Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information
Energetics of paramagnetic oxide clusters: the Fe(III) oxyhydroxy Keggin ion.

C. André Ohlin[1]

[1]Department of Chemistry, Umeå University, Sweden

Department of Chemistry, Umeå University, Sweden

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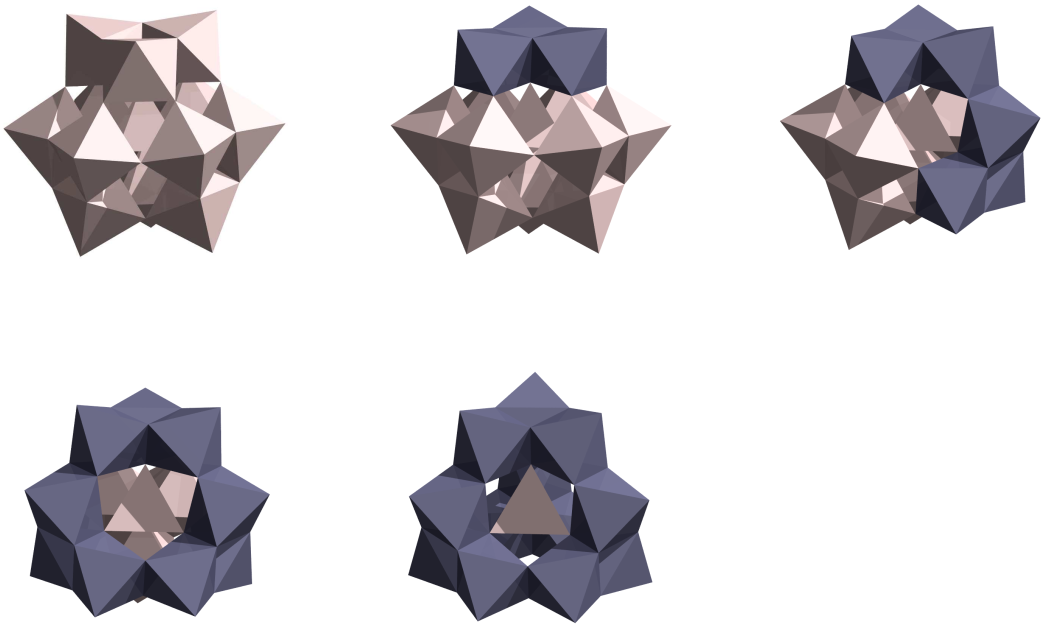

Figure S1: Baker-Figgis isomers of the Keggin ion. The shaded triad indicates one which has been rotated relative to the α isomer. From top left to bottom right: α, β, γ, δ and ϵ.

Table S1: Energies of different Keggin isomers calculated at different levels of theory. All isomers have a spin angular momentum of 32.5. Implicit solvation was included through the use of the polarizable continuum model (PCM).

Isomer	**PBE0**	**B3LYP**	**M06**[a]	**PBE**
α	-19458.5955057	-19465.0044729	-19463.3972482	-19458.3979841
β	-19458.5996921	-19465.0060446	-19463.3990737	-19458.4041281
γ	-19458.6004864	-19465.0069746	-19463.4017116	-19458.4073961
δ	-19458.6002837	-19465.0070946	-19463.4037190	-19458.4091273
ϵ	-19458.5861402	-19464.9963446	-19463.3952253	-19458.395399

def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [a] the 'Solvation Model based on Density' (SMD) was used instead of PCM. See main text for literature references to the PCM and SMD models.

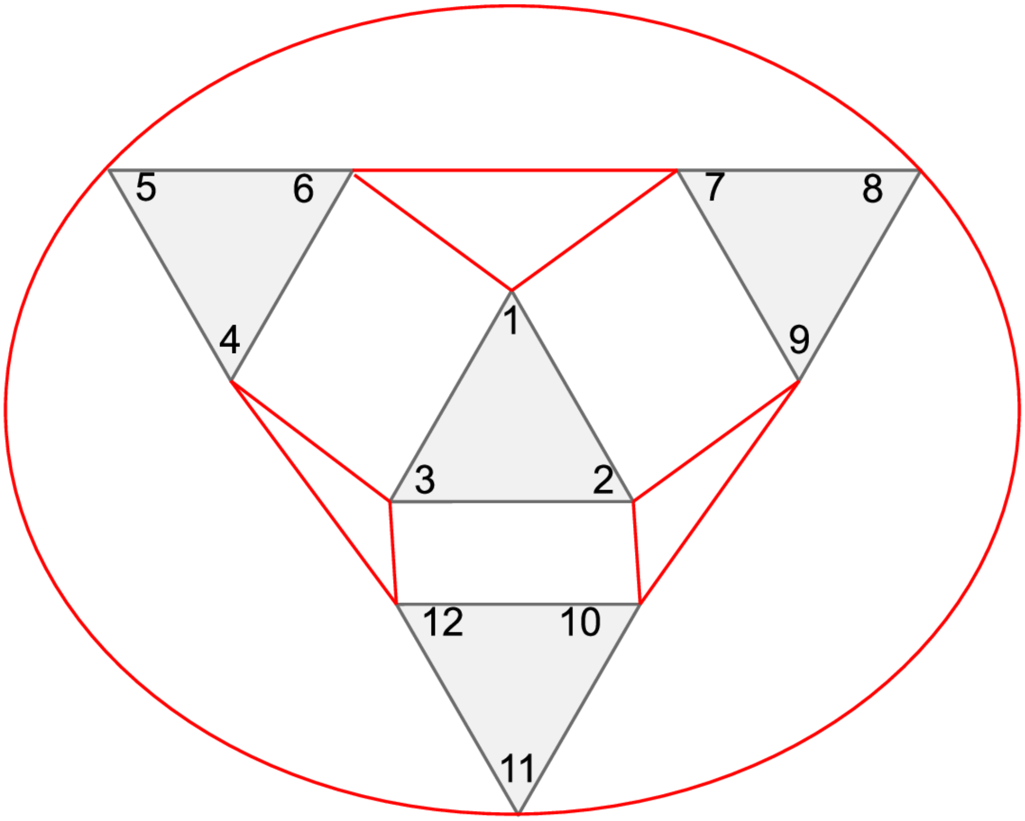

Figure S2: Schematic view of the coupling paths in the α-isomer. Iron centres are indicated as numbers. Intratriad J_{1a} couplings are shown as black lines, and intertriad J_{1b} couplings are shown as red lines. Fe centres 1-12 all couple to centre 13 via J_2.

Table S2: Coupling matrix for the α-isomer

Fe centre												
1	2	3	4	5	6	7	8	9	10	11	12	13
0	J_{1a}	J_{1a}	0	0	J_{1b}	J_{1b}	0	0	0	0	0	J_2
J_{1a}	0	J_{1a}	0	0	0	0	0	J_{1b}	J_{1b}	0	0	J_2
J_{1a}	J_{1a}	0	J_{1b}	0	0	0	0	0	0	0	J_{1b}	J_2
0	0	J_{1b}	0	J_{1a}	J_{1a}	0	0	0	0	0	J_{1b}	J_2
0	0	0	J_{1a}	0	J_{1a}	0	J_{1b}	0	0	J_{1b}	0	J_2
J_{1b}	0	0	J_{1a}	J_{1a}	0	J_{1b}	0	0	0	0	0	J_2
J_{1b}	0	0	0	0	J_{1b}	0	J_{1a}	J_{1a}	0	0	0	J_2
0	0	0	0	J_{1b}	0	J_{1a}	0	J_{1a}	0	J_{1b}	0	J_2
0	J_{1b}	0	0	0	0	J_{1a}	J_{1a}	0	J_{1b}	0	0	J_2
0	J_{1b}	0	0	0	0	0	0	J_{1b}	0	J_{1a}	J_{1a}	J_2
0	0	0	0	J_{1b}	0	0	J_{1b}	0	J_{1a}	0	J_{1a}	J_2
0	0	J_{1b}	J_{1b}	0	0	0	0	0	J_{1a}	J_{1a}	0	J_2
J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	0

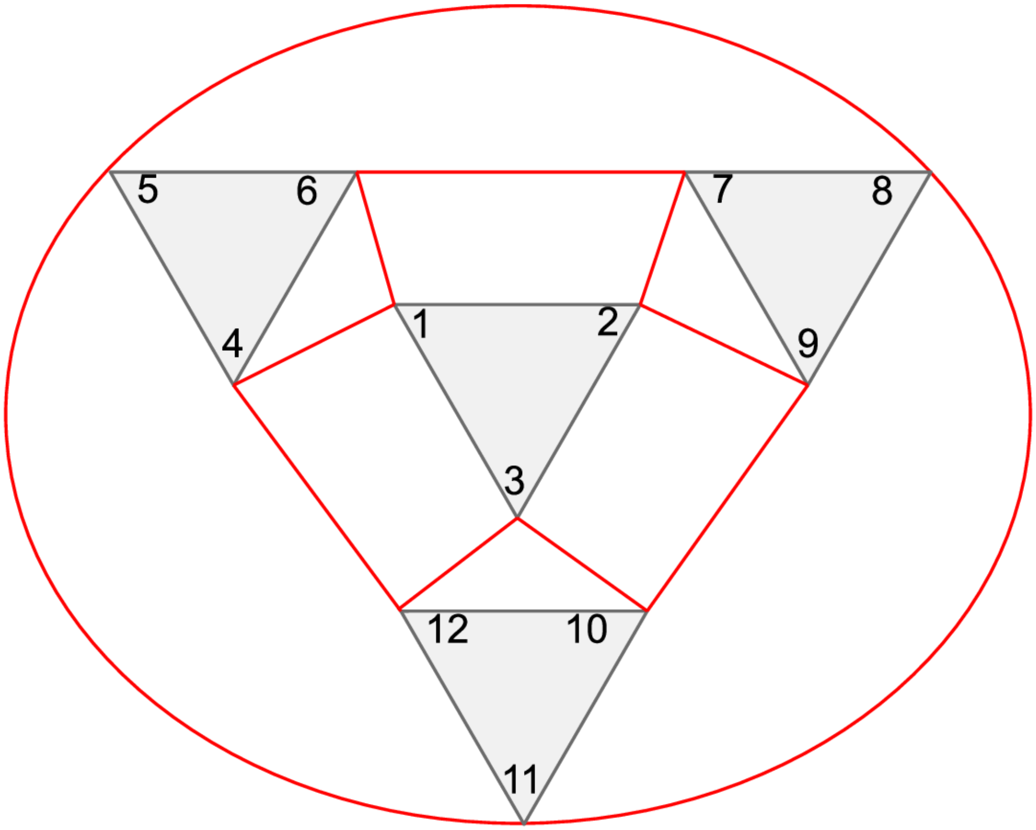

Figure S3: Schematic view of the coupling paths in the β-isomer. Intratriad J_{1a} couplings are shown as black lines, and intertriad J_{1b} couplings are shown as red lines. Fe centres 1-12 all couple to centre 13 via J_2.

Table S3: Coupling matrix for the β-isomer

Fe centre												
1	2	3	4	5	6	7	8	9	10	11	12	13
0	J_{1a}	J_{1a}	J_{1b}	0	J_{1b}	0	0	0	0	0	0	J_2
J_{1a}	0	J_{1a}	0	0	0	J_{1b}	0	J_{1b}	0	0	0	J_2
J_{1a}	J_{1a}	0	0	0	0	0	0	0	0	J_{1b}	J_{1b}	J_2
J_{1b}	0	0	0	J_{1a}	J_{1a}	0	0	0	0	0	J_{1b}	J_2
0	0	0	J_{1a}	0	J_{1a}	0	J_{1b}	0	0	J_{1b}	0	J_2
J_{1b}	0	0	J_{1a}	J_{1a}	0	J_{1b}	0	0	0	0	0	J_2
0	J_{1b}	0	0	0	J_{1b}	0	J_{1a}	J_{1a}	0	0	0	J_2
0	0	0	0	J_{1b}	0	J_{1a}	0	J_{1a}	0	J_{1b}	0	J_2
0	J_{1b}	0	0	0	0	J_{1a}	J_{1a}	0	0	J_{1b}	0	J_2
0	0	0	0	0	0	0	0	0	0	J_{1a}	J_{1a}	J_2
0	0	J_{1b}	0	J_{1b}	0	0	J_{1b}	J_{1b}	J_{1a}	0	J_{1a}	J_2
0	0	J_{1b}	J_{1b}	0	0	0	0	0	J_{1a}	J_{1a}	0	J_2
J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	0

Table S4: Coupling matrix for the γ-isomer

Fe centre												
1	2	3	4	5	6	7	8	9	10	11	12	13
0	J_{1a}	J_{1a}	0	0	J_{1d}	0	0	0	0	0	0	J_2
J_{1a}	0	J_{1a}	0	0	0	J_{1b}	0	J_{1b}	0	0	0	J_2
J_{1a}	J_{1a}	0	0	0	0	0	0	0	0	J_{1b}	J_{1b}	J_2
0	0	0	0	J_{1a}	J_{1a}	0	0	0	J_{1b}	0	J_{1b}	J_2
0	0	0	J_{1a}	0	J_{1a}	J_{1b}	J_{1b}	0	0	0	0	J_2
J_{1d}	0	0	J_{1a}	J_{1a}	0	0	0	0	0	0	0	J_2
0	J_{1b}	0	0	J_{1b}	0	0	J_{1a}	J_{1a}	0	0	0	J_2
0	0	0	0	J_{1b}	0	J_{1a}	0	J_{1a}	J_{1b}	0	0	J_2
0	J_{1b}	0	0	0	0	J_{1a}	J_{1a}	0	0	J_{1b}	0	J_2
0	0	0	J_{1b}	0	0	0	J_{1b}	0	0	J_{1a}	J_{1a}	J_2
0	0	J_{1b}	0	0	0	0	0	J_{1b}	J_{1a}	0	J_{1a}	J_2
0	0	J_{1b}	J_{1b}	0	0	0	0	0	J_{1a}	J_{1a}	0	J_2
J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	0

