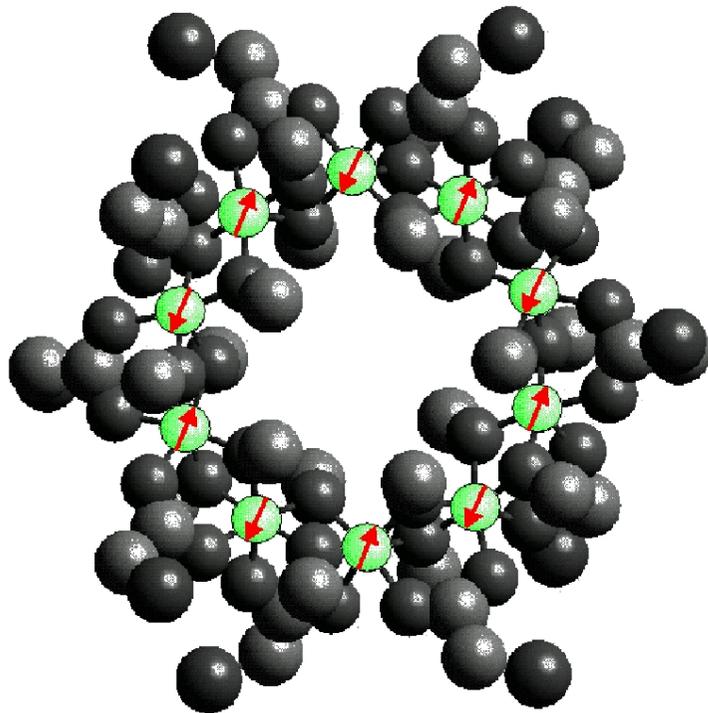


“Espresso-doped multi-core”

128 cores, 384 GB RAM

... but that's not enough!

# Contents for you today



Fe<sub>10</sub>

1. Isotropic case – simple
2. Isotropic case – advanced
3. Anisotropic case – general
4. Single ion anisotropy – examples
5. Thorsten Glaser's molecules
6. Anisotropic exchange

# Isotropic case

## Complete diagonalization: The easy version

Most physicists do this!

## Model Hamiltonian – Heisenberg

$$\tilde{H} = -2 \sum_{i < j} J_{ij} \tilde{\vec{S}}_i \cdot \tilde{\vec{S}}_j + \mu_B B g \sum_i^N \tilde{S}_i^z$$

Why does the Heisenberg model often yield a very good description of a spin system?

**Reason:** Some ions of the iron group have quenched angular momentum  $\langle \tilde{l} \rangle \approx 0$  due to chemical binding (ligand field), remaining spin-orbit coupling treated perturbatively with the help of anisotropy terms or simply neglected. This is different for most ions in the periodic table, e.g. rare earth ions! But let's not care for a moment.

Since the dimension of Hilbert space equals  $(2s + 1)^N$  the Hamiltonian can be diagonalized completely for small molecules. For larger ones approximate methods are used.

## Product basis and symmetries

Product basis, total dimension:  $\dim(\mathcal{H}) = (2s + 1)^N$

$$\tilde{S}_u^z |m_1, \dots, m_u, \dots, m_N\rangle = m_u |m_1, \dots, m_u, \dots, m_N\rangle$$

These states span the Hilbert space and are used to construct symmetry-related basis states. Use  $a_u = s_u - m_u$  for computation (integer).

Symmetries of the Heisenberg model without anisotropy

$$\left[ \tilde{H}, \tilde{S}^2 \right] = 0 \quad , \quad \left[ \tilde{H}, \tilde{S}_z \right] = 0$$

Additional (point group) symmetries are possible, e.g. shifts on a ring molecule.

## Decomposition into mutually orthogonal subspaces

If  $\left[ \underline{H}, \underline{S}_z \right] = 0$ , the Hilbert space  $\mathcal{H}$  can be decomposed into mutually orthogonal subspaces  $\mathcal{H}(M)$  ( $M$  is the quantum number belonging to  $\underline{S}_z$ )

$$\left[ \underline{H}, \underline{S}_z \right] = 0 \quad : \quad \mathcal{H} = \bigoplus_{M=-S_{\max}}^{+S_{\max}} \mathcal{H}(M), \quad S_{\max} = Ns$$

$\mathcal{H}(M)$  contains all states  $|m_1, \dots, m_u, \dots, m_N\rangle$  with  $\sum_i m_i = M$ .

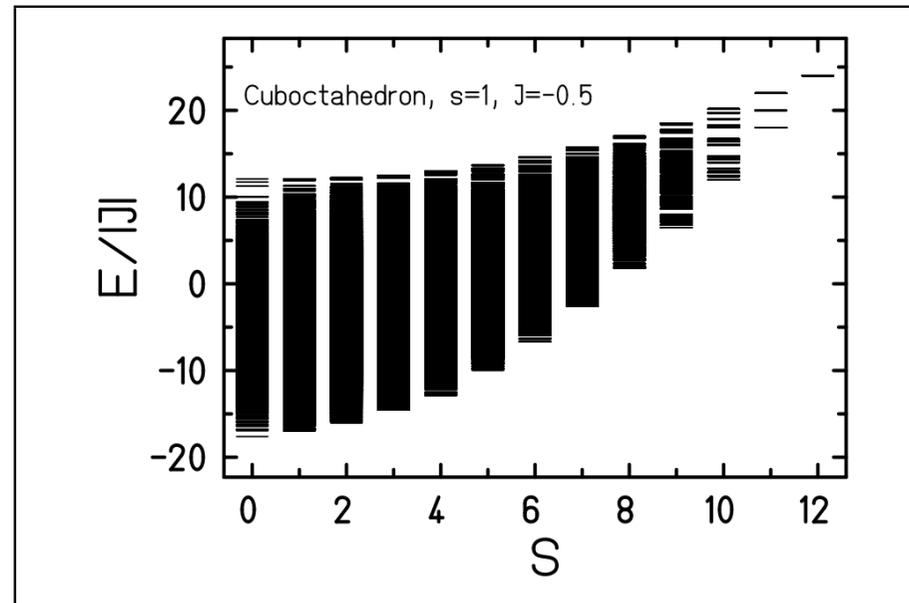
The Hamiltonian is diagonalized in all subspaces separately. The dimension of the largest subspace determines whether a Hamiltonian can be diagonalized completely. If further symmetries apply this dimension will be further reduced.

For practical purposes  $\vec{s}_i \cdot \vec{s}_j = s_i^z s_j^z + \frac{1}{2} \left[ s_i^+ s_j^- + s_i^- s_j^+ \right]$ .

## Example: spin ring with $N = 6, s = 1/2$

- Total dimension of  $\mathcal{H}$ :  $Dim(\mathcal{H}) = (2 \times 1/2 + 1)^6 = 64$ ;
- $M = 3$ :  $|\Omega\rangle = |+++++\rangle$ ;  $Dim(\mathcal{H}(M)) = 1$ ;
- $M = 2$ :  $| - + + + + \rangle$  and cyclic shifts;  $Dim(\mathcal{H}(M)) = 6$ ;
- $M = 1$ :  $| - - + + + \rangle, | - + - + + \rangle, | - + + - + \rangle$  and cyclic shifts;  
 $Dim(\mathcal{H}(M)) = 15$ ;
- $M = 0$ :  $| - - - + + \rangle, | - - + - + \rangle, | - + - - + \rangle, | - + - + - \rangle$   
and cyclic shifts;  $Dim(\mathcal{H}(M)) = 20$ ;
- Dimensional check:  $64 = 1 + 6 + 15 + 20 + 15 + 6 + 1 \checkmark$
- Inclusion of translational symmetry leads to orthogonal subspaces  $\mathcal{H}(M, k)$  with  $k = 0, \dots, 5$ . Then the largest dimension is 4.

# Exact diagonalization



- Numerically exact diagonalization feasible up to RAM size;
- Example: 10,000x10,000 complex\*16, 1.6 GB RAM needed;
- Not much we can do at this point, wait for more RAM 😊

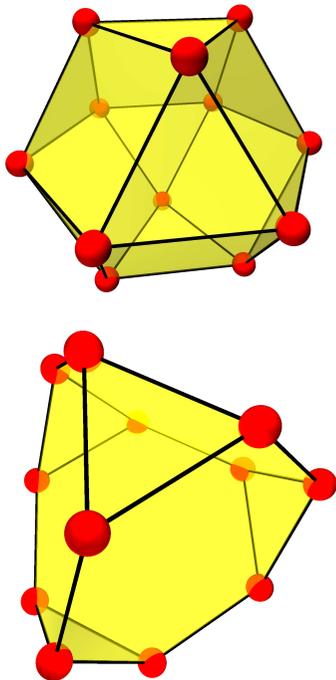
# Isotropic case

## Complete diagonalization: SU(2) & point group symmetry

Quantum chemists need to be much smarter since they have smaller computers!

- (1) D. Gatteschi and L. Pardi, *Gazz. Chim. Ital.* **123**, 231 (1993).
- (2) J. J. Borrás-Almenar, J. M. Clemente-Juan, E. Coronado, and B. S. Tsukerblat, *Inorg. Chem.* **38**, 6081 (1999).
- (3) B. S. Tsukerblat, *Group theory in chemistry and spectroscopy: a simple guide to advanced usage*, 2nd ed. (Dover Publications, Mineola, New York, 2006).

# Irreducible Tensor Operator approach



## Spin rotational symmetry SU(2):

- $\underline{H} = -2 \sum_{i < j} J_{ij} \underline{\tilde{S}}_i \cdot \underline{\tilde{S}}_j + g\mu_B \underline{\tilde{S}} \cdot \underline{\tilde{B}} ;$

- Physicists employ:  $[\underline{H}, \underline{S}_z] = 0;$

- Chemists employ:  $[\underline{H}, \underline{S}^2] = 0, [\underline{H}, \underline{S}_z] = 0;$

Irreducible Tensor Operator (ITO) approach;  
Free program MAGPACK (2) available.

(1) D. Gatteschi and L. Pardi, *Gazz. Chim. Ital.* **123**, 231 (1993).

(2) J. J. Borrás-Almenar, J. M. Clemente-Juan, E. Coronado, and B. S. Tsukerblat, *Inorg. Chem.* **38**, 6081 (1999).

(3) B. S. Tsukerblat, *Group theory in chemistry and spectroscopy: a simple guide to advanced usage*, 2nd ed. (Dover Publications, Mineola, New York, 2006).

# Idea of ITO

$$\begin{aligned}
 \underline{H}_{\text{Heisenberg}} &= -2 \sum_{i < j} J_{ij} \vec{s}_i \cdot \vec{s}_j \\
 &= 2\sqrt{3} \sum_{i < j} J_{ij} \underline{T}^{(0)}(\{k_i\}, \{\bar{k}_i\} | k_i = k_j = 1)
 \end{aligned}$$

## Irreducible Tensor Operator approach

- Express spin operators and functions thereof as ITOs;
- Use vector coupling basis  $|\alpha S M\rangle$  and recursive recoupling.

(1) Gatteschi, Tsukerblat, Coronado, Waldmann, ...  
 (2) R. Schnalle, Ph.D. thesis, Osnabrück University (2009)

# Point Group Symmetry

$$|\alpha' S M \Gamma\rangle = \mathcal{P}^{(\Gamma)} |\alpha S M\rangle = \left( \frac{l_{\Gamma}}{h} \sum_R \left( \chi^{(\Gamma)}(R) \right)^* \mathcal{G}(R) \right) |\alpha S M\rangle$$

## Method:

- Projection onto irreducible representations  $\Gamma$  of the point group (1,2);
- No free program, things are a bit complicated (3,4).

(1) M. Tinkham, *Group Theory and Quantum Mechanics*, Dover.

(2) D. Gatteschi and L. Pardi, *Gazz. Chim. Ital.* **123**, 231 (1993).

(3) O. Waldmann, *Phys. Rev. B* **61**, 6138 (2000).

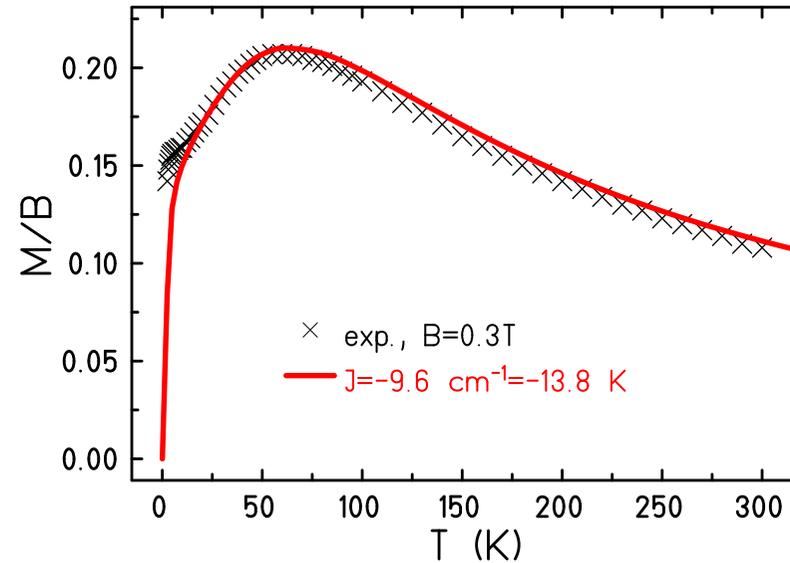
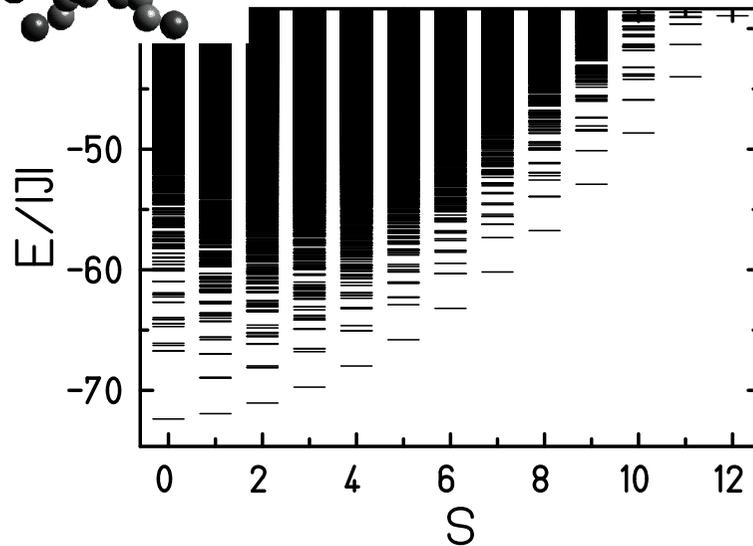
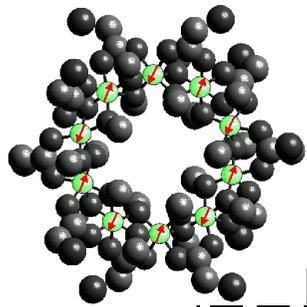
(4) R. Schnalle and J. Schnack, *Int. Rev. Phys. Chem.* **29**, 403-452 (2010)  $\Leftarrow$  contains EVERYTHING.

# Decomposition of Hamiltonian Matrix

$M_1$ $\Gamma_1$	0	0	0
0	$M_1$ $\Gamma_2$	0	0
0	0	$M_2$ $\Gamma_1$	0
0	0	0	$M_2$ $\Gamma_2$

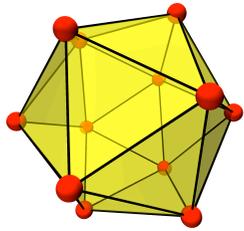
Block diagonal due to symmetry-adapted basis.  
Only separate blocks need to be diagonalized.

# Example: Fe<sub>10</sub>

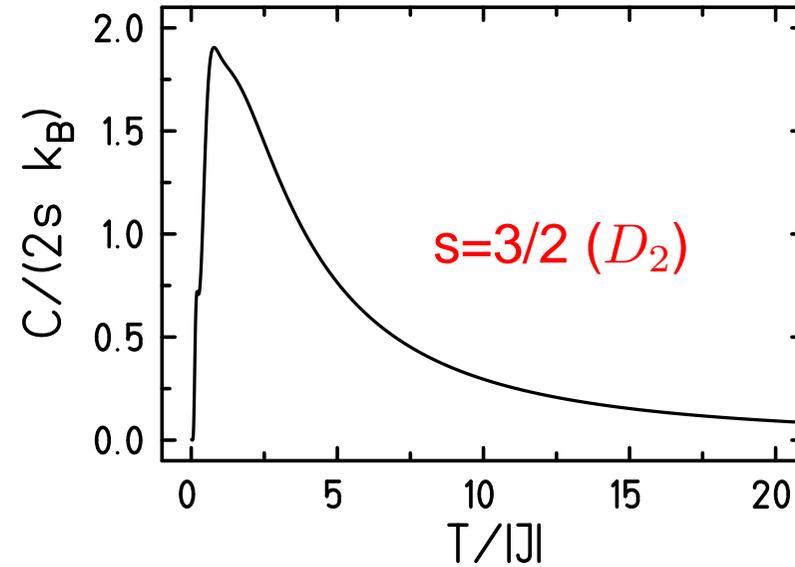
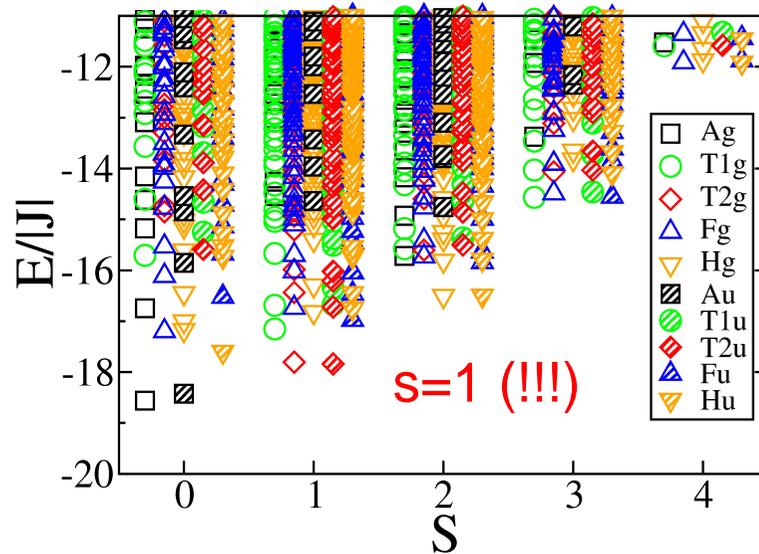


Spin ring,  $N = 10$ ,  $s = 5/2$ , Hilbert space dimension 60,466,176; symmetry  $D_2$  (1).

- (1) R. Schnalle and J. Schnack, *Int. Rev. Phys. Chem.* **29**, 403-452 (2010).
- (2) C. Delfs *et al.*, *Inorg. Chem.* **32**, 3099 (1993).



# Example: Icosahedron



Icosahedron,  $s = 3/2$ , Hilbert space dimension 16,777,216; symmetry  $I_h$ ; Evaluation of recoupling coefficients for  $s = 3/2$  in  $I_h$  **practically impossible** (1).

(1) R. Schnalle and J. Schnack, Int. Rev. Phys. Chem. **29**, 403-452 (2010).

# Anisotropic Hamiltonians

# Model Hamiltonian

$$\tilde{H} = \sum_{i,j} \vec{\tilde{s}}(i) \cdot \mathbf{J}_{ij} \cdot \vec{\tilde{s}}(j) + \sum_{i,j} \vec{D}_{ij} \cdot [\vec{\tilde{s}}(i) \times \vec{\tilde{s}}(j)] + \mu_B \vec{B} \sum_i^N \mathbf{g}_i \vec{\tilde{s}}(i)$$

Exchange/Anisotropy
Dzyaloshinskii-Moriya
Zeeman

1. Addresses many anisotropic contributions (up to bilinear/quadratic order)
2. Other terms, e.g. biquadratic ?
3. Works with spin degrees of freedom
4. Sufficiently general? Strong  $l_s$ -coupling? Replace  $\vec{\tilde{s}}(i)$  by  $\vec{j}(i)$ ?
5. Many open parameters – accurate and detailed magnetic observables needed: low- $T$  magnetization, EPR, INS. Forget  $\chi T$ !

# Anisotropic magnetic molecules – Theory

$$\tilde{H} = \tilde{H}(\vec{B})$$

- $[\tilde{H}, \tilde{S}^2] \neq 0, [\tilde{H}, \tilde{S}_z] \neq 0; \Rightarrow \Rightarrow \Rightarrow$  **MAGPACK does NOT work.**
- **You have to diagonalize  $\tilde{H}(\vec{B})$  for every field (direction and strength)!**  
 $\Rightarrow$  **Orientational average for powder samples.**
- Point group symmetries reduce to inversion (at most) in the presence of a magnetic field.
- **Easy:  $\dim(\mathcal{H}) < 30,000$ ; possible:  $30,000 < \dim(\mathcal{H}) < 140,000$**

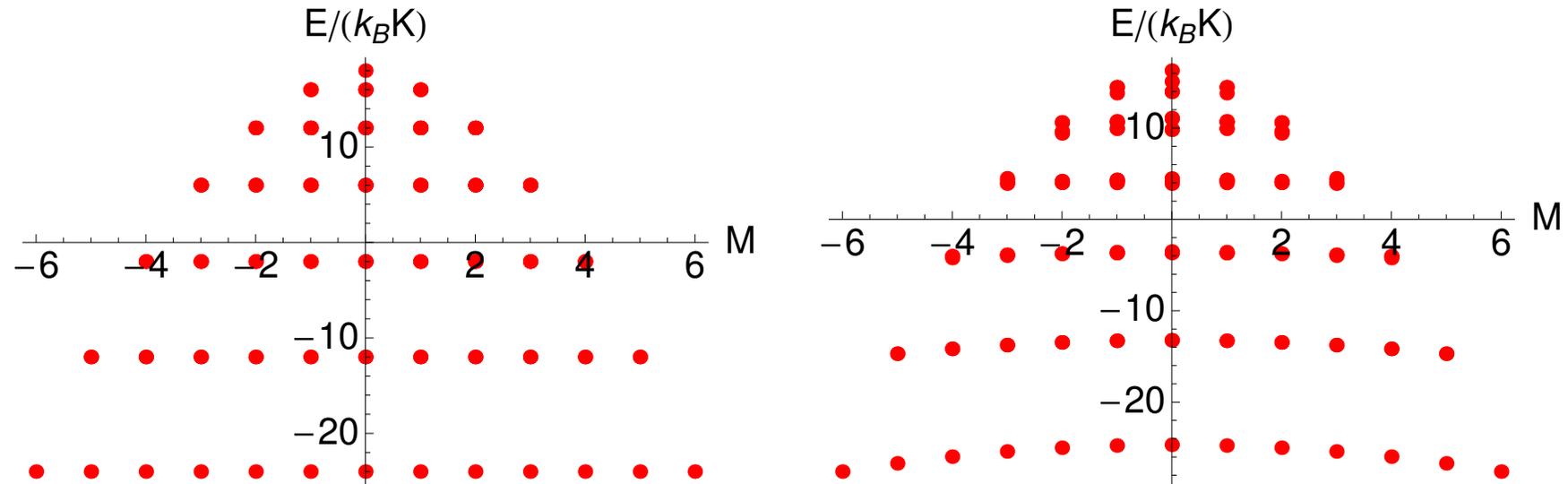
T. Glaser *et al.* et J. Schnack, Inorg. Chem. **48**, 607 (2009).

# Anisotropic magnetic molecules – simpler Hamiltonian

$$\underline{H}(\vec{B}) = -2 \sum_{i < j} J_{ij} \vec{\underline{S}}(i) \cdot \vec{\underline{S}}(j) + \sum_i d_i (\vec{e}_i \cdot \vec{\underline{S}}(i))^2 + \mu_B \vec{B} \cdot \sum_i^N g_i \vec{\underline{S}}(i)$$

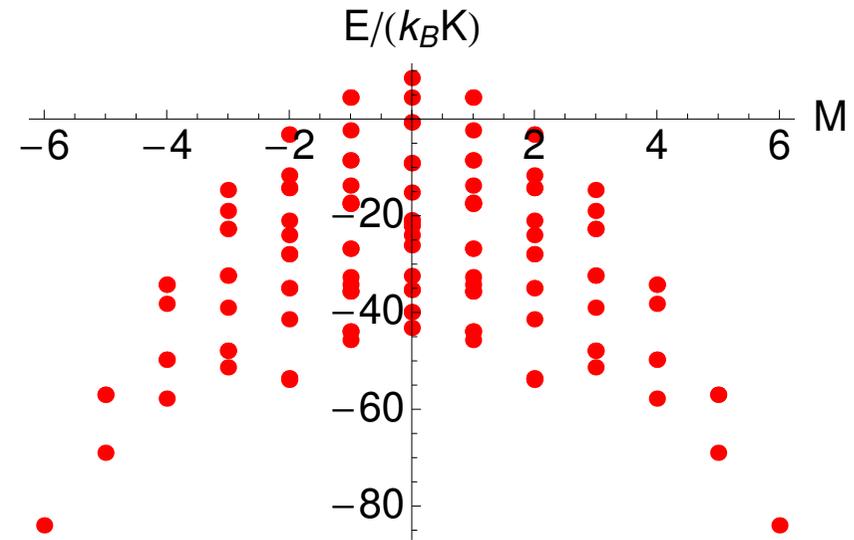
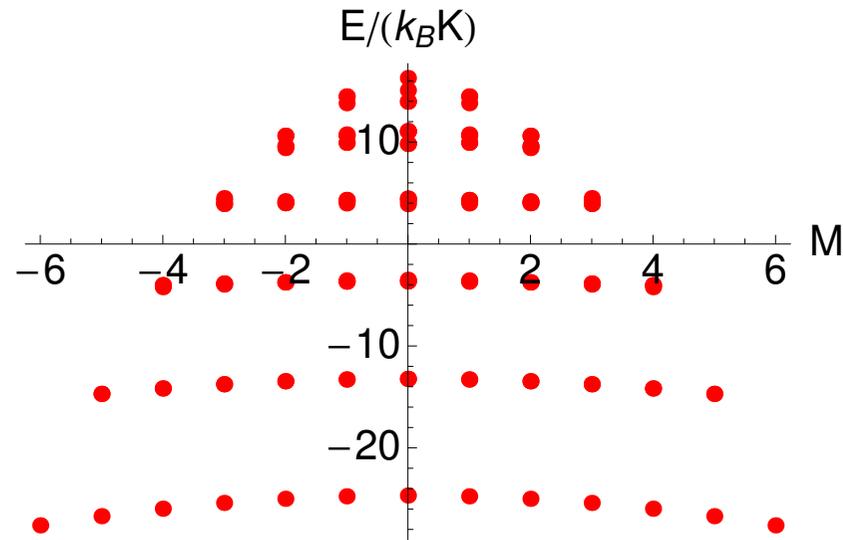
- $\vec{e}_i$  direction of major anisotropy axis at site  $i$ ;
- $d_i$  strength of anisotropy along major axis at site  $i$ ;
- Use of eigenvectors to evaluate observables.
- Alternative: use difference quotient.