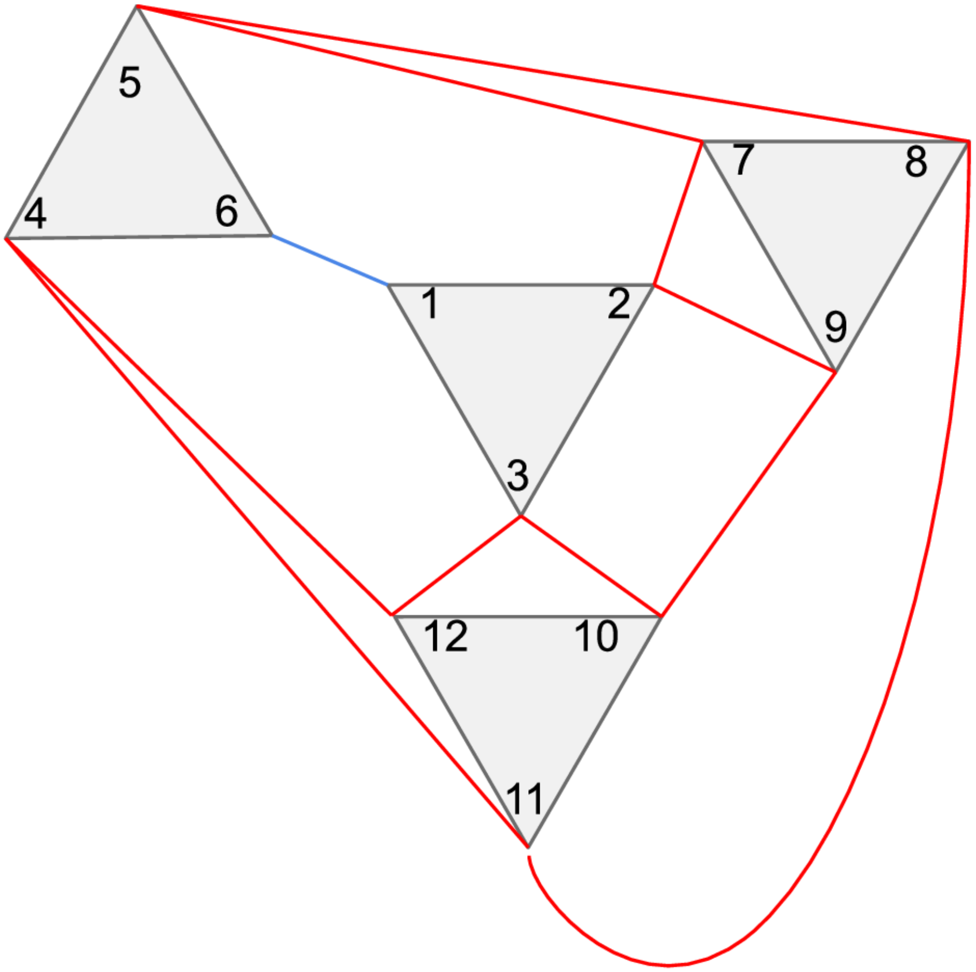

Figure S4: Schematic view of the coupling paths in the γ-isomer. Intratriad J_{1a} couplings are shown as black lines, intertriad J_{1b} couplings are shown as red lines, and intertriad J_{1d} couplings are shown as blue lines. Fe centres 1-12 all couple to centre 13 via J_2.

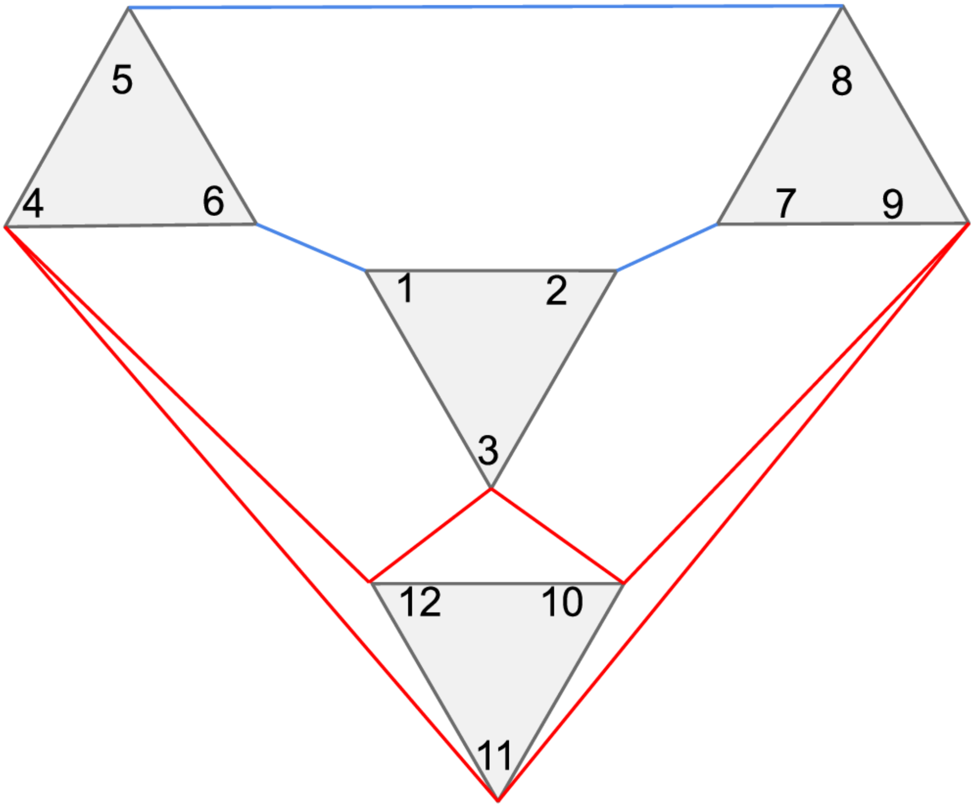

Figure S5: Schematic view of the coupling paths in the δ-isomer. Intratriad J_{1a} couplings are shown as black lines, intertriad J_{1b} couplings are shown as red lines, and intertriad J_{1d} couplings are shown as blue lines. Fe centres 1-12 all couple to centre 13 via J_2.

Table S5: Coupling matrix for the δ-isomer

Fe centre												
1	2	3	4	5	6	7	8	9	10	11	12	13
0	J_{1a}	J_{1a}	0	0	J_{1d}	0	0	0	0	0	0	J_2
J_{1a}	0	J_{1a}	0	0	0	J_{1d}	0	0	0	0	0	J_2
J_{1a}	J_{1a}	0	0	0	0	0	0	0	0	J_{1b}	J_{1b}	J_2
0	0	0	0	J_{1a}	J_{1a}	0	0	0	J_{1b}	0	J_{1b}	J_2
0	0	0	J_{1a}	0	J_{1a}	0	J_{1d}	0	0	0	0	J_2
J_{1d}	0	0	J_{1a}	J_{1a}	0	0	0	0	0	0	0	J_2
0	J_{1d}	0	0	0	0	0	J_{1a}	J_{1a}	0	0	0	J_2
0	0	0	0	J_{1d}	0	J_{1a}	0	J_{1a}	0	0	0	J_2
0	0	0	0	0	0	J_{1a}	J_{1a}	0	J_{1b}	J_{1b}	0	J_2
0	0	0	J_{1b}	0	0	0	0	J_{1b}	0	J_{1a}	J_{1a}	J_2
0	0	J_{1b}	0	0	0	0	0	J_{1b}	J_{1a}	0	J_{1a}	J_2
0	0	J_{1b}	J_{1b}	0	0	0	0	0	J_{1a}	J_{1a}	0	J_2
J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	0

Table S6: Coupling matrix for the ϵ-isomer

Fe centre												
1	2	3	4	5	6	7	8	9	10	11	12	13
0	J_{1a}	J_{1a}	0	0	J_{1d}	0	0	0	0	0	0	J_2
J_{1a}	0	J_{1a}	0	0	0	J_{1d}	0	0	0	0	0	J_2
J_{1a}	J_{1a}	0	0	0	0	0	0	0	0	0	J_{1d}	J_2
0	0	0	0	J_{1a}	J_{1a}	0	0	0	J_{1d}	0	0	J_2
0	0	0	J_{1a}	0	J_{1a}	0	J_{1d}	0	0	0	0	J_2
J_{1d}	0	0	J_{1a}	J_{1a}	0	0	0	0	0	0	0	J_2
0	J_{1d}	0	0	0	0	0	J_{1a}	J_{1a}	0	0	0	J_2
0	0	0	0	J_{1d}	0	J_{1a}	0	J_{1a}	0	0	0	J_2
0	0	0	0	0	0	J_{1a}	J_{1a}	0	0	J_{1d}	0	J_2
0	0	0	J_{1d}	0	0	0	0	0	0	J_{1a}	J_{1a}	J_2
0	0	0	0	0	0	0	0	J_{1d}	J_{1a}	0	J_{1a}	J_2
0	0	J_{1d}	0	0	0	0	0	0	J_{1a}	J_{1a}	0	J_2
J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	J_2	0

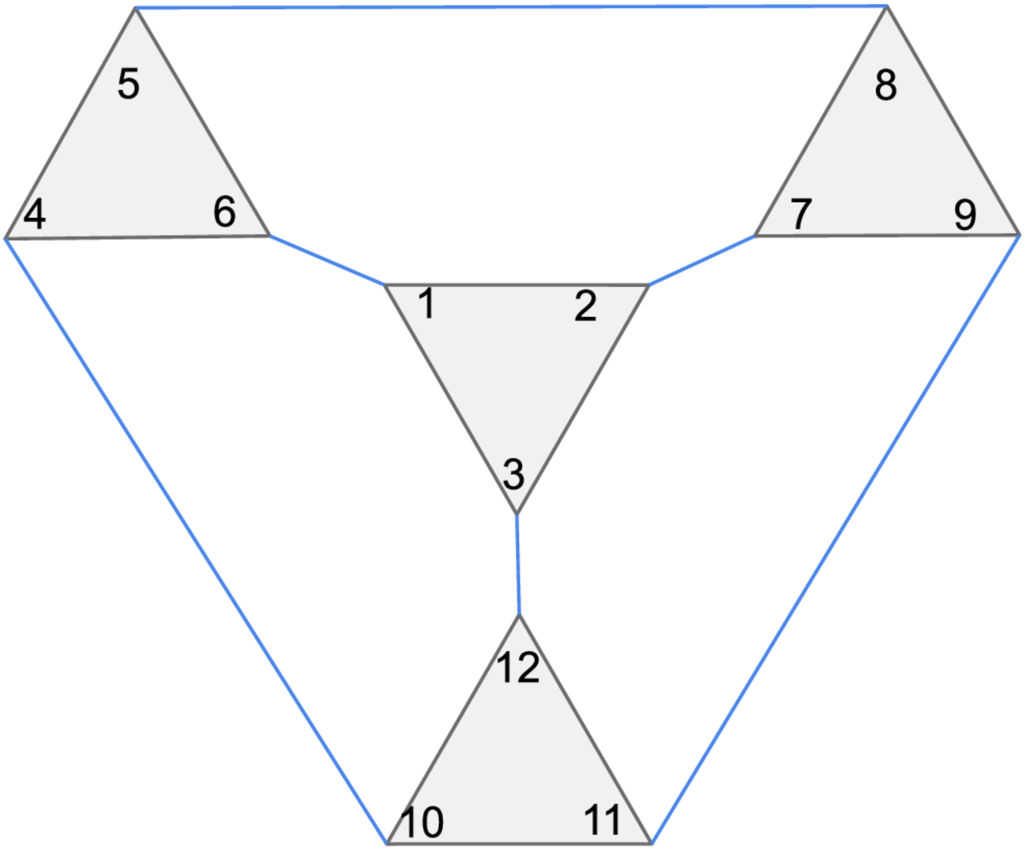

Figure S6: Schematic view of the coupling paths in the ϵ-isomer. Intratriad J_{1a} couplings are shown as black lines, and intertriad J_{1d} couplings are shown as blue lines. Fe centres 1-12 all couple to centre 13 via J_2.

Table S7: Investigated spin configurations for the α-isomer. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1.

Species	Flipped spins[a]	S[b]	J_2	J_{1a}	J_{1b}
S_{max}	–	32.5	–	–	–
BS1	1	27.5	15	30	30
BS2	13	27.5	180	0	0
BS4	1,2,3	17.5	45	0	0
BS5	1,4,9,12	12.5	60	120	90
BS6	1,4,9,12,13	2.5	120	120	90
BS7	1,4,6,7,9,12	2.5	90	120	60
BS8	1,4,6	17.5	45	60	60
BS9	1,4,5,6,8,11	2.5	90	90	60
BS10	1,4,9,11,13	2.5	120	120	120

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.[b] S is the total spin angular momentum.

$$\Delta E = \sum n_i \cdot J_i \tag{S1}$$

The predicted energy difference between the highest spin configuration and a broken spin symmetry can be described as a linear equation, where the prefactors can be obtained from equation 1 in the main text. Prefactors for the broken symmetry configurations used in this study are given in tables S7

Table S8: Energies of different spin configurations for the α-isomer for the B3LYP, PBE0, and M06 exchange and correlation functionals. All geometries were optimised with the indicated method for that particular spin state, and with implicit solvation through the polarizable continuum model (PCM), except where indicated otherwise.