# Strong exchange limit



- Heisenberg, i.e. exchange, term dominant; uniaxial single-ion anisotropy in this example;
- $\Rightarrow$  zero-field split multiplets.

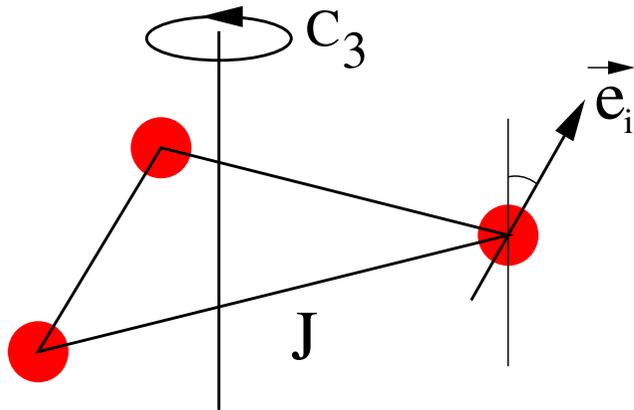
# Weak exchange limit



- (Single ion) anisotropy term dominant;
- $\Rightarrow$  no multiplets at all; nesting; mixing.

# Systematic study of a trimer

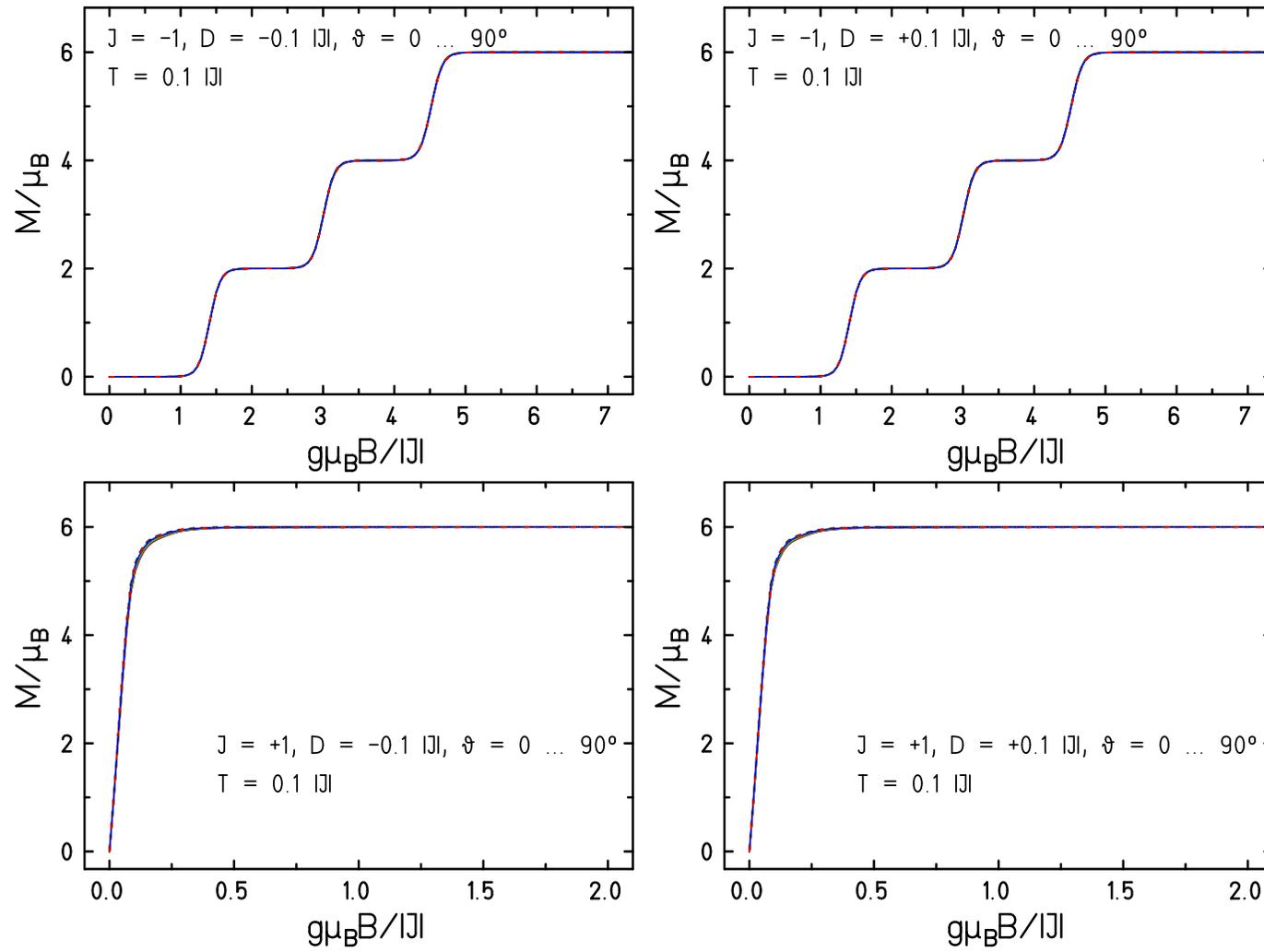
## Anisotropic trimer



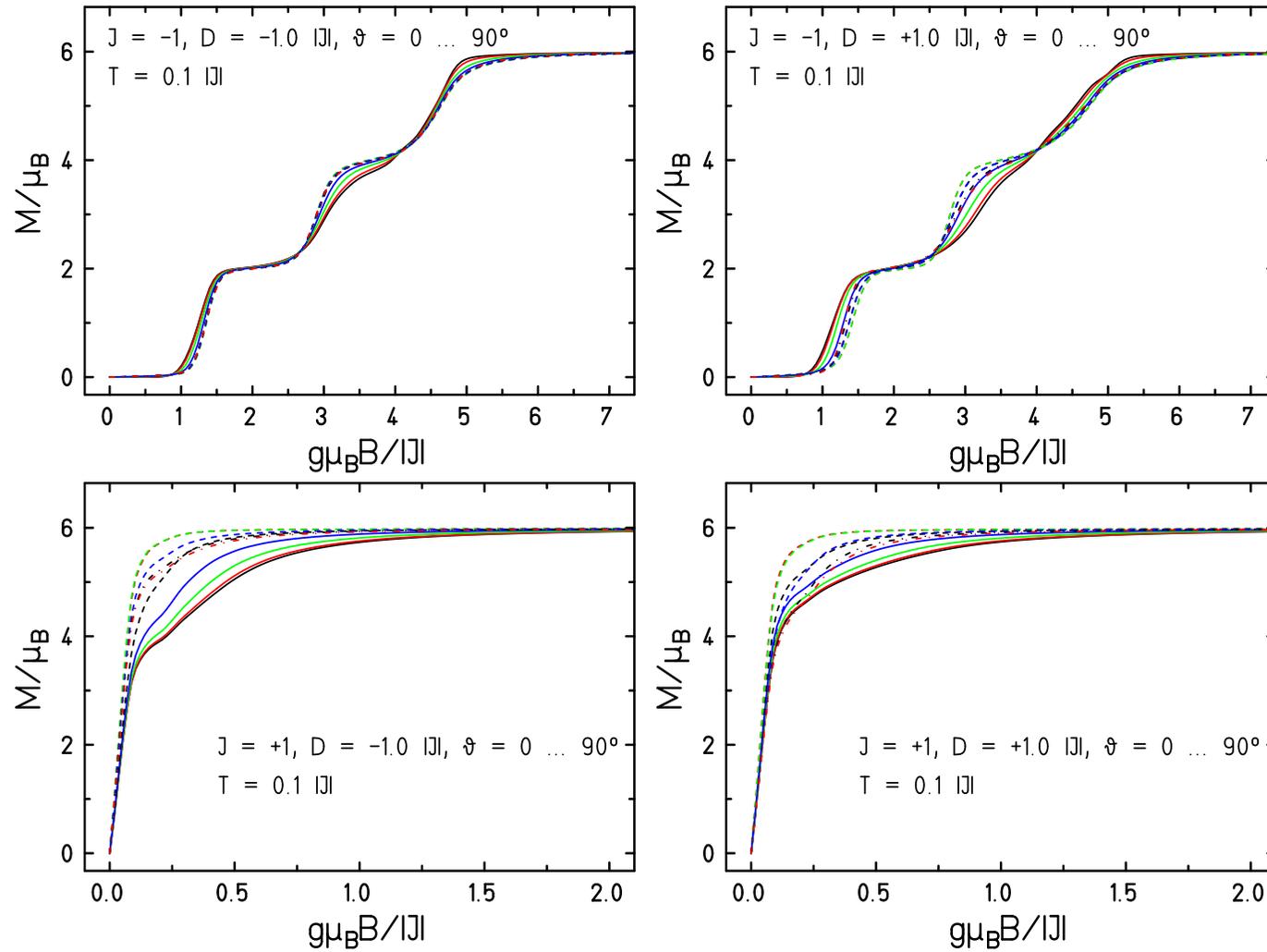
- Ions with  $s = 1$ ;  $C_3$  symmetry;
- 1 exchange interaction;
- Local anisotropy axis with azimuthal angle  $\vartheta$ .
- Powder average.