Spin isomer	ϵ **(Ha)**							
	B3LYP			PBE0			M06	
	def2-svp	def2-tzvp+svp[a]	def2-tzvp	def2-svp	def2-tzvp+svp[a]	def2-tzvp	def2-tzvp+svp[a,b]	def2-tzvp[b]
S_{max}	-19462.6809265	-19465.0044729	-19468.5292324	-19456.2970693	-19458.5955057	-19462.0704952	-19463.3972482	-19466.7370044
BS1	-19462.6893938	-19465.0121735	-19468.5383579	-19456.3044294	-19458.6027443	-19462.0781605	-19463.4016689	-19466.7409931
BS4	-19462.7014248	-19465.0247350	-19468.5504853	-19456.3148111	-19458.6133325	-19462.0890291	-19463.4138835	-19466.7536278
BS5	-19462.7072609	-19465.0301836	-19468.5553959	-19456.3138577	-19458.6157826	-19462.0928525	-19463.4159394	-19466.7561296
BS6	-19462.7176272	-19465.0389620	-19468.5665606	-19456.3275136	-19458.6246327	-19462.1015866	-19463.4248798	-19466.7657280
BS7	-19462.7087254	-19465.0305170	-19468.5575987	-19456.3194237	-19458.6171548	-19462.0940216	-19463.4169950	-19466.7576750
BS8	-19462.6992958	-19465.0221957	-19468.5490593	-19456.3116954	-19458.6109679	-19462.0868693	-19463.4096162	-19466.7493182
BS9	-19462.7079624	-19465.0294930	-19468.5563920	-19456.3192017	-19458.6164300	-19462.1015866	-19463.4175974	-19466.7579748
BS10	-19462.7212893	-19465.0429030	-19468.5703632	-19456.3306695	-19458.6280491	-19462.1055003	-19463.4280362	-19466.7689016

[a] def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [b] the 'Solvation Model based on Density' (SMD) was used instead of PCM. See main text for literature references to the PCM and SMD models.

Table S9: Energies of different spin configurations for the α-isomer for the PBE, and BP86 exchange and correlation functionals. All geometries were optimised with the indicated method for that particular spin state, and with implicit solvation through the polarizable continuum model (PCM).

Spin isomer	**ϵ (Ha)**	
	PBE def2-svp	BP86 def2-svp
S$_{max}$	-19456.0635212	-19464.7295487
BS1	-19456.0865879	-19464.7540167
BS4	-19456.1149618	-19464.7857977
BS5	-19456.1419826	-19464.8184643
BS6	-19456.1685447	-19464.8481586
BS7	-19456.1510087	-19464.832556
BS8	-19456.1180298	-19464.8031144
BS9	-19456.1464679	-19464.8255093
BS10	-19456.1741531	-19464.8491219

$$\sigma_{BS}^2 = \sum_i^n a_i^2 \cdot \sigma_{J_i}^2 \tag{S2}$$

Formula for propagation of uncertainties for a system where all parameters J_i are assumed to be uncorrelated, and where a_i is the pre-factor for J_i for a particular spin state BS.

Table S10: Energies, including enthalpy and entropy correction terms, of different spin configurations for the α-isomer for the B3LYP exchange and correlation functional. All geometries were optimised with the indicated method for that particular spin state, and with implicit solvation through the polarizable continuum model (PCM).

Spin isomer	**def2-tzvp+svp**[a]		
	ϵ (Ha)	H$_{corr}$ (Ha)	S[c] (cal/mol·K)
S$_{max}$	-19465.0044729	.760413	463.045
BS1	-19465.0121735	0.760775	461.202
BS4	-19465.0247350	0.760705	460.067
BS5	-19465.0301836	0.761163	461.578
BS6	-19465.0389620	0.760267	466.057
BS7	-19465.0305170	0.760063	465.906
BS8	-19465.0221957	0.760673	462.351
BS9	-19465.0294930	0.760717	458.401
BS10	-19465.0429030	0.760326	462.694

[a] def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [b] Correction factor for the enthalpy. [c] S here stands for entropy.

Table S11: Additional investigated spin configurations for the α-isomer at the B3LYP/def2-svp+tzvp level of theory. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1. Entries marked with * were used together with the BS set for fitting (dataset X). The others were used to test the predictive ability of the method, using the parameters from dataset X (see table S12). Δ E is relative to S_{max}.

Species	Flipped spins[a]	S[b]	J_2	J_{1a}	J_{1b}	ϵ (Ha)	Found ΔE (cm^{-1})	Predicted ΔE (cm^{-1})
x1	13	27.5	180	0	0	-19465.03038	-5686	-5773 ± 82
x2	1,13	22.5	165	30	30	-19465.03357	-6385	-6462± 77
x3	1,8	22.5	30	60	60	-19465.01415	-3620	-3302± 42
x4*	1,4,8,11,12,13	2.5	105	120	90	-19465.0364		
x5	8,11	22.5	30	60	30	-19465.01424	-2143	-2332±33
x6	8,9,11,12	12.5	60	60	90	-19465.02869	-5316	-5234±57
x7	8,9,12	17.5	45	60	90	-19465.02552	-4620	-4753± 55
x8	1,11,13	17.5	150	60	60	-19465.03409	-6500	-7151±79
x9*	2,3,6,8,12,13	2.5	105	120	120	-19465.04128		
x10	2,3,4,6,7,8	7.5	90	90	120	-19465.03753	-7255	-7366 ± 81
x11	3,6,7,9,10	7.5	75	120	90	-19465.03194	-6029	-6114± 77
x12*	1,6,7,8,10	7.5	75	120	60	-19465.02741		
x13*	3,4,8,12,13	7.5	120	120	30	-19465.03023		
x14	3,5,6,7,8,13	2.5	105	90	90	-19465.03655	-7039	-6877 ± 76
x15	10,11,12,13	12.5	135	0	90	-19465.03761	-7273	-7241 ± 75
x16	3,5,6,8,10,13	2.5	105	120	120	-19465.04079	-7971	-8047 ± 92
x17*	1,2,3,4,8,13	2.5	105	60	120	-19465.03923		
x18	2,6,8,10,11,12	2.5	90	90	120	-19465.03673	-7079	-7366 ± 81
x20*	1,6,7	17.5	45	90	0	-19465.01379		
x21*	11,12	22.5	30	30	60	-19465.01813		
x22	2,3,4	17.5	45	60	60	-19465.02186	-3816	-3783 ± 44
x23*	1,4,12	17.5	45	90	60	-19465.02238		
x24*	9,12,13	17.5	150	60	60	-19465.03682		
x25*	3,4,13	17.5	150	60	30	-19465.03263		
x26	1,2,6,7	12.5	60	90	30	-19465.02011	-3432	-3493 ± 51
x27	1,3,4,7	12.5	60	90	60	-19465.02506	-4519	-4464 ± 57
x28	1,2,3,4	12.5	60	30	90	-19465.02954	-5502	-5035 ± 53
x29	6,9,12,13	12.5	135	90	90	-19465.04024	-7850	-7839 ± 85

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.[b] S is the total spin angular momentum.

Table S12: Fitted coupling constants in cm^{-1} for the α-isomer as a function of basis set and exchange correlation functional.

Method	$J_{1a} \pm \sigma$	$J_{1b} \pm \sigma$	$J_2 \pm \sigma$	Fitting set[b]
PBE0/def2-svp	5.52647 ± 3.455	-20.3274 ± 3.672	-46.5883 ± 5.321	BS
PBE0/def2-tzvp+svp	-2.06856 ± 0.9474	-26.5474 ± 1.007	-28.2093 ± 1.459	BS
PBE0/def2-tzvp	-1.56321 ± 9.298	-22.1933 ± 9.880	-43.7769 ± 14.32	BS
B3LYP/def2-svp	-6.91382 ± 1.563	-30.766 ± 1.66	-37.3467 ± 2.406	BS
B3LYP/def2-tzvp+svp[a]	-6.65384 ± 1.082	-32.8274 ± 1.150	-31.8966 ± 1.667	BS
B3LYP/def2-tzvp+svp[a]	-6.59149 ± 0.4495	-32.3395 ± 0.4761	-32.0749± 0.4535	X
B3LYP/def2-tzvp+svp[a]	-6.15383± 1.107	-32.4851 ± 1.221	-31.8131± 0.8257	All
B3LYP/def2-tzvp	-6.04695 ± 2.865	-32.5504 ± 3.044	-38.0232 ± 4.413	BS
M06/def2-tzvp+svp[a]	1.35205 ± 1.574	-22.5191 ± 1.672	-35.2112 ± 2.423	BS
M06/def2-tzvp	1.21197 ± 2.202	-20.9939 ± 2.340	-38.2017 ± 3.391	BS
PBE/def2-svp	-42.8857 ± 11.85	-66.8562 ± 12.59	-103.32 ± 18.25	BS
BP86/def2-svp	-60.0534 ± 27.36	-72.9388 ± 29.07	-107.911 ± 42.13	BS

[a] def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [b] Denotes which data was used for the fitting. BS used only the BS entries, X used BS and select X entries (see table S11) and All used all BS and X entries.

Table S13: Investigated spin configurations for the β-isomer. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1.

Species	Flipped spins[a]	S[b]	J_2	J_{1a}	J_{1b}
S_{max}	–	32.5	–	–	–
BS1	13	27.5	180	0	0
BS2	1	27.5	15	30	30
BS3	1,6	22.5	30	60	45
BS4	5,13	22.5	165	30	30
BS5	5,10	22.5	30	60	60
BS6	1,2,3	17.5	45	0	90
BS7	1,5,8,10	12.5	60	120	90
BS8	1,5,6,9,12	7.5	75	120	165
BS9	1,4,5,8,10,12	2.5	90	120	90
BS10	2	27.5	15	30	30
BS11	2,13	22.5	165	30	30
BS12	2,11	22.5	30	60	75
BS13	4,5,6	17.5	45	0	120
BS14	7,8,9	17.5	45	0	120
BS15	2,7,8,9	12.5	60	30	90
BS16	1,2,11,12,13	7.5	120	60	150
BS17	1,7,9,11,12,13	2.5	105	90	210

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.[b] S is the total spin angular momentum.

Table S14: Energies, including enthalpy and entropy correction terms, of different spin configurations for the β-isomer for the B3LYP exchange and correlation functional. All geometries were optimised with the indicated method for that particular spin state, and with implicit solvation through the polarizable continuum model (PCM). Entries marked with * were used for fitting, together with those in table S15. Δ E is relative to S_{max} at B3LYP/def2-tzvp+svp.

Spin isomer	**def2-tzvp+svp**^{a}			**def2-tzvp**	Found	Predicted
	ϵ (Ha)	H_{corr} (Ha)	S^{c} (cal/mol·K)	ϵ (Ha)	ΔE (cm^{-1})	ΔE (cm^{-1})
S_{max}	-19465.0060446	0.758785	467.93	-19468.5314174		
BS1	-19465.0320581	0.758800	466.978	-19468.5589450	-5709	-5413±593
BS2*	-19465.0127479	0.758723	468.287	-19468.5388696		
BS3	-19465.0164453	0.758967	466.055	-19468.5427421	-2283	-2215± 269
BS4	-19465.0359471	0.759000	465.391	-19468.5630956	-6563	-6005±571
BS5*	-19465.0165482	0.759081	463.491	-19468.5426237		
BS6	-19465.0250003	0.758976	465.382	-19468.5514735	-4160	-3672±446
BS7*	-19465.0222049	0.758935	464.048	-19468.5488536		
BS8	-19465.0372426	0.758998	463.830	-19468.5646203	-6847	-6427±739
BS9*	-19465.0263369	0.759117	460.341	-19468.5533583		
BS10	-19465.0129812	0.758894	466.887	-19468.5388754	-1522	-1494±181
BS11	-19465.0354276	0.758966	465.958	-19468.5624713	-6449	-6005±571
BS12	-19465.0198463	0.758887	465.299	-19468.5462200	-3029	-3761±479
BS13*	-19465.0251729	0.759229	466.010	-19468.5517930		
BS14	-19465.0261444	0.759151	465.713	-19468.5524703	-4411	-3672 ± 446
BS15*	-19465.0239121	0.759052	464.923	-19468.5506443		
BS16*	-19465.0415024	0.759229	463.925	-19468.5690747		
BS17	-19465.0403924	0.759587	457.636	-19468.5678754	-7538	-7833±841

[a] def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [b] Correction factor for the enthalpy. [c] S here stands for entropy.

Table S15: Additional investigated spin configurations for the β-isomer at the B3LYP/def2-svp+tzvp level of theory. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1. Entries marked with * were used for fitting, and make up dataset X, together with those in table S14. The other entries were used to test the predictive ability of the method using parameters fitted using dataset X. Δ E is relative to S_{max}.

Species	Flipped spins[a]	J_2	J_{1a}	J_{1b}	ϵ (Ha)	Found ΔE (cm^{-1})	Predicted ΔE (cm^{-1})
x1	1,2,4,5,8	75	90	90	-19465.0324578	-5797	-5384 ± 578
x2	1,4,5,7,9	75	90	120	-19465.035981	-6570	-6157 ± 687
x3*	3,4,7,8,10	75	120	120	-19465.0369565		
x4*	2,6,7,10,12	75	120	60	-19465.032154		
x5	7,8,10	45	60	60	-19465.0238205	-3901	-3439 ± 378
x6	3,7,8	45	60	90	-19465.0270833	-4617	-4212 ± 492
x7	3,11,13	150	60	60	-19465.0337652	-6084	-6597 ± 605
x8*	5,6,8,10,11,13	105	90	60	-19465.0312718		
x9*	2, 6, 7, 9, 10, 12	90	120	60	-19465.0339487		
x10*	1,2,3,4,10,13	105	60	90	-19465.0403164		
x11*	2,4,6,9,10	75	120	90	-19465.0359853		
x12*	1,2,6,7,13	120	90	30	-19465.0302632		
x13*	3,5,6,8,10,13	105	120	90	-19465.0323229		
x14	6,7,9,11,12	75	90	120	-19465.0322424	-5750	-6157 ± 687
x15*	1,6,9,11,13	120	120	90	-19465.0345145		
x16	1,2,4,5,8,13	105	90	90	-19465.0368681	-6765	-6287 ± 627
x17	2,3,5,8,10,11	90	120	60	-19465.0311811	-5517	-5332 ± 581
x18*	3,4,8,11,12,13	105	120	60	-19465.0330416		
x20*	10	15	30	0	-19465.0133087		
x21*	12,13	165	30	30	-19465.0355234		
x22*	11,13	165	30	60	-19465.0351647		
x23*	2,4,6,11,13	120	90	150	-19465.0421248		
x24*	1,4,10	45	90	30	-19465.0228944		
x25	2,4,7	45	90	60	-19465.0225154	-3615	-3709 ± 444
x26	2,7,13	150	60	30	-19465.0341141	-6161	-5824 ± 554
x27*	1,11,13	150	60	90	-19465.0366544		
x28*	11,12,13	150	30	90	-19465.0375886		
x29	6, 11,12,13	135	60	120	-19465.0388999	-7211	-7692 ± 745

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.

Table S16: Investigated spin configurations for the γ-isomer. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1.

Species	Flipped spins[a]	S^b	J_2	J_{1a}	J_{1b}	J_{1d}
S_{max}	–	32.5	–	–	–	–
BS1	13	27.5	180	0	0	0
BS2	1	27.5	15	30	0	15
BS3	2	27.5	15	30	30	0
BS4	10	27.5	15	30	30	0
BS5	1,6	22.5	30	60	0	0
BS6	1,13	22.5	165	30	0	15
BS7	1,2	22.5	30	30	30	15
BS9	1,2,3	17.5	45	0	60	15
BS11	2,7,9	17.5	45	60	30	0
BS12	1,2,3,6	12.5	60	30	60	0
BS13	1,2,3,5,6	7.5	75	30	90	0
BS14	1,2,3,5,6,13	2.5	105	30	90	0
BS15	3,4,7,8,9,13	2.5	105	60	150	0

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.[b] S is the total spin angular momentum.

Table S17: Energies, including enthalpy and entropy correction terms, of different spin configurations for the γ-isomer for the B3LYP exchange and correlation functional. All geometries were optimised with the indicated method for that particular spin state, and with implicit solvation through the polarizable continuum model (PCM). Entries marked with * were used for fitting, together with those in table S18. Δ E is relative to S_{max} at B3LYP/def2-tzvp+svp.

Spin isomer	**def2-tzvp+svp**[a]			**def2-tzvp**	Found	Predicted
	ϵ (Ha)	H_{corr} (Ha)	S^c (cal/mol·K)	ϵ (Ha)	ΔE (cm^{-1})	ΔE (cm^{-1})
S_{max}	-19465.0069746	0.757718	471.544	-19468.5331620		
BS1*	-19465.0324851	0.758163	465.467	-19468.5601869		
BS2*	-19465.0115025	0.758395	467.082	-19468.5381436		
BS3*	-19465.0139500	0.757937	470.362	-19468.5407071		
BS4	-19465.0140785	0.758165	466.014	-19468.5407627	-1559	-1546 ± 42
BS5*	-19465.0129057	0.758168	468.770	-19468.5397790		
BS6	-19465.0329328	0.758183	468.313	-19468.5610626	-5697	-5759 ± 110
BS7	-19465.0176921	0.758527	466.136	-19468.5447557	-2352	-2371±85
BS9	-19465.0232730	0.758813	462.142	-19468.5504205	-3577	-3541± 93
BS11	-19465.0195939	0.758091	465.885	-19468.5468350	-2770	-2684 ± 71
BS12*	-19465.0245284	0.758372	465.381	-19468.5518415		
BS13*	-19465.0304660	0.758467	466.499	-19468.5581326		
BS14	-19465.0345995	0.759008	460.330	-19468.5627121	-6063	-6161 ± 100
BS15*	-19465.0433843	0.759060	459.339	-19468.5717761		

[a] def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [b] Correction factor for the enthalpy. [c] S here stands for entropy.

Table S18: Additional investigated spin configurations for the γ-isomer at the B3LYP/def2-svp+tzvp level of theory. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1. Entries marked with * were used for fitting, and make up dataset X, together with those in table S17. The other entries were used to test the predictive ability of the method using parameters fitted using dataset X. Δ E is relative to S_{max}.

Species	Flipped spins[a]	J_2	J_{1a}	J_{1b}	J_{1d}	ϵ (Ha)	Found ΔE (cm^{-1})	Predicted ΔE (cm^{-1})
x1	2,3,4,7,10,13	105	120	90	0	-19465.03721	-6635	-6726 ± 156
x2	1,3,5,7,13	120	90	60	12	-19465.0368	-6545	-6478 ± 141
x3*	1,4,5,6,12	75	60	60	0	-19465.02847		
x4	2,6,8,9	60	90	60	15	-19465.0315	-5382	-4580 ± 133
x5*	5,6,8,13	135	60	30	15	-19465.03405		
x6	4,9,10,13	135	90	60	0	-19465.03669	-6522	-6603 ± 124
x7*	1,3,5,8,12,13	105	120	60	15	-19465.03453		
x8*	3,5,6,10,11,13	105	90	90	15	-19465.03861		
x9*	2,7,9,10,11,12	90	60	90	0	-19465.03487		
x10	2,6,7,8,10,12	90	120	90	15	-19465.03634	-6446	-6601 ± 170
x11*	1,4,5,8,10	75	120	30	15	-19465.02674		
x12	1,6,9,10,11	75	120	60	0	-19465.02889	-4809	-4893 ± 139
x13	3,6,7,12	60	120	60	15	-19465.02763	-4534	-4768 ± 153
x14*	2,3,7,10,12,13	105	90	90	0	-19465.03652		
x15	1,3,5,8,9,13	105	90	90	15	-19465.03798	-6804	-6887 ± 151
x16	1,2,3,7,11,13	105	60	60	15	-19465.0337	-5865	-5816 ± 120
x17*	2,5,6,8,9,10	90	120	60	15	-19465.03314		
x18	1,6,7,8,11,12	90	120	120	0	-19465.03863	-6949	-7135 ± 170
x20*	6	15	30	0	15	-19465.01174		
x21*	2,7	30	60	30	0	-19465.01715		
x22*	1,12	30	60	30	15	-19465.01867		
x23*	2,10	30	60	60	0	-19465.02176		
x24*	10,13	165	30	30	0	-19465.03677		
x25*	9,12,13	150	60	60	0	-19465.03717		
x26*	2,3,13	150	30	60	0	-19465.03751		
x27	3,12,13	150	60	30	0	-19465.03406	-5944	-6006 ± 97
x28*	3,4,7	45	90	90	0	-19465.02779		
x29	2,11,12	45	60	90	0	-19465.02788	-4588	-4451 ± 105

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.

Table S19: Investigated spin configurations for the δ-isomer. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1.

Species	Flipped spins[a]	S^b	J_2	J_{1a}	J_{1b}	J_{1d}
S_{max}	–	32.5	–	–	–	–
BS1	13	27.5	180	0	0	0
BS2	8,13	22.5	165	30	0	15
BS3	5,8	22.5	30	60	0	0
BS4	1,2,6,7	12.5	60	90	0	0
BS5	10,11,12	12.5	45	0	90	0
BS6	11,12	22.5	30	30	60	0
BS7	7,8	22.5	30	30	0	30
BS8	6,7,8	17.5	45	60	0	45
BS9	6,7,8,9	12.5	60	30	30	45
BS10	5,7,8,9,10,11	2.5	90	60	30	45
BS11	7,8,10,11,12,13	2.5	105	30	90	30
BS12	6,8,10,11,12	7.5	75	60	90	30
BS13	3,4,9,13	12.5	75	30	90	0
BS14	3,4,8,9,13	7.5	120	90	90	15
BS15	10,11,12,13	7.5	135	0	90	0

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.[b] S is the total spin angular momentum.

Table S20: Energies, including enthalpy and entropy correction terms, of different spin configurations for the δ-isomer for the B3LYP exchange and correlation functional. All geometries were optimised with the indicated method for that particular spin state, and with implicit solvation through the polarizable continuum model (PCM). Entries marked with * were used for fitting, together with those in table S21. Δ E is relative to S_{max} at B3LYP/def2-tzvp+svp.

Spin isomer	**def2-tzvp+svp**[a]			**def2-tzvp**	Found	Predicted
	ϵ (Ha)	H_{corr} (Ha)	S^c (cal/mol·K)	ϵ (Ha)	ΔE (cm^{-1})	ΔE (cm^{-1})
$S_m ax$	-19465.0070946	0.769287	456.165	-19468.5344167		
BS1*	-19465.0311457	0.758155	471.070	-19468.5602286		
BS2	-19465.0316664	0.758374	468.546	-19468.5611106	-5393	-5309±100
BS3*	-19465.0121696	0.757964	470.297	-19468.5404629		
BS4*	-19465.0184402	0.758285	466.678	-19468.5470871		
BS5*	-19465.0256962	0.758635	463.903	-19468.5542097		
BS6*	-19465.0195784	0.758743	465.253	-19468.5478371		
BS7	-19465.0145524	0.758538	467.454	-19468.5428957	-1637	-1601±66
BS8	-19465.0181586	0.758482	470.744	-19468.5468719	-2428	-2475 ±104
BS9*	-19465.0237666	0.758587	466.287	-19468.5525870		
BS10	-19465.0257929	0.758416	466.008	-19468.5548099	-4104	-4132 ± 80
BS11	-19465.0370372	0.759088	459.886	-19468.5664779	-6572	-6497 ± 121
BS12*	-19465.0331178	0.759231	464.033	-19468.5624778		
BS13*	-19465.0392050	0.759273	462.314	-19468.5689249		
BS14	-19465.0391452	0.759221	462.647	-19468.5688558	-7034	-6952± 131
BS15*	-19465.0381709	0.758641	464.608	-19468.5673980		

[a] def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [b] Correction factor for the enthalpy. [c] S here stands for entropy.

Table S21: Additional investigated spin configurations for the δ-isomer at the B3LYP/def2-svp+tzvp level of theory. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1. Entries marked with * were used for fitting, and make up dataset X, together with those in table S20. The other entries were used to test the predictive ability of the method using parameters fitted using dataset X. Δ E is relative to S_{max}.

Species	Flipped spins[a]	J_2	J_{1a}	J_{1b}	J_{1d}	ϵ (Ha)	Found ΔE (cm^{-1})	Predicted ΔE (cm^{-1})
x1*	3,5,6,8,13	120	90	30	15	-19465.03091		
x2*	2,3,6,11,12,13	105	90	30	30	-19465.02918		
x3	4,8,10,11,12,13	105	60	60	15	-19465.03327	-5745	-5468 ± 98
x4	1,5,7,8,10,12	90	120	60	30	-19465.03133	-5320	-5604 ± 134
x5*	1,3,7,9,11,13	105	90	30	30	-19465.03173		
x6	2,4,6,9,10,12	90	120	30	30	-19465.02898	-4803	-4711 ± 125
x7*	3,6,8,13	135	90	30	30	-19465.03428		
x8	3,5,8,10	60	120	60	0	-19465.0251	-3951	-4150 ± 114
x9*	2,4,7,8,10	75	120	30	15	-19465.02517		
x10	2,6,7,12,13	120	120	30	15	-19465.03114	-5277	-5315 ± 122
x11	2,3,4,5,11,13	105	90	60	30	-19465.0345	-6015	-5899 ± 123
x12	1,3,5,7,9,12	90	120	60	45	-19465.03286	-5655	-5887 ± 150
x13*	1,2,3,5,6,9	90	60	60	30	-19465.03165		
x14	3,4,5,7,12	75	120	30	30	-19465.02562	-4067	-4267 ± 122
x15	4,6,8,10,11	75	90	60	30	-19465.03031	-5096	-5012 ± 116
x16*	4,6,7,8,12,13	105	90	30	45	-19465.03036		
x17	1,2,3,4,5,8	90	60	60	30	-19465.03079	-5201	-5308 ± 107
x18*	3,4,9,10,11,13	105	120	30	0	-19465.02756		
x20*	11	15	30	30	0	-19465.01328		
x21*	1,7	30	60	0	30	-19465.01466		
x22*	9,13	165	30	30	0	-19465.03343		
x23*	9,12	30	60	60	0	-19465.02045		
x23*	5,9	30	60	30	15	-19465.01785		
x25	1,5,8	45	90	0	15	-19465.01567	-1882	-2057 ± 80
x26	1,4,10	45	90	30	15	-19465.0195	-2722	-2950 ± 85
x27	1,2,12	45	60	30	30	-19465.0202	-2876	-3085 ± 85
x28*	3,4,13	150	60	60	0	-19465.03661		
x29	1,3,8,13	135	60	30	30	-19465.03378	-5856	-5746 ± 111

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.