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

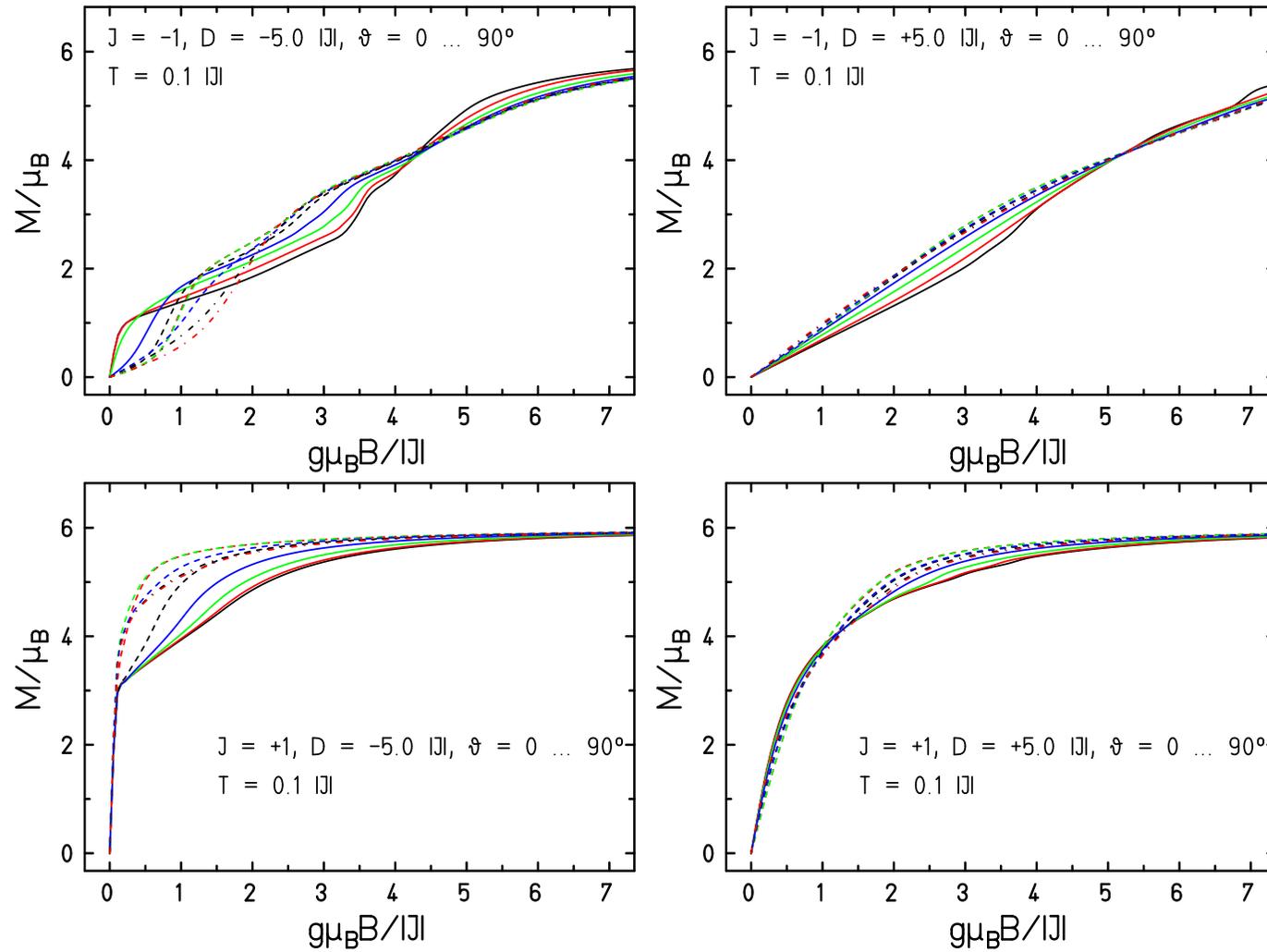
# Strong coupling



# Intermediate coupling



# Weak coupling



# Single-ion anisotropy – examples

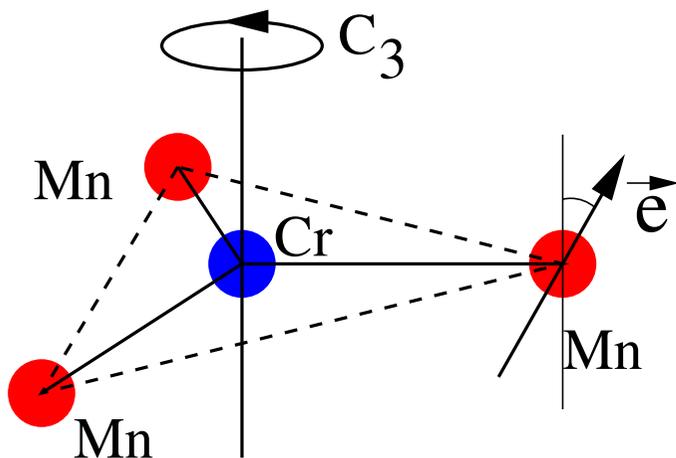
# Anisotropic magnetic molecules – simpler Hamiltonian

$$\tilde{H}(\vec{B}) = -2 \sum_{i < j} J_{ij} \vec{\tilde{S}}(i) \cdot \vec{\tilde{S}}(j) + \sum_i d_i (\vec{e}_i \cdot \vec{\tilde{S}}(i))^2 + \mu_B \vec{B} \cdot \sum_i^N g_i \vec{\tilde{S}}(i)$$

- $\vec{e}_i$  direction of major anisotropy axis at site  $i$ ;
- $d_i$  strength of anisotropy along major axis at site  $i$ ;
- Use of eigenvectors to evaluate observables.
- Alternative: use difference quotient.

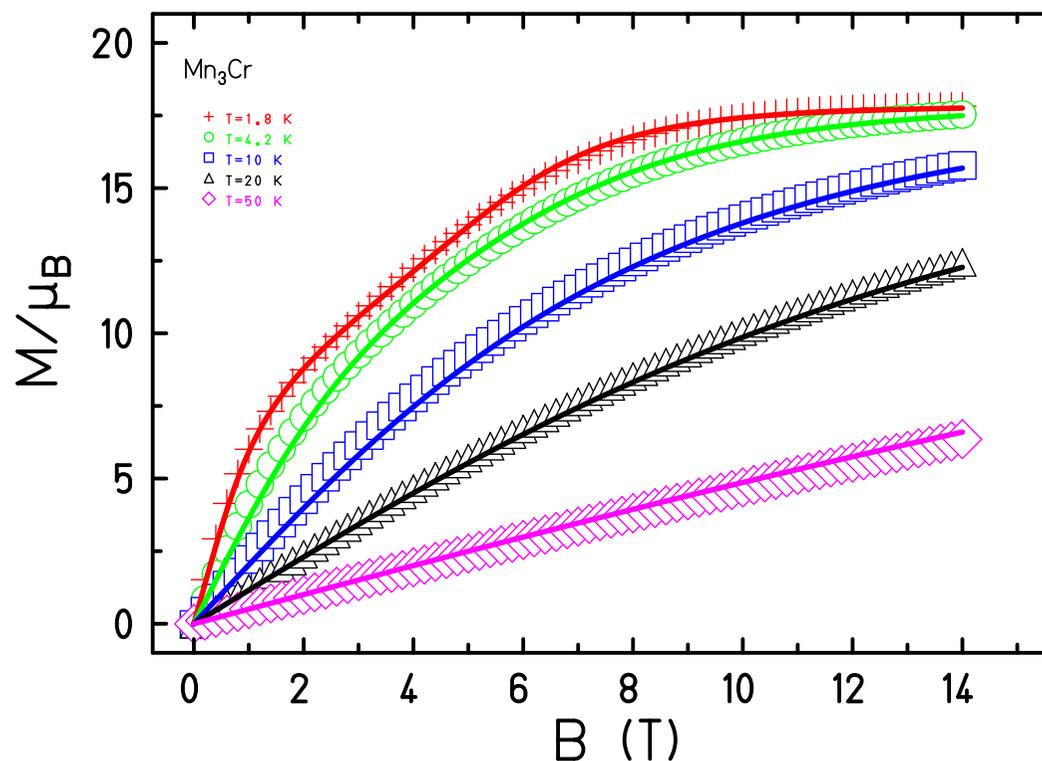
# Anisotropic magnetic molecules – Mn<sub>3</sub>Cr

## What can be achieved? Mn<sub>3</sub>Cr:



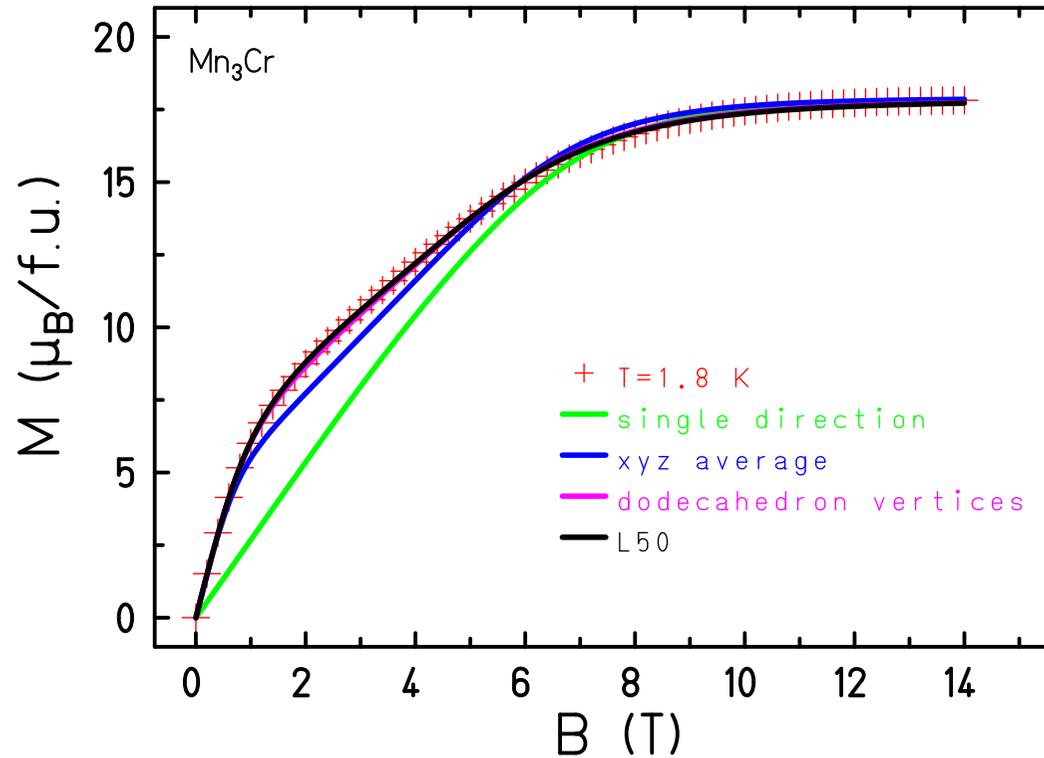
- Two couplings:  $J_1$  to central Cr,  $J_2$  between Mn; Mn:  $s=5/2$ ,  $g=2.0$ ; Cr:  $s=3/2$ ,  $g=1.95$
- Model Mn anisotropy by local axis  $\vec{e}(\vartheta, \phi)$ . Due to  $C_3$  symmetry  $\vartheta_{\text{Mn1}} = \vartheta_{\text{Mn2}} = \vartheta_{\text{Mn3}}$ . Only relative  $\phi = 120^\circ$  determined.
- Model Cr anisotropy by local axis  $\vec{e}(\vartheta, \phi)$ . Due to  $C_3$  symmetry  $\vartheta_{\text{Cr}} = 0$ ,  $\phi_{\text{Cr}} = 0$ .
- Result:  $J_1 = -0.29 \text{ cm}^{-1}$ ,  $J_2 = -0.08 \text{ cm}^{-1}$ ,  $d_{\text{Mn}} = -1.21 \text{ cm}^{-1}$ ,  $\vartheta_{\text{Mn}} = 22^\circ$ ,  $d_{\text{Cr}} = +0.17 \text{ cm}^{-1}$ .
- ab initio calculations needed.

# Anisotropic magnetic molecules – Mn<sub>3</sub>Cr



Manuel Prinz, Karsten Kuepper, Christian Taubitz, Michael Raekers, Sumit Khanra, Biplab Biswas, Thomas Weyhermüller, Marc Uhlarz, Joachim Wosnitza, Jürgen Schnack, Andrei V. Postnikov, Christian Schröder, Simon J. George, Manfred Neumann, and Phalguni Chaudhuri, *Inorg. Chem.* **49** (2010) 2093

# Mn<sub>3</sub>Cr III – Angular averaging



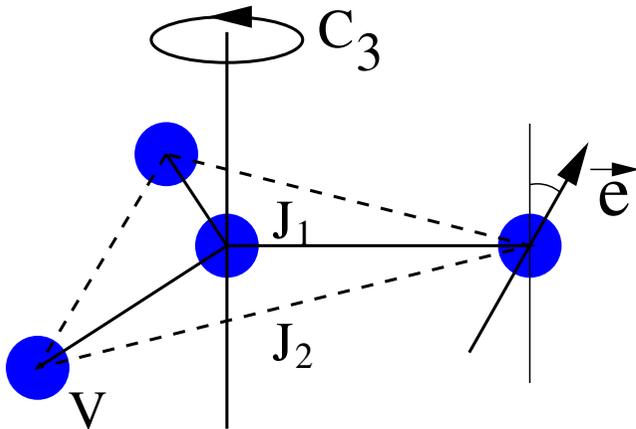
For a good fit you need several directions, at least 10.