Table S22: Investigated spin configurations for the ϵ-isomer. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1.

Species	Flipped spins[a]	S[b]	J_2	J_{1a}	J_{1b}	J_{1d}
S_{max}	–	32.5	–	–	–	–
BS1	13	27.5	180	0	0	0
BS2	1	27.5	165	30	0	15
BS3	1,6	22.5	30	60	0	0
BS4	1,2,3	17.5	60	90	0	0
BS5	1,4,8,10	12.5	45	0	90	0
BS6	1,2,6,7,12	7.5	30	30	60	0
BS7	1,2,3,6,7,12	7.5	30	30	0	30
BS8	1,2,3,4,5,6	2.5	45	60	0	45
BS9	3,5,8,12	12.5	60	30	30	45
BS11	5,8,9,11	12.5	90	60	30	45
BS12	10,11,12,	17.5	105	30	90	30
BS13	7,8,9,10,11,12	2.5	75	60	90	30

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.[b] S is the total spin angular momentum.

Table S23: Energies, including enthalpy and entropy correction terms, of different spin configurations for the ϵ-isomer for the B3LYP exchange and correlation functional. All geometries were optimised with the indicated method for that particular spin state, and with implicit solvation through the polarizable continuum model (PCM). Entries marked with * were used for fitting, together with those in table S24. Δ E is relative to S_{max} at B3LYP/def2-tzvp+svp.

Spin isomer	**def2-tzvp+svp**[a]			**def2-tzvp**	Found	Predicted
	ϵ (Ha)	H_{corr} (Ha)	S[c] (cal/mol·K)	ϵ (Ha)	ΔE (cm^{-1})	ΔE (cm^{-1})
S_{max}	-19464.9963446	0.757269	466.024	-19468.5279268		
BS1*	-19465.0187709	0.757565	465.704	-19468.5516775		
BS2*	-19465.0002740	0.756912	473.450	-19468.5321476		
BS3	-19465.0011233	0.757152	468.128	-19468.5333139	-1049	-1014 ± 36
BS4	-19465.0067713	0.757054	469.938	-19468.5389996	-2248	-2111 ± 53
BS5	-19465.0077015	0.756619	471.388	-19468.5403874	-2493	-2610 ± 79
BS6*	-19465.0131694	0.756894	468.557	-19468.5463908		
BS7	-19465.0121423	0.756929	466.913	-19468.5450399	-3467	-2759 ± 62
BS8*	-19465.0132411	0.756737	466.114	-19468.5457561		
BS9	-19465.0058395	0.756955	468.167	-19468.5386937	-2048	-2028 ± 71
BS11	-19465.0052641	0.756957	465.699	-19468.5380585	-1958	-1934 ± 56
BS12*	-19465.0053570	0.757022	468.413	-19468.5375754		
BS13	-19465.0132030	0.756308	470.576	-19468.5457873	-3700	-3639 ± 76

[a] def2-tzvp was used for all Fe atoms; def2-svp was used for all other atoms. [b] Correction factor for the enthalpy. [c] S here stands for entropy.

Table S24: Additional investigated spin configurations for the ϵ-isomer at the B3LYP/def2-svp+tzvp level of theory. The integers given in each row for J_i are prefactors n_i used to construct a linear equation according to equation S1. Entries marked with * were used for fitting, and make up dataset X, together with those in table S23. The other entries were used to test the predictive ability of the method using parameters fitted using dataset X. Δ E is relative to S_{max}.

Species	Flipped spins[a]	J_2	J_{1a}	J_{1d}	ϵ (Ha)	Found ΔE (cm^{-1})	Predicted ΔE (cm^{-1})	
x1	2,13	165	30	0	15	-19465.0185617	-4876	-4924 ± 72
x2	2,7,13	150	60	0	0	-19465.0158955	-4291	-4315 ± 70
x3	3,12,13	150	60	0	0	-19465.0156031	-4227	-4315 ± 70
x4	1,2,6,7,13	120	90	0	0	-19465.0127536	-3601	-3584 ± 70
x5*	5,8,13	150	60	0	0	-19465.0159445	-4302	
x6*	3,5,8,10	60	120	0	30	-19465.0079799	-2554	
x7*	1,12	30	60	0	30	-19465.0038232	-1641	
x8	2,3	30	30	0	30	-19465.003784	-1633	-1501 ± 39
x9*	1,3	30	30	0	30	-19465.0042545	-1736	
x10*	1,5,7,8,11,13	105	120	0	45	-19465.0145123	-3987	
x11*	2,4,6,7,12	75	120	0	45	-19465.0113905	-3302	
x12*	3,5,12,13	135	90	0	15	-19465.0156888	-4246	
x13	4,5,7,8,11,13	105	90	0	45	-19465.0134133	-3746	-4044 ± 83
x14*	1,3,4,9,10,11	90	120	0	30	-19465.0121495	-3469	
x15*	5,6,8,9,11,12	90	90	0	30	-19465.0120362	-3444	

[a] Fe(III) centres for which the spins have been set to -5/2. All other Fe(III) centres have spins of 5/2.

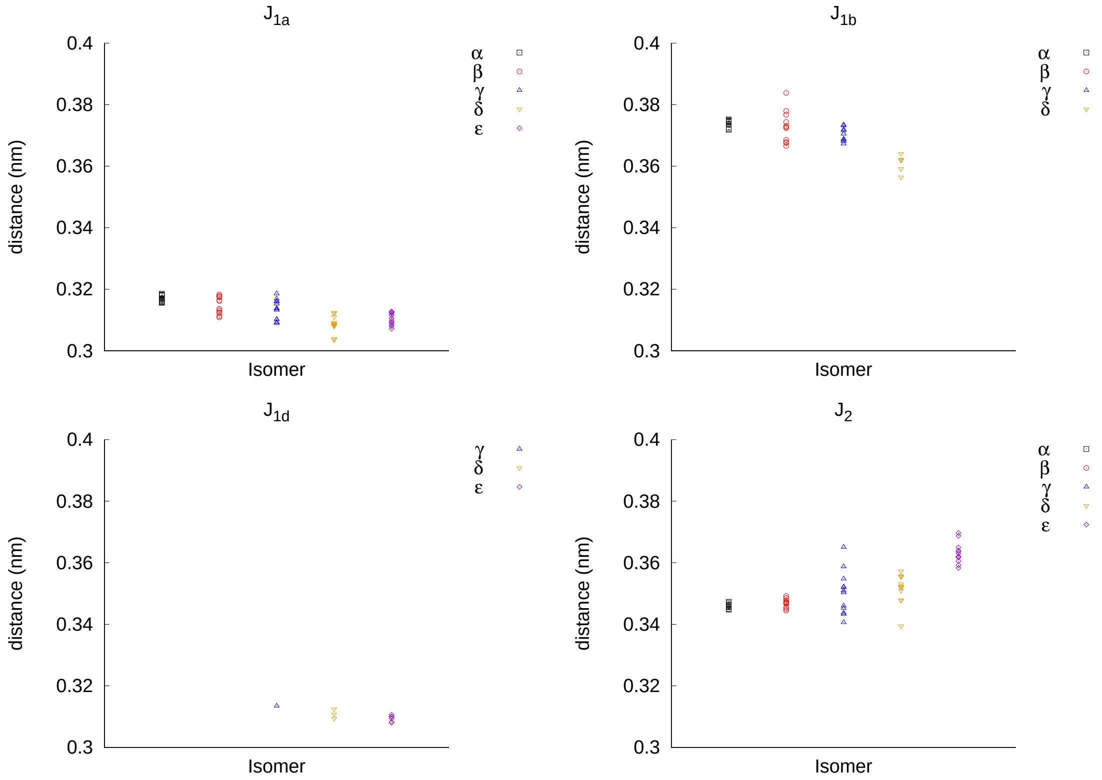

Figure S7: Distances for spin couplings in the S_{max} spin state of different Keggin isomers. Geometries optimised at B3LYP/def2-tzvp+svp. Only the BS data sets were used.

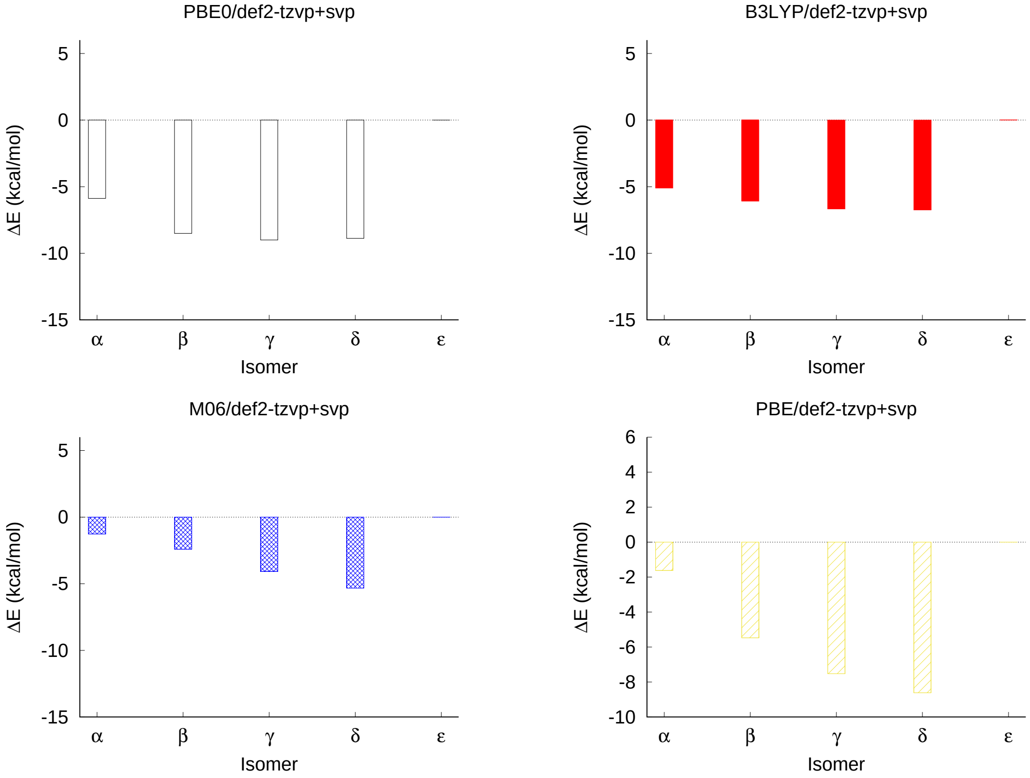

Figure S8: Energies of the different isomers in their highest spin state relative to the ϵ isomer in the highest spin state for geometries optimised using different exchange correlation functionals with the def2-tzvp+svp basis set combination. PCM was used for PBE0, B3LYP and PBE. SMD was used for M06. Only the BS data set was used.

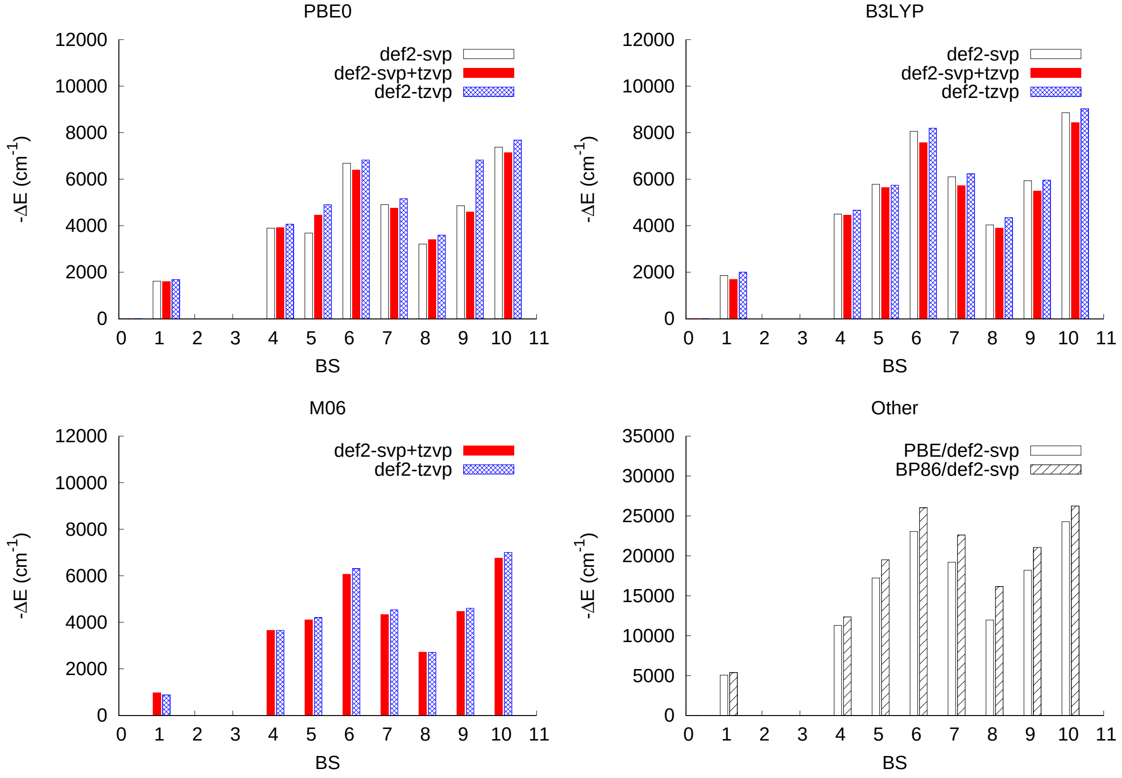

Figure S9: Energies of the different broken symmetry states of the α-isomer relative to the highest spin state for different combinations of basis sets and exchange correlation functionals. Only the BS data set was used. Note that the vertical axis shows -ΔE.