V. I. Lebedev and D. N. Laikov, Dokl. Akad. Nauk **366**, 741 (1999); and link to program on [www.molmag.de](http://www.molmag.de)

# V<sub>4</sub> I

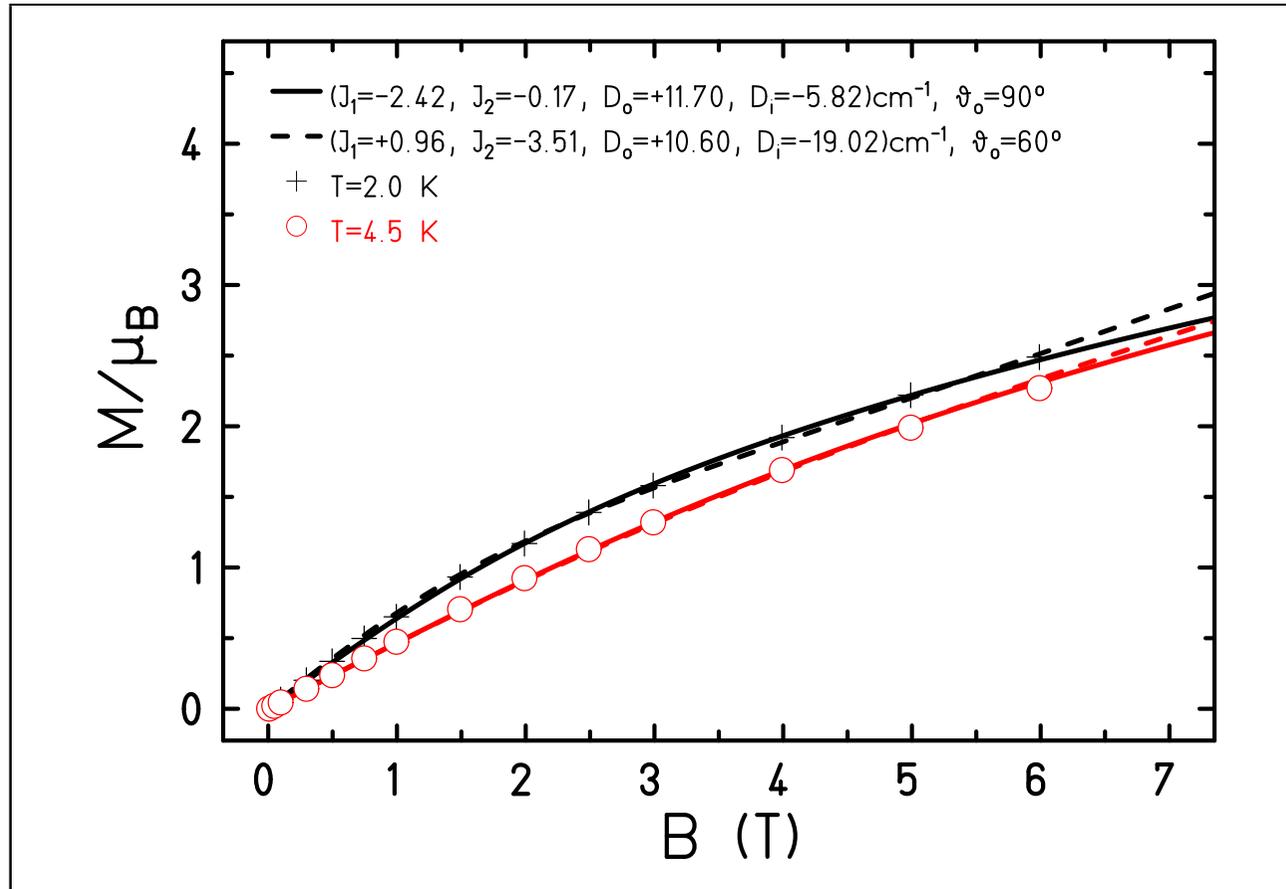


- 4 V<sub>4</sub><sup>III</sup> ions with  $s = 1$ ; approximate  $C_3$  symmetry;
- 2 exchange interactions;
- Central V: axial anisotropy;
- Outer Vs: local anisotropy axis with azimuthal angle  $\vartheta$ .
- Powder average.



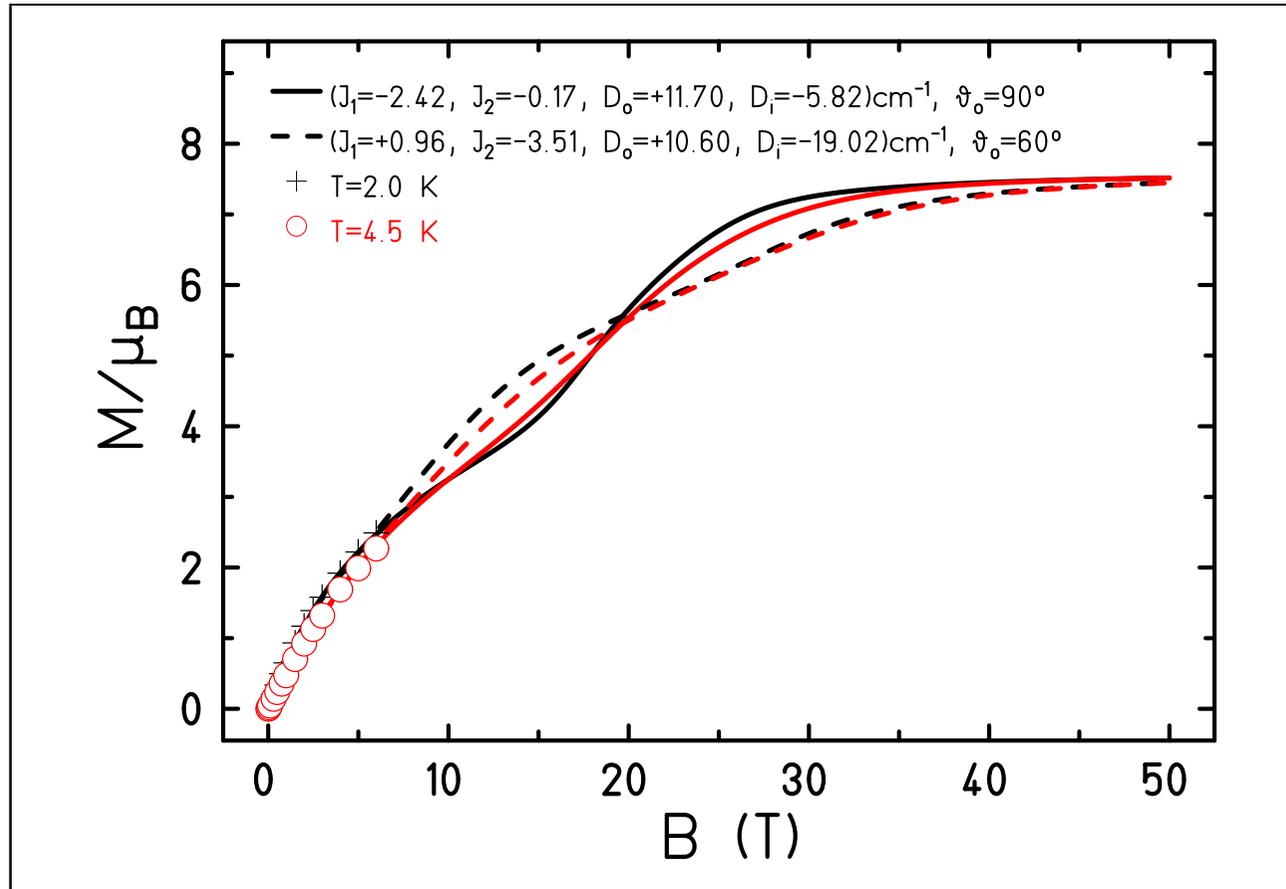
Ian S. Tidmarsh, Luke J. Batchelor, Emma Scales, Rebecca H. Laye, Lorenzo Sorace, Andrea Caneschi, Jürgen Schnack and Eric J.L. McInnes, Dalton Trans. (2009) 9402-9409

# V<sub>4</sub> II



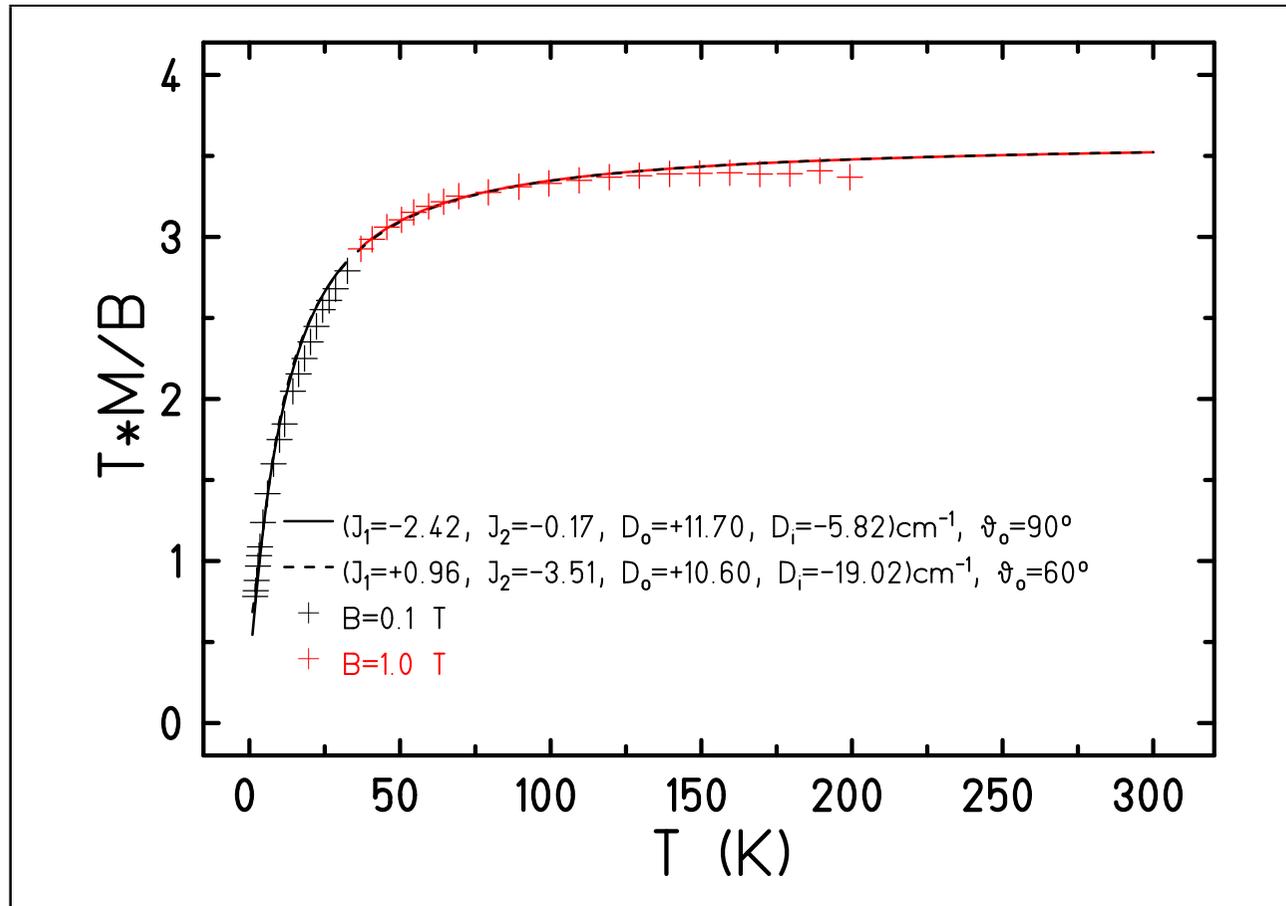
Two equally good parameter sets.

# V<sub>4</sub> III



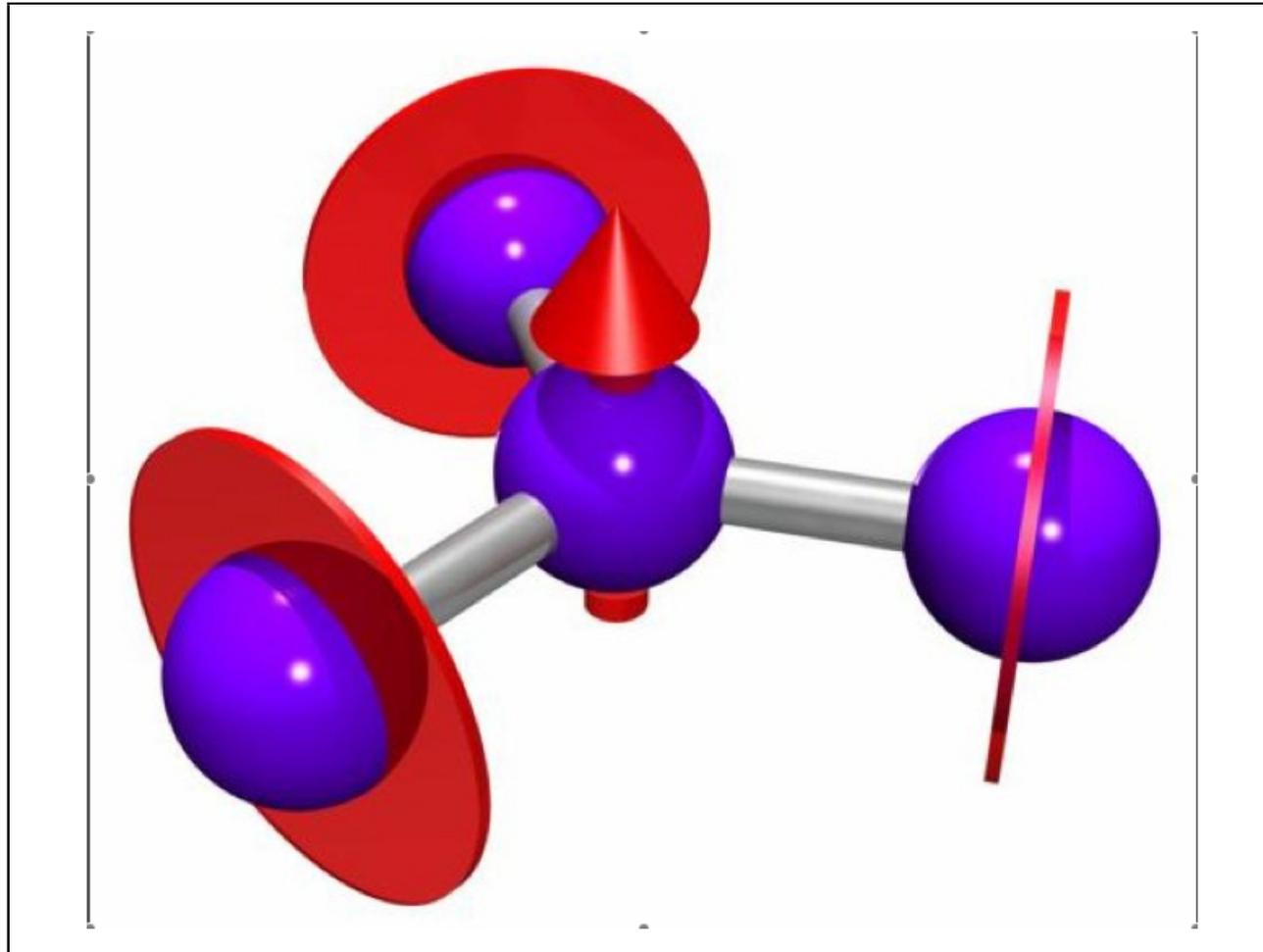
High fields could distinguish.