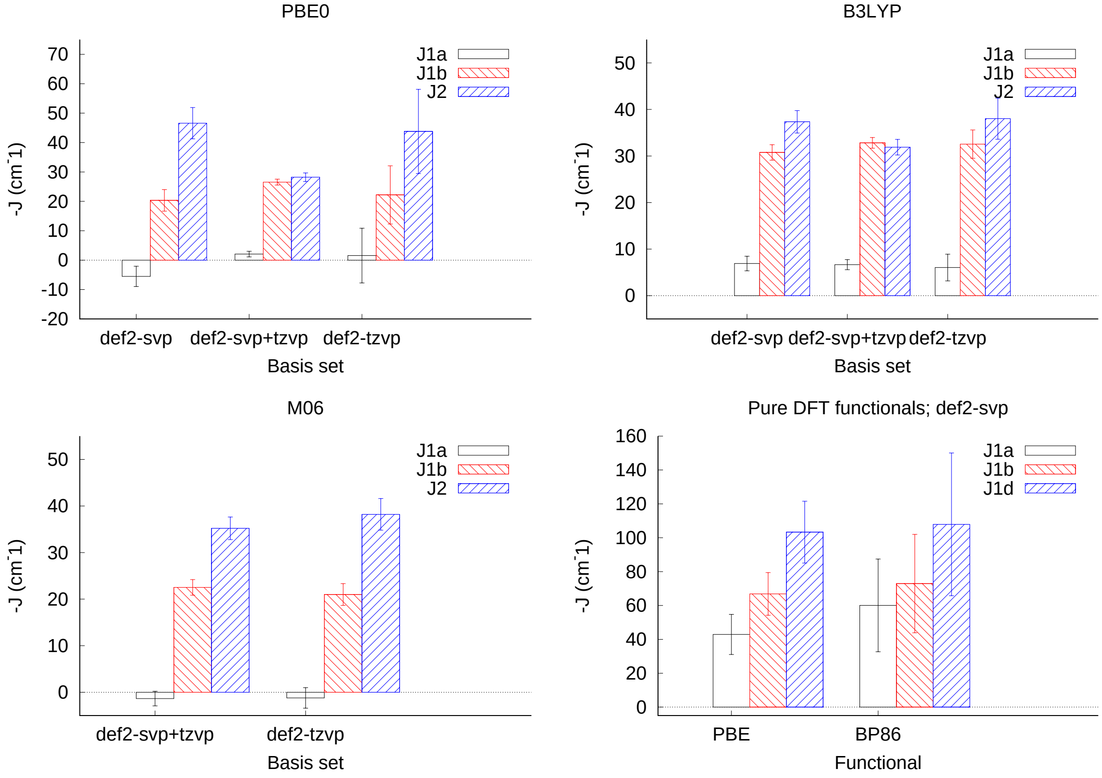

Figure S10: Fitted antiferromagnetic coupling constants for the α isomer for different combinations of basis sets and exchange correlation functionals. Note that the vertical axis shows -J. Only the BS data set was used.

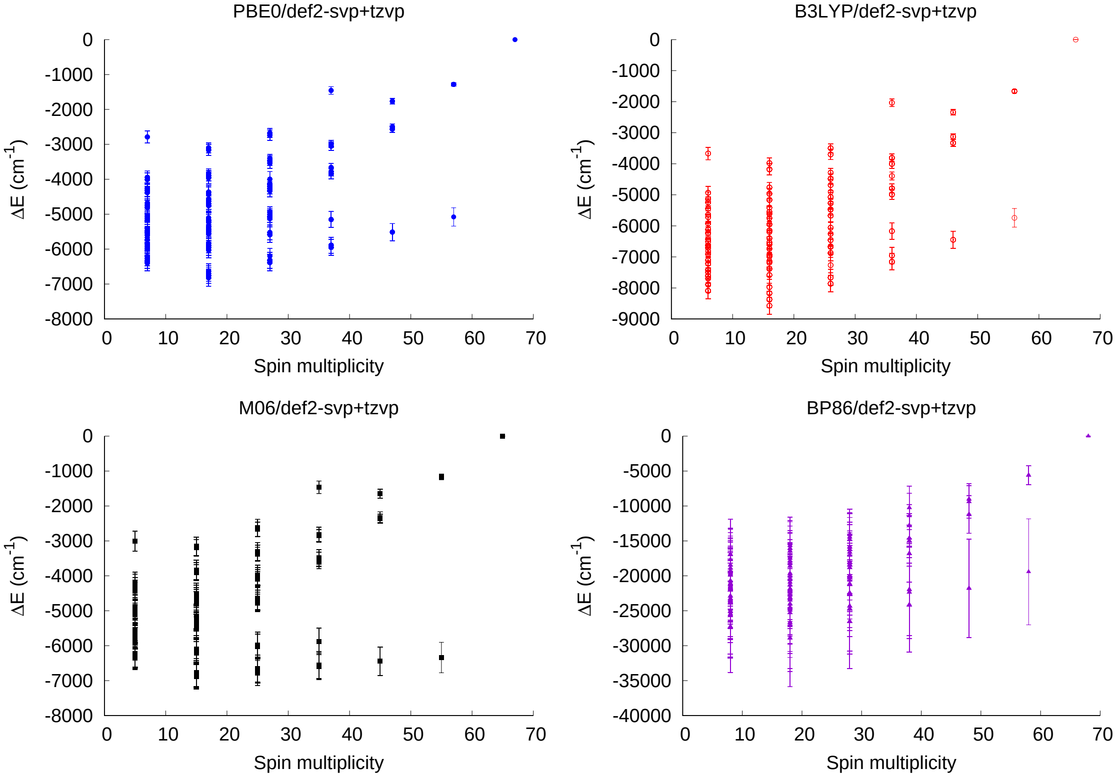

Figure S11: Predicted energies of the different broken symmetry states of the α-isomer relative to the highest spin state for different combinations of basis sets and exchange correlation functionals. Uncertainties propagated according to equation $S2$. Only the BS data set was used.

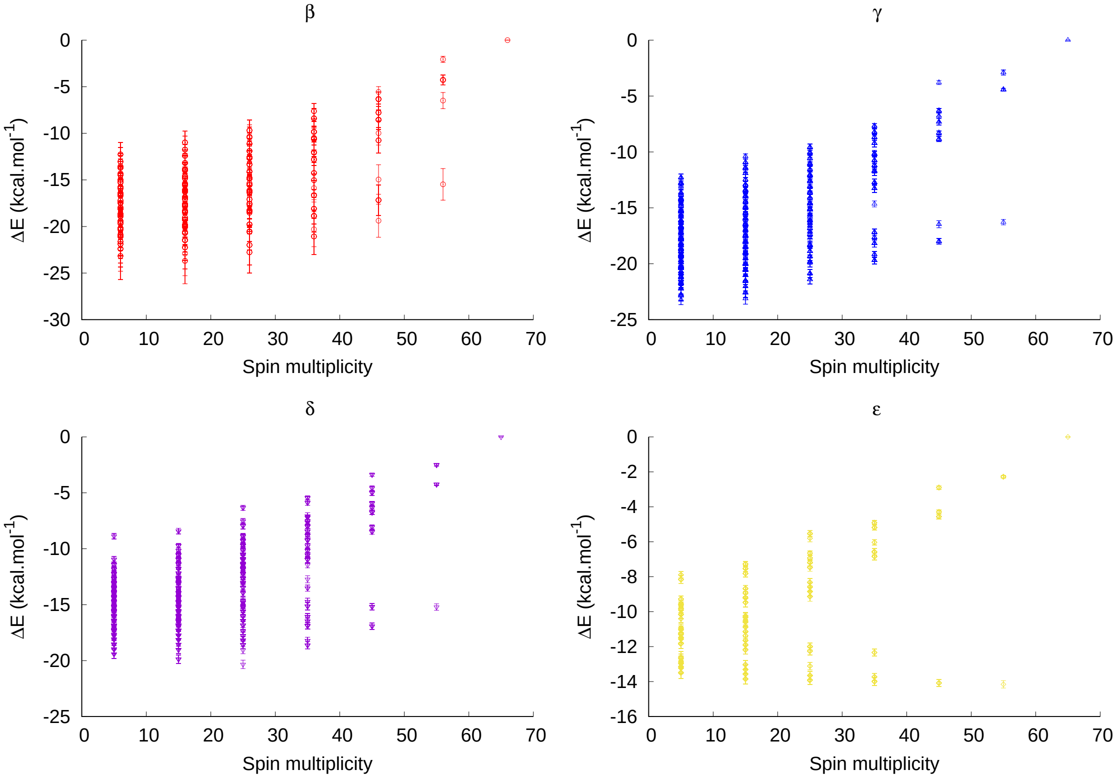

Figure S12: Predicted energies at B3LYP/def2-tzvp+svp of the different broken symmetry states of the β-ϵ isomers, relative to the highest spin state of each isomer. Uncertainties propagated according to equation $S2$. The extended data set was used

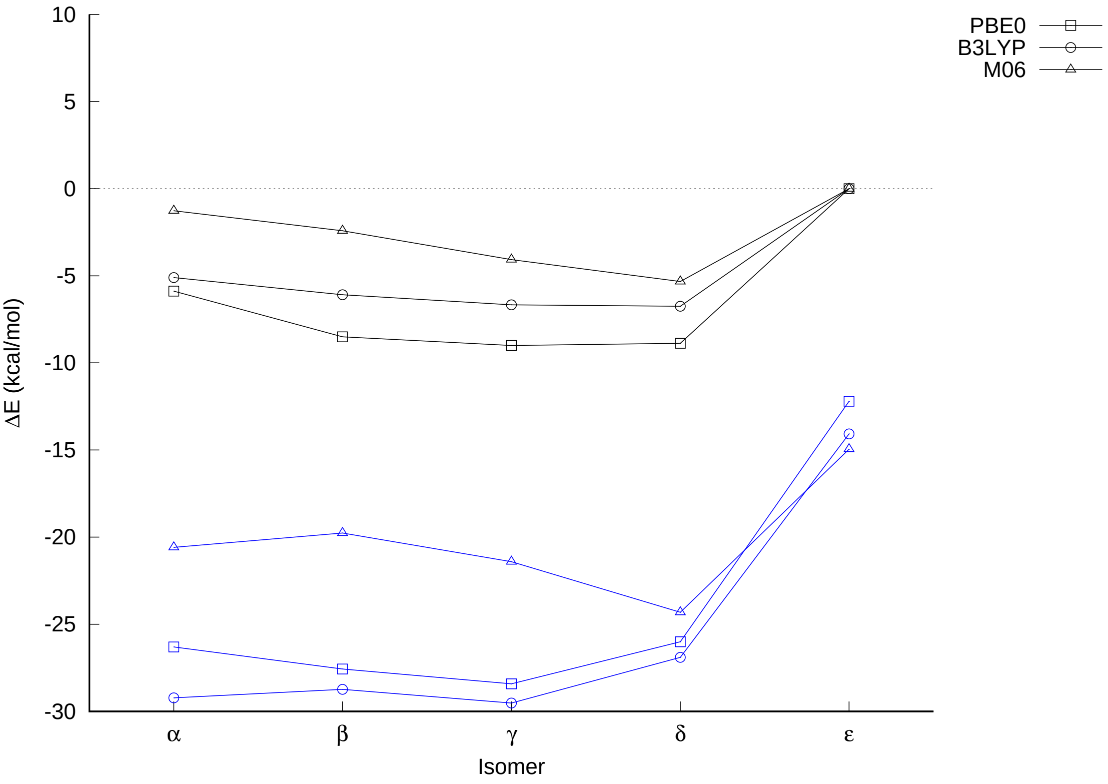

Figure S13: Computed energies of the S_{max} (black) and lowest energy (blue) spin configuration for each isomer at PBE0, B3LYP and M06 with the def2-tzvp+svp basis set. Implicit solvation was used (PCM for PBE0 and B3LYP; SMD for M06).

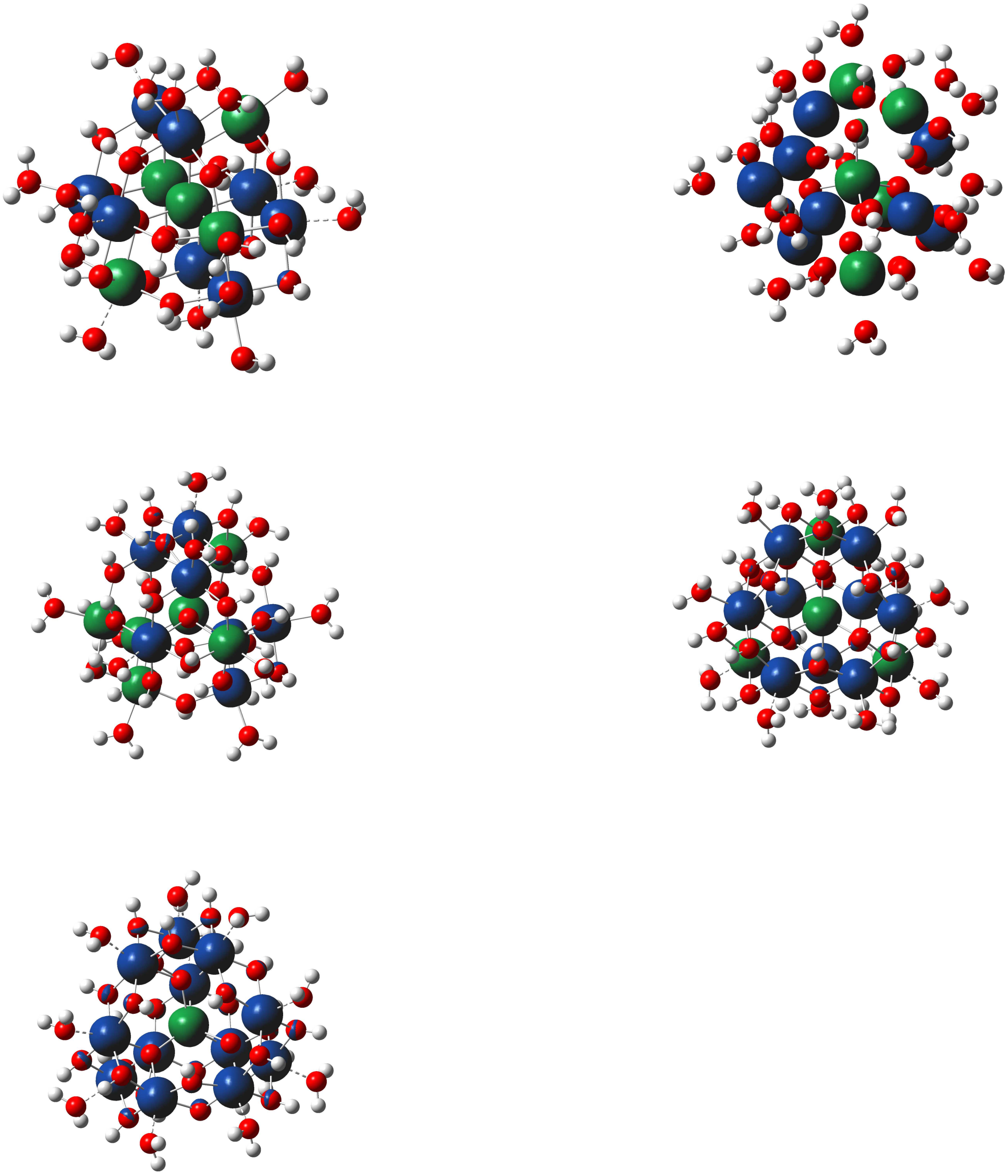

Figure S14: The lowest spin configurations for each Baker-Figgis isomer of the Keggin ion. Blue and green indicate positive and negative spin, respectively. An isodensity value of 0.04 was used to render the figures. Top:α (left), β (right). Middle: γ (left), δ (right). Bottom: ϵ.

J_generator

The source code for J_generator.py is given below (listing S2). Usage is described in the comments in the code, and consists of providing three arguments – which Keggin isomer to use, whether to remove energy/J coupling duplicates, and whether to generate sets of linear equations or to compute energies based on fitted coupling constants.

A partial example output for the command `./J_generator.py a 1 0` is given below. This command can be used to generate sets of linear equations for ΔE as a function of the coupling constants.

```
#Spin   E   dE   J2 J1a J1b  J2 J1a J1b  Spins

66  0.00 0.00 0 0 0 0.00 0.00 0.00 []
56 180.00 180.00 180 0 0 1.00 0.00 0.00 [13]
56 75.00 45.00 15 30 30 0.20 0.40 0.40 [12]
46 225.00 170.37 165 30 30 0.73 0.13 0.13 [12, 13]
46 120.00 73.48 30 30 60 0.25 0.25 0.50 [11, 12]
```

The first row is a header row.

The first row of output is for the S_{max} state with a multiplicity of 66. The second row of output states that there is a spin state (header 'Spin') with a multiplicity of 56. The next two items, 180.00 (header 'E') and 180.00 (header 'dE') have no meaning here, since no energy is computed. The next three items, 180, 0 and 0 (headers 'J2', 'J1a' and 'J1b') shows how the linear equation for ΔE is constructed: $\Delta E = 180 \cdot J_2 + 0 \cdot J_{1a} + 0 \cdot J_{1b}$. The next three items (the second set of headers 'J2', 'J1a' and 'J1b') are not relevant here since no energy is computed. The final [13] (header 'Spins') states that the spin state is achieved by inverting the spin of atom 13.

A partial example output for the command `./J_generator.py a 1 1` is given below. This command computes the energies of the different spin states based on fitted coupling constants. The coupling constants are provided by the user directly in the code.

```
#Spin   E   dE   J2 J1a J1b  J2 J1a J1b  Spins

66  0.00 0.00 0 0 0 0.00 0.00 0.00 []
56 -5773.48 81.63 -5773 0 0 1.00 -0.00 -0.00 [13]
56 -1650.85 20.79 -481 -199 -970 0.29 0.12 0.59 [12]
46 -6462.09 77.36 -5292 -199 -970 0.82 0.03 0.15 [12, 13]
46 -3102.16 34.39 -962 -199 -1940 0.31 0.06 0.63 [11, 12]
```

The first row is a header row.

The first row of output is for the S_{max} state with a multiplicity of 66. The second row of output states that there is a spin state (header 'Spin') with a multiplicity of 56. The next two items, -5773.48 (header 'E') and 81.63 (header 'dE') are the energy ΔE (in cm^{-1}) and uncertainty of the spin state relative to the S_{max} state. The next three items, -5773, 0 and 0 (headers 'J2', 'J1a' and 'J1b') shows the absolute contribution of each coupling constant to the computed energy. The next three items (the second set of headers 'J2', 'J1a' and 'J1b') Show the relative (i.e. fraction) contribution of each coupling constant to the energy. The final [13] (header 'Spins') states that the spin state is achieved by inverting the spin of atom 13.

Systems are defined as functions in spinmatrices.py. An example function is

```
def getExample():
  #Mini is for testing/development purposes. The atoms are at the corner of a square. Direct neighbours couple via J1a, diagonals couple via J2.
  JName=['0','J2','J1a','J1b','J1c','0','0','0','0','0','0','0','0']

  J=[[0,4,3,4], \
     [4,0,2,1], \
     [3,2,0,2], \
```

```
    [4,1,2,0]]
  SpinArray  =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0]
  JValue=[0,-28.2502,-3.92415,1,1,0,0,0,0,0,0,0] # For testing
  JValueError=[0,1.13,1.206,2,2,0,0,0,0,0,0,0]# For testing

  return J, JName, SpinArray, JValue, JValueError
```

JName defines arbitrary names for the different coupling constants.

J is the spin coupling matrix.For example, atom 2 couple with atom 4 via coupling constant number 1 (here J_2; arrays in python start at 0) and with atom 1 via coupling constant number 4 (J_{1c}).

The spin array defines the spin of the atoms in the spin matrix.

JValue and JValueError contain the fitted values of the coupling constants and the standard errors. If they aren't known, the following can be used instead:

```
  JValue= [0 if x=='0' else 1 for x in JName]
  JValueError= [0 if x=='0' else 1 for x in JName]
```

Once a system has been defined in spinmatrices.py, it needs to be added to the getData(Isomer) routine at the end of the spinmatrices.py file.

```
def getData(Isomer):
  if Isomer=='a':
    J,JName,SpinArray,JValue,JValueError=getAlpha()
..
  elif Isomer=='example': #For testing/development purposes
    J,JName,SpinArray,JValue,JValueError=getExample()

  return J,JName,SpinArray,JValue,JValueError
```

It can now be called with `./J_generator.py example 1 0`.

The full program listings follow:

```
#!/usr/bin/python
import sys
import itertools
import numpy as np
from heapq import nlargest
from math import sqrt
import spinmatrices

'''
 Written by Andy Ohlin
 Umea University, Sweden

 20/11/2019
 * Can handle mixed valence
 * Systems are defined in a module file (spinmatrices.py)
 * DO NOT EDIT THIS FILE

 Usage Examples:

 general command: program isomer terse mode
 * isomer can be any system defined in spinmatrices.py, such as a which is presently corresponding to the alpha-epsilon isomers of the Keggin ion,
 or mini, which is a test system. ALL systems should be defined in spinmatrices.py
 * terse is 0 or 1. If 1, then all duplicates (i.e. energetically degenerate states) with the same J formulae are remove
```

```
 * mode is 0 or 1. If 0, J formulae are generated. If 1, energies are calculated, with error propagation, using provided coupling constants.

 Examples:
 python J_generator.py a 0  0 -- compute all permutations of couplings for isomer a (alpha).
 python J_generator.py a 1  0 -- compute all permutations of couplings, but removes all duplicates, whether incidental or symmetry-based. Terse=1
 python J_generator.py a 0  1 -- compute energies from fitted parameters. Terse=0 will allow duplicates.
'''

def GenSpecies(J):
  AllPermutationsX = list(itertools.product([1,-1],repeat=len(J)))
  AllSpecies=[]
  for n in range(0,len(AllPermutationsX)):
    Spins=[]
    for m in range(0,len(AllPermutationsX[n])):
      Spins+=[AllPermutationsX[n][m]*SpinArray[m]]
    AllSpecies+=[Spins]
  return AllSpecies

def getMax(J):
  maximum=0
  for n in J:
    for m in n:
      if m>maximum:
        maximum=m
  return maximum

def GenCoupling(n,J):
  JList=[0]*(getMax(J)+1)

  for m in range(0,len(n)):
    for k in range(0,len(n)):
      if not (m==k) and not(n[m]==n[k]) and not (abs(n[m])/abs(n[k])==(n[m]/n[k])):
        JList[J[m][k]]= JList[J[m][k]] + 2*(SpinArray[m]*SpinArray[k])+SpinArray[k]

  for l in range(0,len(JList)):
    JList[l]=JList[l]/2.0

  Spin=0
  for l in n:
    Spin+=l
  Spin=2*abs(Spin)

  return JList,Spin

def checkpresence(stuff,mylist):
  TF=0
  for n in mylist:
    if stuff == n[4]:
      TF=1
  return TF

def checkjeq(jeq,spin,mylist):
  TF=0
  for n in mylist:
    if jeq==n[2]:
      if int(spin)==n[0]:
        TF=1
  return TF

if __name__ == "__main__":
  Isomer=sys.argv[1]
```

```
  Terse=int(sys.argv[2])
  Predict=int(sys.argv[3])

## DON'T EDIT THIS FILE
## ALL DATA IS COLLECTED FROM SPINMATRICES.PY
  J,JName, SpinArray, JValue, JValueError = spinmatrices.getData(Isomer)

  if Predict==0:
    JValue= [0 if x=='0' else 1 for x in JName]
    JValueError= [0 if x=='0' else 1 for x in JName]


  JList=[0]*(max(max(J))+1)


#Check symmetry of spin matrix
  for n in range(0,len(J)):
    for m in range(0,len(J)):
      if not (J[n][m]-J[m][n]==0):
        print 'Asymmetry', n,m

  #Generates all possible spin flip combinations
  AllSpecies=GenSpecies(J)
  #Generate linear equations and compute spins
  Species=[]

  for n in AllSpecies:
    Couplings, Spin=GenCoupling(n,J)

    Js=Couplings
    JTot=0.0

    # Energy
    EnergyDifference=0
    EnergyError=0
    Jeq=[0]*(getMax(J)+1)

    for m in range(0,(getMax(J)+1)):
      Jeq[m]+=Js[m]*JValue[m]
      JTot+=Jeq[m]
      EnergyDifference+=JValue[m]*Js[m]
      EnergyError+=JValueError[m]*JValueError[m]*Js[m]*Js[m]

    # Generate percentage contributions
    JContrib=[0]*(getMax(J)+1)
    for m in range(0,(getMax(J)+1)):
      if JTot==0:
        JContrib[m]=0.0
      else:
        JContrib[m]=float(Jeq[m]/JTot)

    #Find flipped spins
    positions=[i+1 for i,x in enumerate(n) if x < 0]
    Flipped=positions

    if len(Flipped)>(len(J)/2): #Fixed
      positions=list(set(range(1,len(J)+1))-set(Flipped)) #Fixed
      positions.sort()

    #Weed out dupes:
    if not checkpresence(positions,Species):
      if Terse==1:
        if not ( checkjeq(Jeq,Spin, Species)):
          Species+=[[int(Spin)+1,EnergyDifference,Jeq,JContrib, positions,sqrt(EnergyError)
    ]]
```

```
      elif Terse==0:
        Species+=[[int(Spin)+1,EnergyDifference,Jeq,JContrib, positions,sqrt(EnergyError)]]

# print Species
  JNames=''
  for n in JName:
    if not n=='0':
      JNames+=str(n)+'\t'
  StringToWrite='#Spin \t E \t dE \t %s %s Spins \n' % (str(JNames),str(JNames))

  print StringToWrite
  for Specie in Species:

    StringToWrite=''

    StringToWrite='%s\t' % str(Specie[0])
    StringToWrite+='%5.2f\t' % float(Specie[1])
    StringToWrite+='%3.2f\t' % float(Specie[5])

    #J coupling equation
    Jeqstr=''

    for n in range(0,len(Specie[2])):

      if not JName[n]=='0':
        Jeqstr+="%d\t"%(Specie[2][n])
    StringToWrite+=Jeqstr

    #J contribution
    Jeqstr=''
    for n in range(0,len(Specie[3])):
      if not JName[n]=='0':
        Jeqstr+="%1.2f\t"%(Specie[3][n])

    StringToWrite+=Jeqstr
    StringToWrite+=str(Specie[4])
    print StringToWrite
```