# V<sub>4</sub> IV



Accuracy of measurement limits modeling.

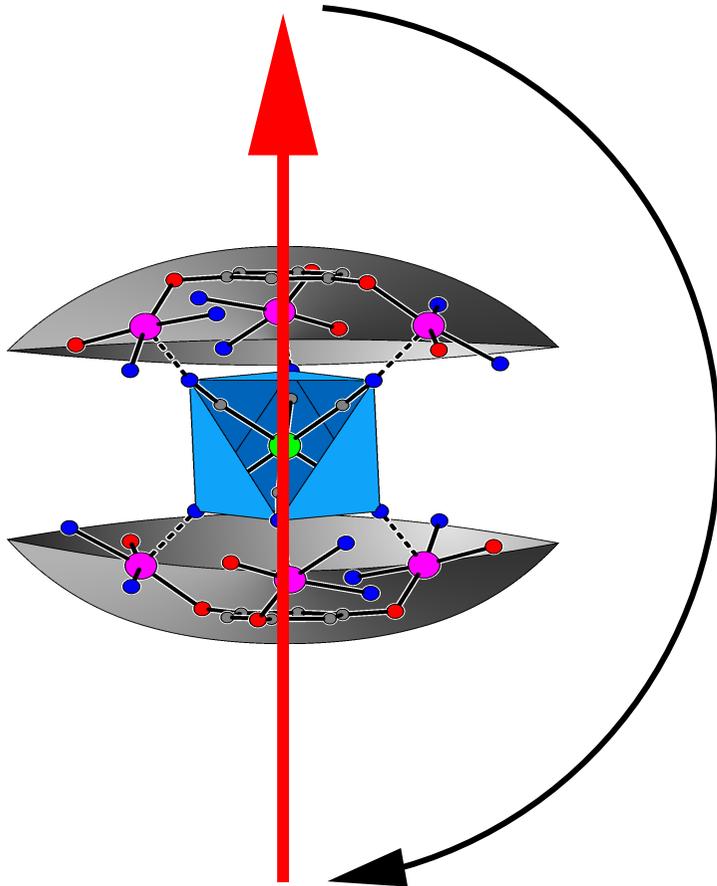
# $V_4$ – Anisotropy tensors



Cartoon of anisotropy tensors.

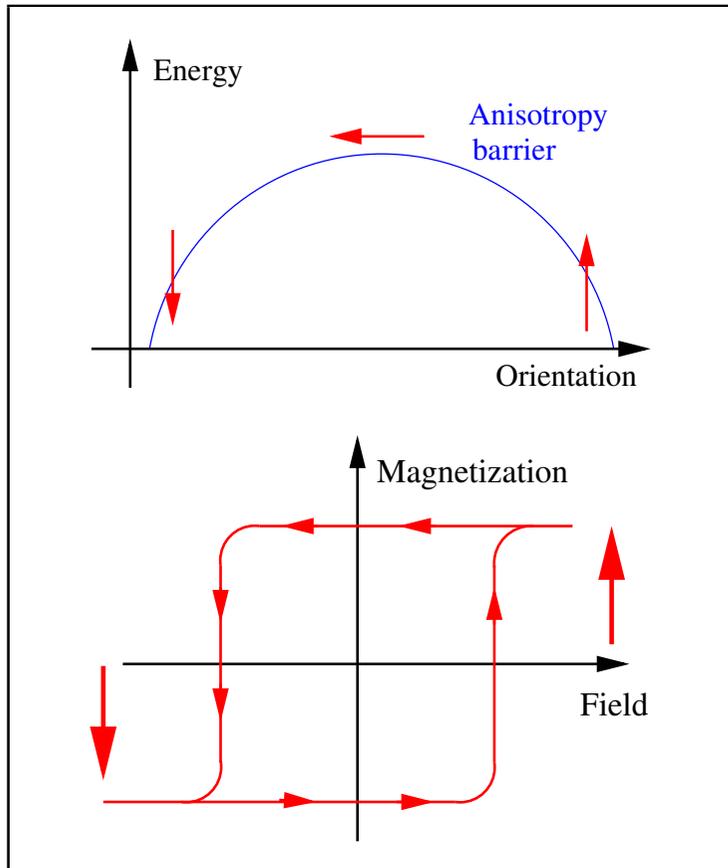
# Thorsten Glaser's molecules

# Single Molecule Magnets I



- Magnetic Molecules may possess a large ground state spin, e.g.  $S = 10$  for Mn<sub>12</sub> or Fe<sub>8</sub>;
- Ground state spin can be stabilized by anisotropy (easy axis).

# Single Molecule Magnets II



- Single Molecule Magnets (SMM): large ground state moment; anisotropy barrier dominates at low  $T$ .

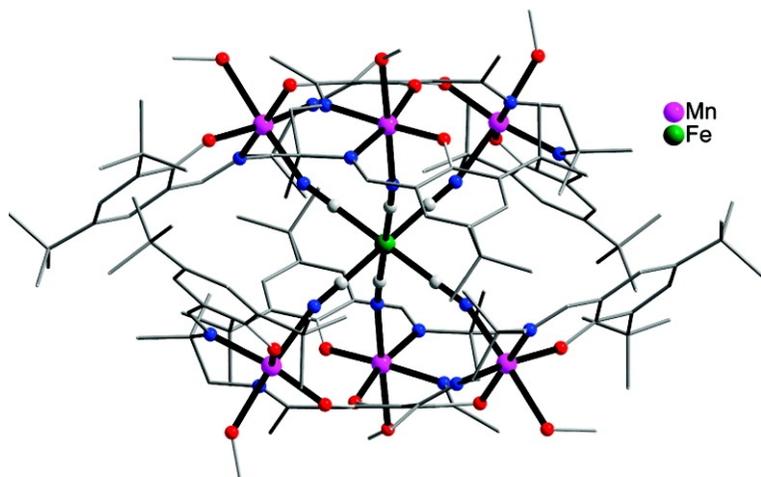
$$\tilde{H} \approx DS_z^2$$

- Metastable magnetization and hysteresis;
- But also magnetization tunneling due to non-commuting terms, e.g.  $E, B_x, B_y$ .

$$\tilde{H} \approx DS_z^2 + E(S_x^2 - S_y^2)$$

# Thorsten Glaser's molecules

## Rational design of strict $C_3$ symmetry:

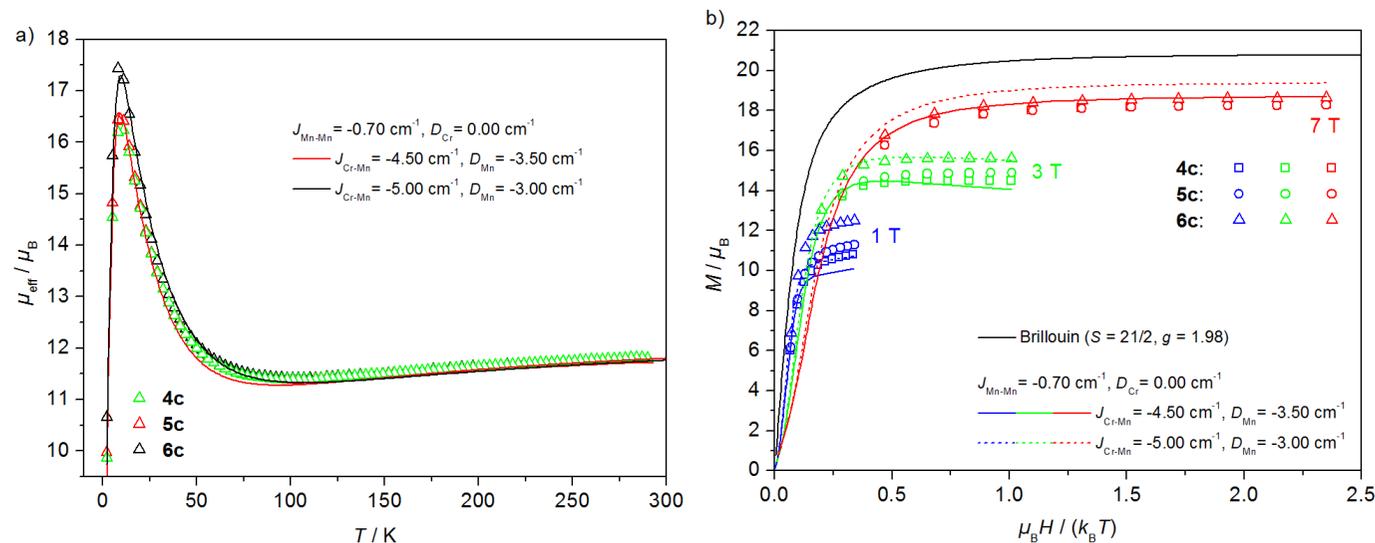
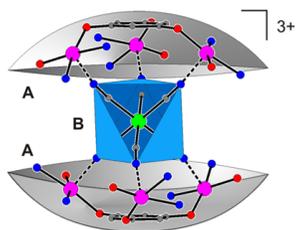


- Idea of Thorsten Glaser (Bielefeld):  $C_3$  symmetric alignment of local easy axes (easy axis  $\equiv$  Jahn-Teller axis);
- Various ions could be used so far, e.g.  $Mn_6Cr$  (1),  $Mn_6Fe$  (2), ...
- Advantage: no  $E$ -terms, i.e. no (less) tunneling;
- Problem: exchange interaction sometimes antiferromagnetic.

T. Glaser *et al.*, *Angew. Chem.-Int. Edit.* **45**, 6033 (2006).

T. Glaser *et al.*, *Inorg. Chem.* **48**, 607 (2009).

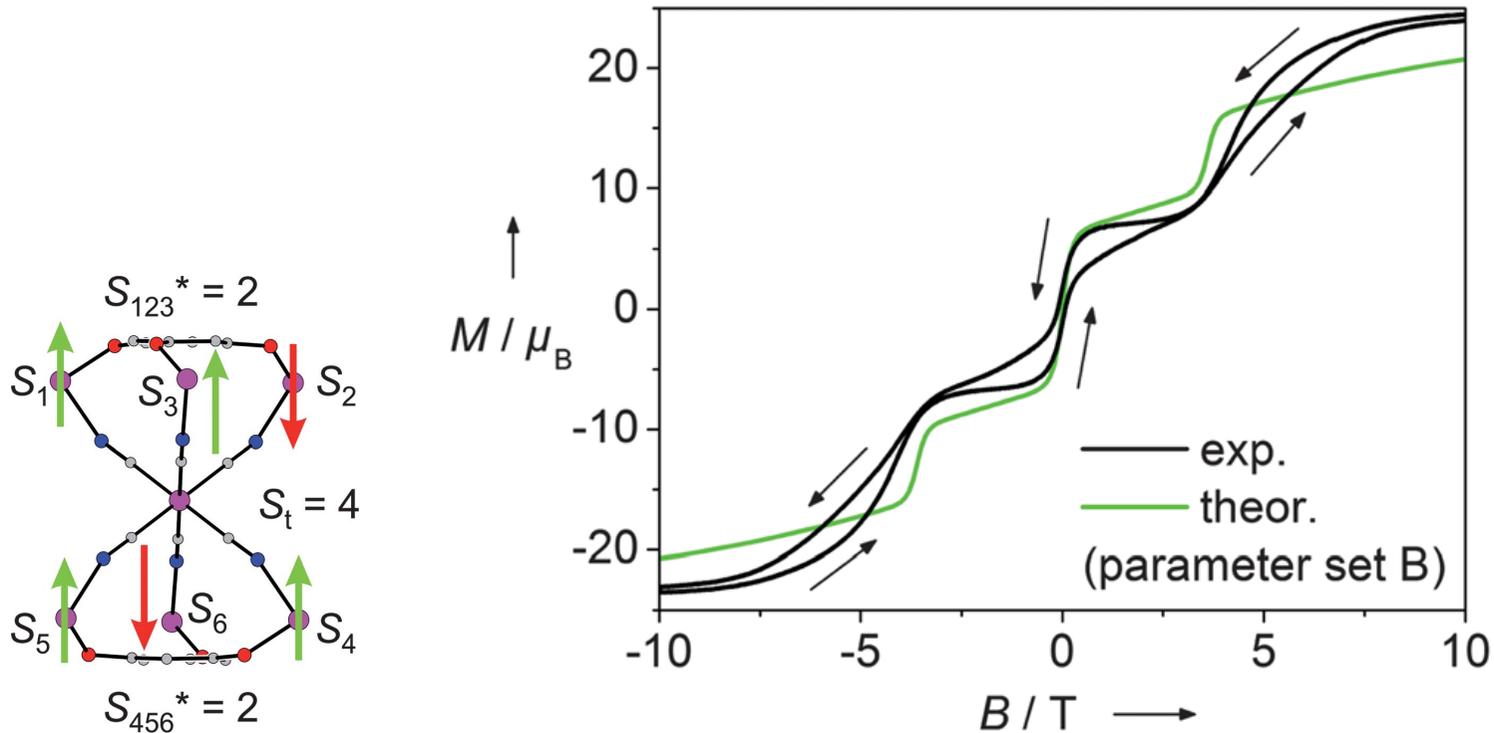
# Thorsten Glaser's molecules – Mn<sub>6</sub>Cr



- Dimension of Hilbert space: 62,500; inversion symmetry applied.
- Ferrimagnetic alignment due to antiferromagnetic exchange.