Listing S1: Source code for the J_generator.py software

```
''' For each system the following must be defined:
J --
JName --
SpinArray --

If 'mode' is 1, for each system the following also needs to be defined:
JValue --
JValueError  --


NOTE: You also need to point to the right function in getData() at the end of this file, which takes the
command-line argument regarding system to use

'''


def getAlpha():
  # The alpha Fe(III)13 Baker-Figgis-Keggin isomer
  JName=['0','J2','J1a','J1b','0','0','0','0','0','0','0','0','0']
  #Spin coupling matrix
  J=[[0, 2, 2, 0, 0, 3, 3, 0, 0, 0, 0, 0, 1], \
     [2, 0, 2, 0, 0, 0, 0, 0, 3, 3, 0, 0, 1], \
     [2, 2, 0, 3, 0, 0, 0, 0, 0, 0, 0, 3, 1], \
     [0, 0, 3, 0, 2, 2, 0, 0, 0, 0, 0, 3, 1], \
```

```
     [0, 0, 0, 2, 0, 2, 0, 3, 0, 0, 3, 0, 1], \
     [3, 0, 0, 2, 2, 0, 3, 0, 0, 0, 0, 0, 1], \
     [3, 0, 0, 0, 0, 3, 0, 2, 2, 0, 0, 0, 1], \
     [0, 0, 0, 0, 3, 0, 2, 0, 2, 0, 3, 0, 1], \
     [0, 3, 0, 0, 0, 0, 2, 2, 0, 3, 0, 0, 1], \
     [0, 3, 0, 0, 0, 0, 0, 0, 3, 0, 2, 2, 1], \
     [0, 0, 0, 0, 3, 0, 0, 3, 0, 2, 0, 2, 1], \
     [0, 0, 3, 3, 0, 0, 0, 0, 0, 2, 2, 0, 1], \
     [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0]]

  #Spins of the centres in the coupling matrix
  SpinArray
    =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/


#   Fitted data:
#   Only used when mode is 1. Not needed for mode 0.
  #JValue=[0,-35.2112,1.35205,-22.5191,0,0,0,0,0,0,0,0] # M06/svp+tzvp w smd
  #JValueError=[0,2.423,1.574,1.672,0,0,0,0,0,0,0,0] # M06/svp+tzvp w smd
  #JValue=[0,-107.911,-60.0534,-72.9388,0,0,0,0,0,0,0,0] #BP86/svp+tzvp w pcm
  #JValueError=[0,42.13,27.36,29.07,0,0,0,0,0,0,0,0] # BP86/svp+tzvp w pcm
  #JValue=[0,-28.2093,-2.06856,-26.5474,0,0,0,0,0,0,0,0] #PBE0/svp+tzvp w pcm
  #JValueError=[0,1.459,0.9474,1.007,0,0,0,0,0,0,0,0] # PEB0/svp+tzvp w pcm
  #JValue=[0,-31.8966,-6.65384,-32.874,0,0,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm  -- only BS
    set
  #JValueError=[0,1.667,1.082,1.150,0,0,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm -- only BS set
  JValue=[0,-32.0749,-6.65149,-32.3395,0,0,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm  X set
  JValueError=[0,0.4535,0.4495,0.4761,0,0,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm X set

  return J, JName, SpinArray, JValue, JValueError

def getBeta():
  # The beta Fe(III)13 Baker-Figgis-Keggin isomer
  # beta 2=j1a, 3=j1b, 1=j2, 4=j1c
  JName=['0','J2','J1a','J1b','0','0','0','0','0','0','0','0','0']
  J=[[0, 2, 2, 3, 0, 3, 0, 0, 0, 0, 0, 0, 1], \
     [2, 0, 2, 0, 0, 0, 3, 0, 3, 0, 0, 0, 1], \
     [2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 3, 3, 1], \
     [3, 0, 0, 0, 2, 2, 0, 0, 0, 0, 0, 3, 1], \
     [0, 0, 0, 2, 0, 2, 0, 3, 0, 0, 3, 0, 1], \
     [3, 0, 0, 2, 2, 0, 3, 0, 0, 0, 0, 0, 1], \
     [0, 3, 0, 0, 0, 3, 0, 2, 2, 0, 0, 0, 1], \
     [0, 0, 0, 0, 3, 0, 2, 0, 2, 0, 3, 0, 1], \
     [0, 3, 0, 0, 0, 0, 2, 2, 0, 0, 3, 0, 1], \
     [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 2, 1], \
     [0, 0, 3, 0, 3, 0, 0, 3, 3, 2, 0, 2, 1], \
     [0, 0, 3, 3, 0, 0, 0, 0, 0, 2, 2, 0, 1], \
     [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0]]

  SpinArray
    =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/


  #JValue=[0,-32.9785,1.83288,-29.7841,0,0,0,0,0,0,0,0]#  b3lyp/svp+tzvp w pcm -- only BS set
  #JValueError=[0,1.566,2.684,2.274,0,0,0,0,0,0,0,0]#  b3lyp/svp+tzvp w pcm -- only BS set
  JValue=[0,-30.0717,-8.99948,-25.7675,0,0,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm X set
  JValueError=[0,3.295,3.445,4.675,0,0,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm X set
  return J, JName, SpinArray, JValue, JValueError

def getGamma():
  # The gamma Fe(III)13 Baker-Figgis-Keggin isomer

  JName=['0','J2','J1a','J1b','0','J1d','0','0','0','0','0','0','0']
  J=[[0, 2, 2, 0, 0, 5, 0, 0, 0, 0, 0, 0, 1], \
     [2, 0, 2, 0, 0, 0, 3, 0, 3, 0, 0, 0, 1], \
```

```
      [2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 3, 3, 1], \
      [0, 0, 0, 0, 2, 2, 0, 0, 0, 3, 0, 3, 1], \
      [0, 0, 0, 2, 0, 2, 3, 3, 0, 0, 0, 0, 1], \
      [5, 0, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 1], \
      [0, 3, 0, 0, 3, 0, 0, 2, 2, 0, 0, 0, 1], \
      [0, 0, 0, 0, 3, 0, 2, 0, 2, 3, 0, 0, 1], \
      [0, 3, 0, 0, 0, 0, 2, 2, 0, 0, 3, 0, 1], \
      [0, 0, 0, 3, 0, 0, 0, 3, 0, 0, 2, 2, 1], \
      [0, 0, 3, 0, 0, 0, 0, 0, 3, 2, 0, 2, 1], \
      [0, 0, 3, 3, 0, 0, 0, 0, 0, 2, 2, 0, 1], \
      [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0]]

  SpinArray
    =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/

  #JValue=[0,-31.1054,-6.77049,-29.046,0,-24.4109,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm
  #JValueError=[0,0.2046,0.4864,0.2716,0,1.717,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm
  JValue=[0,-31.6417,-6.27393,-29.4497,0,-23.3231,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm X set
  JValueError=[0,0.4647,1.026,0.9103,0,4.839,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm X set
  return Jgamma, JNameGamma, SpinArray, JValueGamma, JValueGammaError

def getDelta():
  JName=['0','J2','J1a','J1b','0','J1d','0','0','0','0','0','0','0']

  J=[[0, 2, 2, 0, 0, 5, 0, 0, 0, 0, 0, 0, 1], \
      [2, 0, 2, 0, 0, 0, 5, 0, 0, 0, 0, 0, 1], \
      [2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 3, 3, 1], \
      [0, 0, 0, 0, 2, 2, 0, 0, 0, 3, 0, 3, 1], \
      [0, 0, 0, 2, 0, 2, 0, 5, 0, 0, 0, 0, 1], \
      [5, 0, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 1], \
      [0, 5, 0, 0, 0, 0, 0, 2, 2, 0, 0, 0, 1], \
      [0, 0, 0, 0, 5, 0, 2, 0, 2, 0, 0, 0, 1], \
      [0, 0, 0, 0, 0, 0, 2, 2, 0, 3, 3, 0, 1], \
      [0, 0, 0, 3, 0, 0, 0, 0, 3, 0, 2, 2, 1], \
      [0, 0, 3, 0, 0, 0, 0, 0, 3, 2, 0, 2, 1], \
      [0, 0, 3, 3, 0, 0, 0, 0, 0, 2, 2, 0, 1], \
      [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0]]
  SpinArray
    =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/


  #JValue=[0,-29.806,-5.07834,-30.0776,0,-15.1673,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm
  #JValueError=[0,0.7859,1.42,1.18,0,2.581,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm
  JValue=[0,-29.5641,-4.92424,-29.759,0,-18.8791,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm X set
  JValueError=[0,0.5596,0.7783,0.9269,0,1.995,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm X set

  return J, JName, SpinArray, JValue, JValueError

def getEpsilon():
  JName=['0','J2','J1a','0','0','J1d','0','0','0','0','0','0','0']
  JValue= [0 if x=='0' else 1 for x in JName]
  JValueError= [0 if x=='0' else 1 for x in JName]

  J=[[0, 2, 2, 0, 0, 5, 0, 0, 0, 0, 0, 0, 1], \
      [2, 0, 2, 0, 0, 0, 5, 0, 0, 0, 0, 0, 1], \
      [2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 5, 1], \
      [0, 0, 0, 0, 2, 2, 0, 0, 0, 5, 0, 0, 1], \
      [0, 0, 0, 2, 0, 2, 0, 5, 0, 0, 0, 0, 1], \
      [5, 0, 0, 2, 2, 0, 0, 0, 0, 0, 0, 0, 1], \
      [0, 5, 0, 0, 0, 0, 0, 2, 2, 0, 0, 0, 1], \
      [0, 0, 0, 0, 5, 0, 2, 0, 2, 0, 0, 0, 1], \
      [0, 0, 0, 0, 0, 0, 2, 2, 0, 0, 5, 0, 1], \
      [0, 0, 0, 5, 0, 0, 0, 0, 0, 0, 2, 2, 1], \
      [0, 0, 0, 0, 0, 0, 0, 0, 5, 2, 0, 2, 1], \
      [0, 0, 5, 0, 0, 0, 0, 0, 0, 2, 2, 0, 1], \
```

```
      [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0]]

  SpinArray =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/

  #JValue=[0,-28.2502,-3.92415,0,0,-18.7115,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm
  #JValueError=[0,1.13,1.206,0,0,2.474,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm
  JValue=[0,-27.5094,-3.14517,0,0,-19.3922,0,0,0,0,0,0] # b3lyp/svp+tzvp w pcm X set
  JValueError=[0,0.4107,0.5585,0,0,1.115,0,0,0,0,0,0]# b3lyp/svp+tzvp w pcm X set
  return J, JName, SpinArray, JValue, JValueError

def getExample():
  #Example is for testing/development purposes. The atoms are at the corner of a square. Direct neighbours couple via J1a, diagonals couple via J2.
  JName=['0','J2','J1a','J1b','J1c','0','0','0','0','0','0','0','0']

  J=[[0,4,3,4], \
      [4,0,2,1], \
      [3,2,0,2], \
      [4,1,2,0]]
  SpinArray =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0]
  #JValue=[0,-28.2502,-3.92415,1,1,0,0,0,0,0,0,0] # For testing
  #JValueError=[0,1.13,1.206,2,2,0,0,0,0,0,0,0]# For testing
  JValue= [0 if x=='0' else 1 for x in JName]
  JValueError= [0 if x=='0' else 1 for x in JName]

  return J, JName, SpinArray, JValue, JValueError

def getIs():
  #is -- iron-sulfur cluster -- [Fe6S6Cl6]-. Atom 6 is Fe(II), rest are Fe(III). S bridges. Cl terminal.
  # Czerwinski, INt J. Quant Chem, 1999, 72, 39
  JName=['0','J1','J2','J3','J4','0','0','0','0','0','0','0','0']

  J=[[0,3,4,2,2,1], \
      [3,0,2,4,2,1], \
      [4,2,0,3,2,1], \
      [2,4,3,0,2,1], \
      [2,2,2,2,0,1], \
      [1,1,1,1,1,0]]

  SpinArray =[5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,5.0/2.0,4.0/2.0]

  #JValue=[0,-28.2502,-3.92415,1,1,0,0,0,0,0,0,0] # For testing
  #JValueError=[0,1.13,1.206,2,2,0,0,0,0,0,0,0]# For testing
  JValue= [0 if x=='0' else 1 for x in JName]
  JValueError= [0 if x=='0' else 1 for x in JName]

  return J, JName, SpinArray, JValue, JValueError

def getData(Isomer):
  if Isomer=='a':
    J,JName,SpinArray,JValue,JValueError=getAlpha()
  elif Isomer=='b':
    J,JName,SpinArray,JValue,JValueError=getBeta()
  elif Isomer=='g':
    J,JName,SpinArray,JValue,JValueError=getGamma()
  elif Isomer=='d':
    J,JName,SpinArray,JValue,JValueError=getDelta()
  elif Isomer=='e':
    J,JName,SpinArray,JValue,JValueError=getEpsilon()
  elif Isomer=='example': #For testing/development purposes
    J,JName,SpinArray,JValue,JValueError=getExample()
  elif Isomer=='is': #For testing/development purposes
    J,JName,SpinArray,JValue,JValueError=getIs()
```

```
    return J,JName,SpinArray,JValue,JValueError
```

Listing S2: Source code for spinmatrices.py software