Veronika Hoeke, Maik Heidemeier, Erich Krickemeyer, Anja Stammner, Hartmut Bögge, Jürgen Schnack, Andrei Postnikov, Thorsten Glaser, *Inorg. Chem.* **51** (2012) 10929-10954

# Thorsten Glaser's molecules – Mn<sub>6</sub>Mn



- Central Mn<sup>III</sup> has  $s = 0$ !!!
- Hysteresis cannot be modeled by static observables.

Veronika Hoeke, Klaus Gieb, Paul Müller, Liviu Ungur, Liviu F. Chibotaru, Maik Heidemeier, Erich Krickemeyer, Anja Stammler, Hartmut Bögge, Christian Schröder, Jürgen Schnack, Thorsten Glaser, Chem. Sci. **3** (2012) 2868

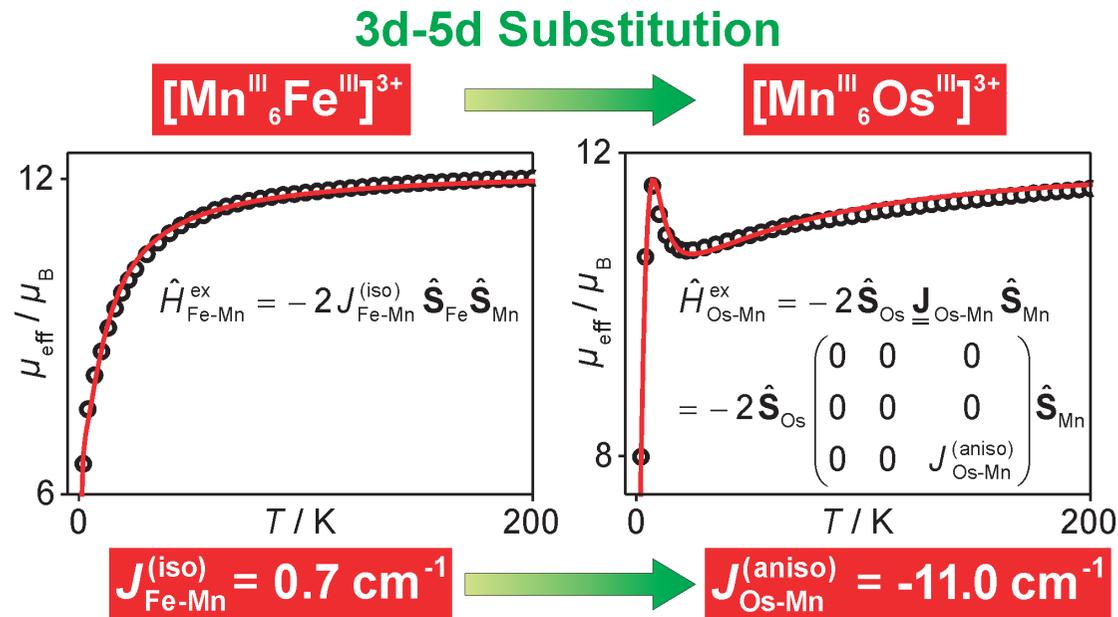
# Anisotropic exchange

# Anisotropic exchange

$$\begin{aligned} \underline{H} &= \sum_{i,j} \underline{\vec{s}}(i) \cdot \mathbf{J}_{ij} \cdot \underline{\vec{s}}(j) \\ &= -2 \sum_{i < j} \underline{\vec{s}}(i) \cdot \left( J_{ij}^{11} \vec{e}_{ij}^1 \otimes \vec{e}_{ij}^1 + J_{ij}^{22} \vec{e}_{ij}^2 \otimes \vec{e}_{ij}^2 + J_{ij}^{33} \vec{e}_{ij}^3 \otimes \vec{e}_{ij}^3 \right) \cdot \underline{\vec{s}}(j) \end{aligned}$$

1. Each bond could have a different exchange tensor.
2.  $\mathbf{J}_{ij}$  can be represented in its eigenbasis.
3. Ions with anisotropic exchange:  $\text{Os}^{\text{III}}$ , .....

# Anisotropic exchange – Mn<sub>6</sub>Os



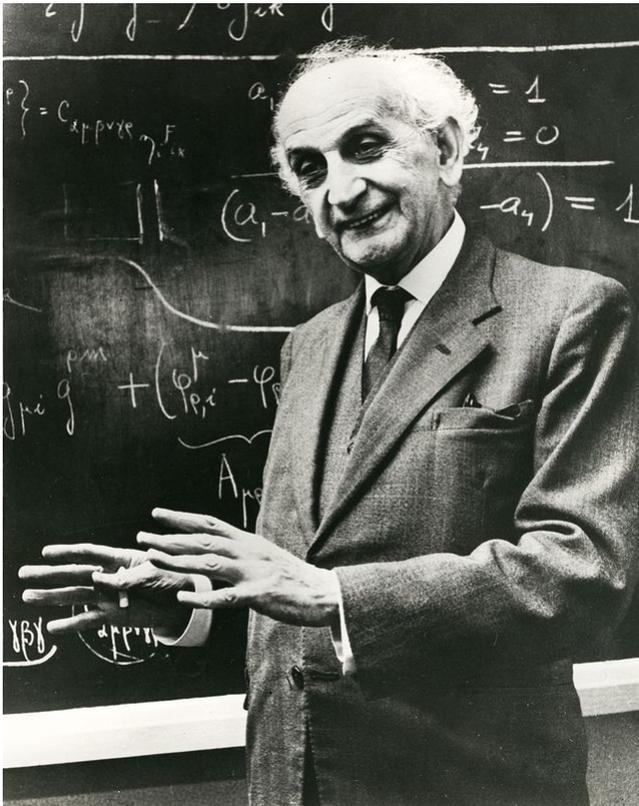
**Central Os<sup>III</sup> has pseudo spin  $s = 1/2$ !** For sake of simplicity exchange Ising like.

Veronika Hoeke, Anja Stammler, Hartmut Bögge, Jürgen Schnack, Thorsten Glaser, submitted.

# Finite-temperature Lanczos Method

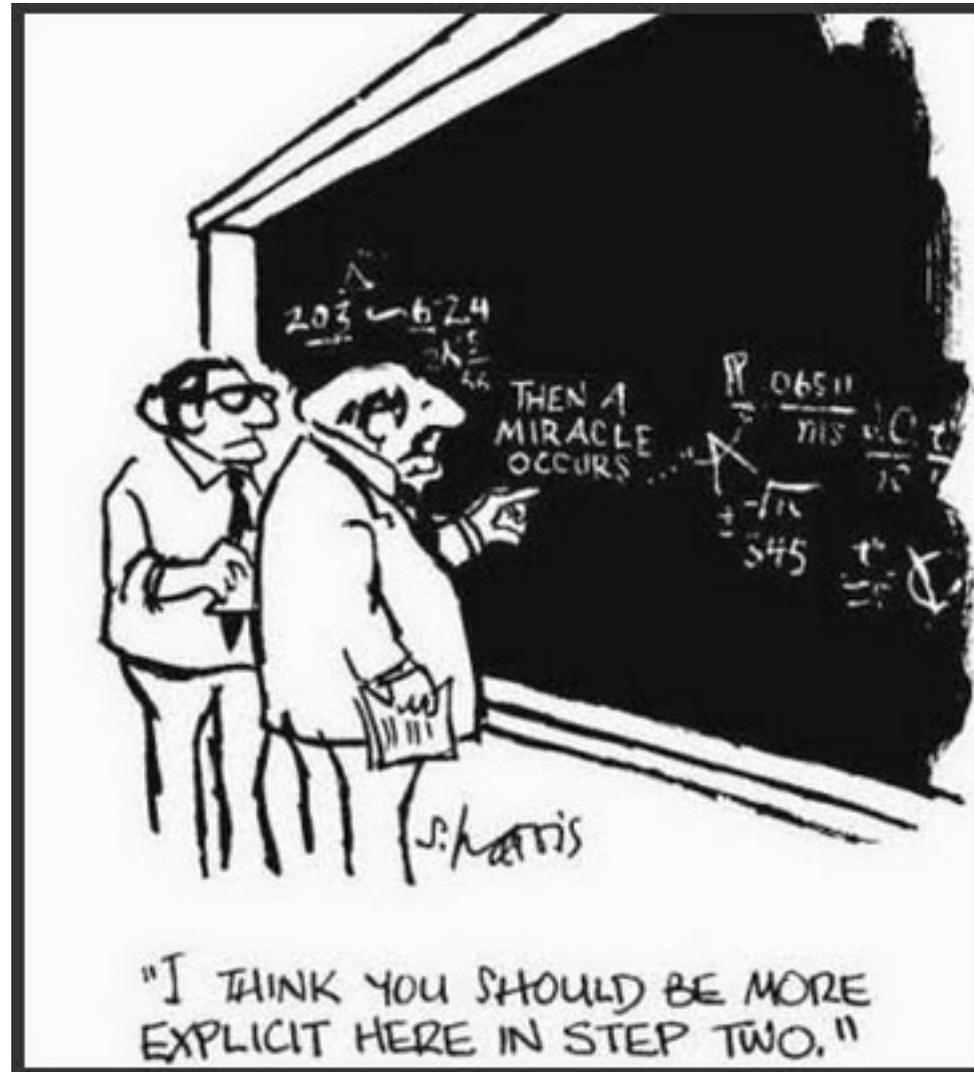
(Good for dimensions up to  $10^{10}$ .)

# Lanczos – a Krylov space method



- Idea: exact diagonalization in reduced basis sets.
- But which set to choose???
- Idea: generate the basis set with the operator you want to diagonalize:  
 $\{ |\phi\rangle, \tilde{H} |\phi\rangle, \tilde{H}^2 |\phi\rangle, \tilde{H}^3 |\phi\rangle, \dots \}$
- But which starting vector to choose???
- Idea: almost any will do!
- Cornelius Lanczos (Lánczos Kornél, 1893-1974)

(1) C. Lanczos, J. Res. Nat. Bur. Stand. **45**, 255 (1950).



# Finite-temperature Lanczos Method I

$$Z(T, B) = \sum_{\nu} \langle \nu | \exp \{ -\beta \tilde{H} \} | \nu \rangle$$

$$\langle \nu | \exp \{ -\beta \tilde{H} \} | \nu \rangle \approx \sum_n \langle \nu | n(\nu) \rangle \exp \{ -\beta \epsilon_n \} \langle n(\nu) | \nu \rangle \quad (\text{Step 2})$$

$$Z(T, B) \approx \frac{\dim(\mathcal{H})}{R} \sum_{\nu=1}^R \sum_{n=1}^{N_L} \exp \{ -\beta \epsilon_n \} |\langle n(\nu) | \nu \rangle|^2$$

- $|n(\nu)\rangle$  n-th Lanczos eigenvector starting from  $|\nu\rangle$
- Partition function replaced by a small sum:  $R = 1 \dots 10, N_L \approx 100$ .

J. Jaklic and P. Prelovsek, Phys. Rev. B **49**, 5065 (1994).

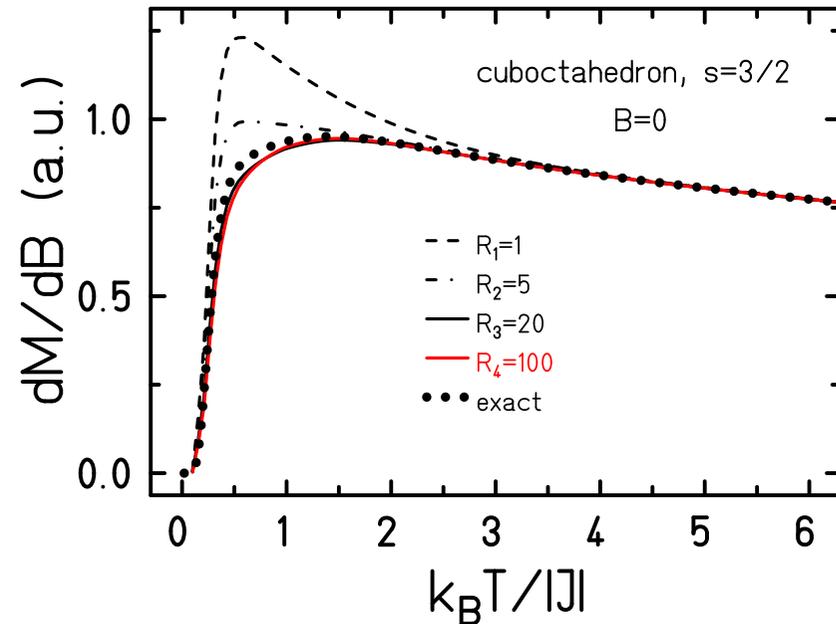
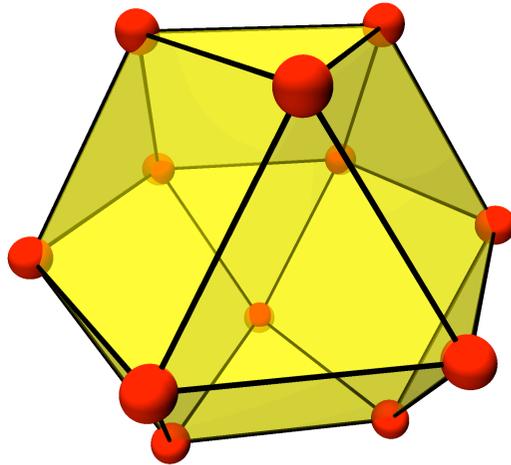
## Finite-temperature Lanczos Method II

$$Z(T, B) \approx \sum_{\Gamma} \frac{\dim(\mathcal{H}(\Gamma))}{R_{\Gamma}} \sum_{\nu=1}^{R_{\Gamma}} \sum_{n=1}^{N_L} \exp\{-\beta\epsilon_n\} |\langle n(\nu, \Gamma) | \nu, \Gamma \rangle|^2$$

- Approximation better if symmetries taken into account.
- $\Gamma$  denotes the used irreducible representations.

J. Schnack and O. Wendland, Eur. Phys. J. B **78** (2010) 535-541

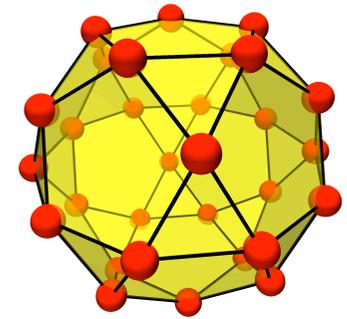
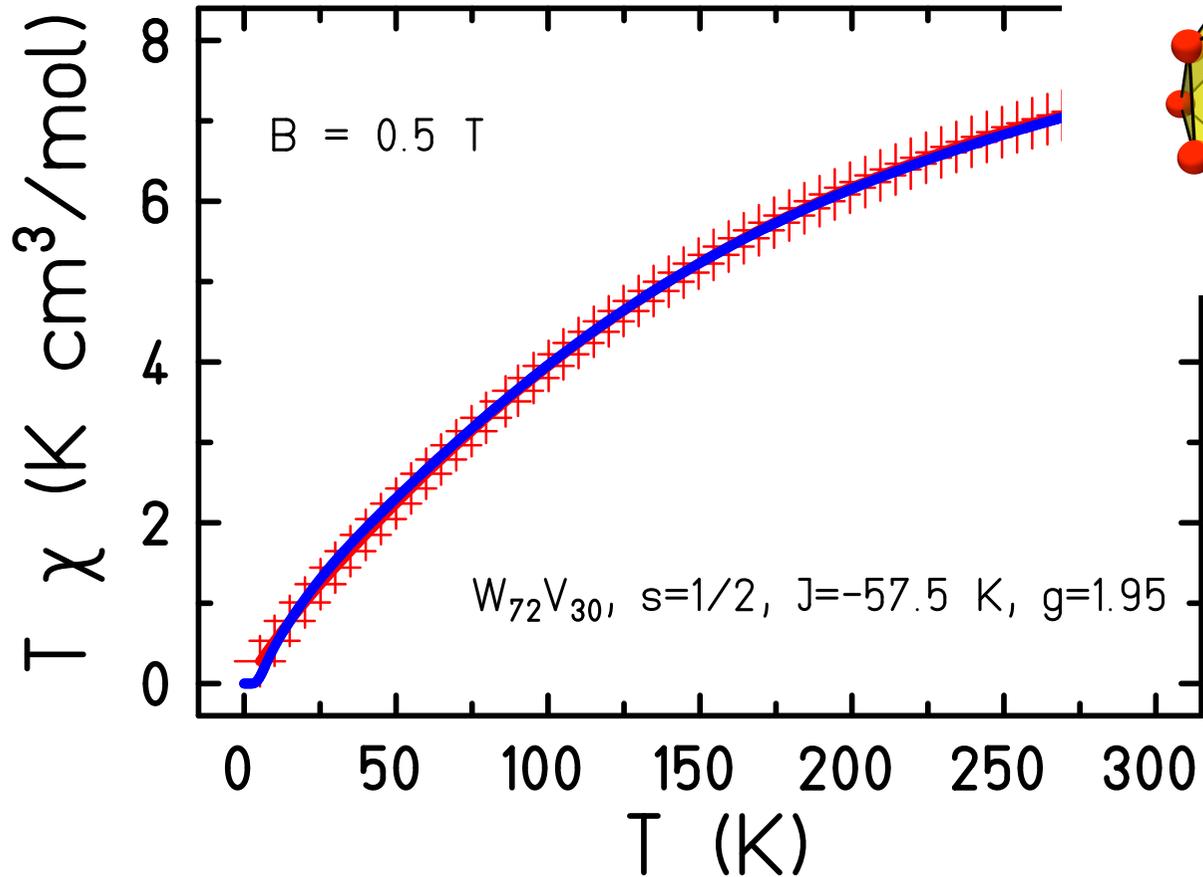
# How good is finite-temperature Lanczos?



- Works very well: compare frustrated cuboctahedron.
- $N = 12, s = 3/2$ : Considered  $< 100,000$  states instead of 16,777,216.

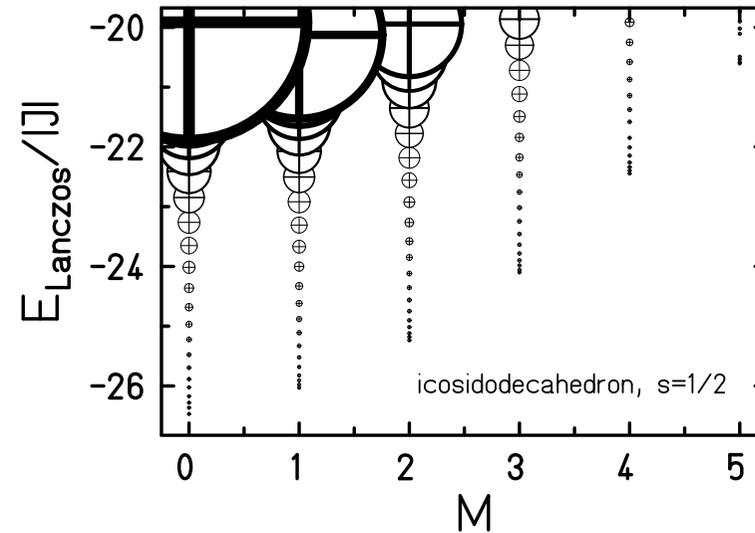
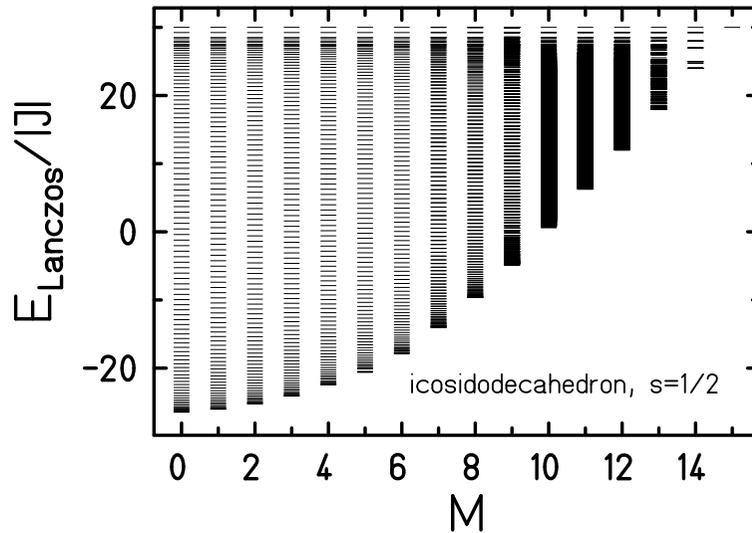
Exact results: R. Schnalle and J. Schnack, *Int. Rev. Phys. Chem.* **29**, 403-452 (2010).  
 FTLM: J. Schnack and O. Wendland, *Eur. Phys. J. B* **78**, 535-541 (2010).

# Icosidodecahedron $s = 1/2$



Exp. data: A. M. Todea, A. Merca, H. Bögge, T. Glaser, L. Engelhardt, R. Prozorov, M. Luban, A. Müller, Chem. Commun., 3351 (2009).

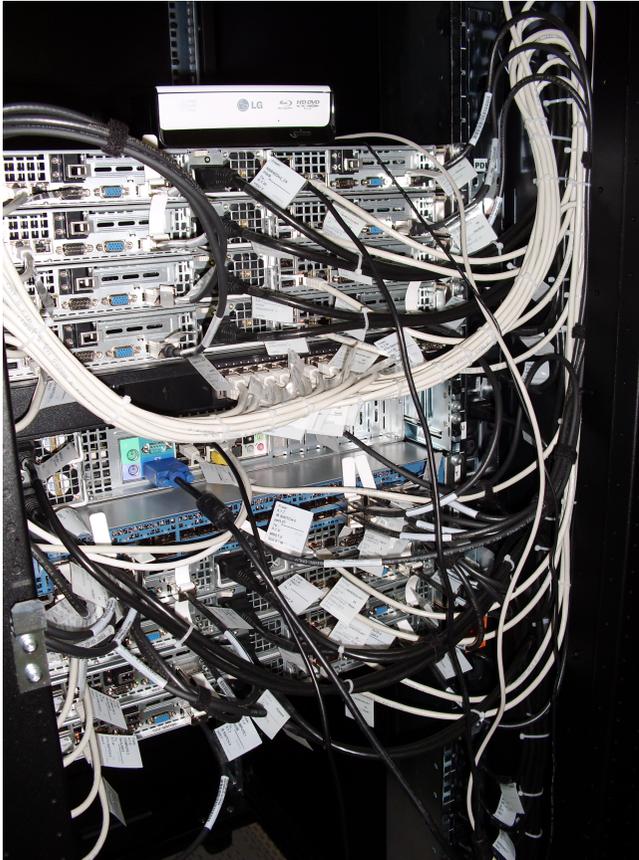
# Icosidodecahedron $s = 1/2$



- The true spectrum will be much denser. This is miraculously compensated for by the weights.

$$Z(T, B) \approx \frac{\dim(\mathcal{H})}{R} \sum_{\nu=1}^R \sum_{n=1}^{N_L} \exp \{ -\beta \epsilon_n \} |\langle n(\nu, \Gamma) | \nu, \Gamma \rangle|^2$$

# Summary



- Exact diagonalization is great but limited.
- Finite-temperature Lanczos is a good approximate method for Hilbert space dimensions smaller than  $10^{10}$ , also for anisotropic molecules.
- Modeling of dynamic quantities, e.g. AC susceptibility, very complicated.
- Anisotropic exchange is a new active direction.

## Many thanks to my collaborators worldwide

- T. Glaser, Chr. Heesing, M. Höck, N.B. Ivanov, S. Leiding, A. Müller, R. Schnalle, Chr. Schröder, J. Ummethum, O. Wendland (Bielefeld)
- K. Bärwinkel, H.-J. Schmidt, M. Neumann (Osnabrück)
- M. Luban (Ames Lab, USA); P. Kögerler (Aachen, Jülich, Ames); R.E.P. Winpenny, E.J.L. McInnes (Man U, UK); L. Cronin, M. Murrie (Glasgow, UK); E. Brechin (Edinburgh, UK); H. Nojiri (Sendai, Japan); A. Postnikov (Metz, France); M. Evangelisti (Zaragoza, Spain)
- J. Richter, J. Schulenburg (Magdeburg); A. Honecker (Göttingen); U. Kortz (Bremen); A. Tennant, B. Lake (HMI Berlin); B. Büchner, V. Kataev, H.-H. Klauß (Dresden); P. Chaudhuri (Mühlheim); J. Wosnitza (Dresden-Rossendorf); J. van Slageren (Stuttgart); R. Klingeler (Heidelberg); O. Waldmann (Freiburg)

Thank you very much for your  
attention.

The end.

Molecular Magnetism Web

[www.molmag.de](http://www.molmag.de)

Highlights. Tutorials. Who is who. Conferences.