Predicting paramagnetic ^{1}H NMR chemical shifts and state-energy separations in spin-crossover host-guest systems

William C. Isley III,[a] Salvatore Zarra,[b] Rebecca K. Carlson,[a] Rana A. Bilbeisi,[b] Tanya K. Ronson,[b] Jonathan R. Nitschke,[b]* Laura Gagliardi,[a]* and Christopher J. Cramer[a]*

[a] *Department of Chemistry, Chemical Theory Center, and Supercomputer Institute, University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455, U.S.A.*

[b] *Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, U.K.*

Supporting Information

Contents

I. Computational Methods

A. Optimization and Thermochemistry

Geometry optimizations were performed for all species at the M06-L[1] level of density functional theory (the M06-L functional was chosen based on its benchmarked performance for the prediction of structural and energetic properties of molecules incorporating transition metals[2, 3]). For Fe and Co atoms, the Stuttgart-Dresden (SDD) ECP10MDF [8s7p6d2f | 6s5p3d2f] basis set and associated pseudopotentials[4, 5] were used; the MIDI! basis[6] was used C, N, and H atoms; the 6-31+G(d) basis was used for S and O atoms. The nature of stationary points was assessed in all cases by computation of analytic vibrational frequencies, which were also used to compute the molecular partition functions necessary to predict 298 K thermochemical quantities using the conventional ideal-gas, rigid-rotator, quantum-mechanical quasi-harmonic-oscillator[7] approximation.[8] Improved electronic energies were computed, as single-point calculations, using the same SDD basis set for Fe and Co but replacing MIDI! or 6-31+G(d), with 6-311+G(2df,p) for all other atoms. We will refer to enthalpies and free energies computed by adding lower level thermal contributions to this higher level electronic energy as simply M06-L enthalpies and free energies, respectively.

B. Spin State Splitting

Spin state splitting energies were computed at the CASSCF/PT2 level of theory. All multiconfigurational calculations were performed with the MOLCAS 7.8 package.[9] The basis sets used were the relativistic all electron ANO-RCC basis sets[10, 11] with the following contractions: [7s6p4d2f1g] for Fe, [5s4p2d1f] for N, [3s2p], and [2s1p] for H. For CASPT2, an imaginary level shift of 0.2 was used to reduce the presence of intruder states.[12] The symmetry group of the cluster is C_1, with an electronic symmetry of ^{1}A. All integrals were computed with the RICD approximation.[13]

In addition, several functionals were compared to the CAS splitting energies including M06-L, M06, M06-2X, M11-L, B3LYP, PBE, PBE0, O3LYP, and OPBE. The basis set used for these computations was the same as for the improved electronic energies as stated above.

C. Paramagnetic NMR

The paramagnetic NMR chemical shift can be approximated[14] for S = ½ as

$$\delta = \delta_{orb} + \delta_{FC} + \delta_{SD} \quad \text{(S1)}$$

where the three contributors to the total isotropic chemical shift are an orbital term, computed analogously as for diamagnetic systems, a Fermi contact term, and a spin–dipole term. The Fermi contact (FC) shift originates from the Fermi contact interaction between the nuclear magnetic moment, and the average spin density at the nucleus.[14] The spin–dipole (SD) term derives from the dipolar interaction between the magnetic moment of unpaired electron density and the nuclear magnetic moment of interest. The spin-dipole term has unfortunately been termed the "pseudocontact" shift; and has been the cause of some confusion in the literature. The pseudocontact interaction originates from the spin-orbit correction to the FC interaction.

For an S = ½ system, the absolute chemical shielding can be expressed as

$$\sigma_K = \sigma_{K,orb} - \frac{S(S+1)}{3k_B T} \frac{\mu_B}{g_{N,K}\mu_{N,K}} g \cdot A_K^T \quad \text{(S2)}$$

where $\sigma_{K,orb}$ is the orbital shielding for nuclei K, S is the effective spin, μ_B and $\mu_{N,K}$ are the Bohr and nuclear magneton, respectively, $g_{N,K}$ is the nuclear g-value of nucleus K (note that the nuclear g-value is commonly substituted for the nuclear gyromagnetic ratio $\gamma_K = \mu_{N,K} g_{N,K}/\hbar$), k_B is the Boltzmann constant, T is the temperature, the g tensor is the electronic g-tensor, and A_K is the hyperfine coupling tensor at nucleus K, the T superscript denotes the transpose. The non-relativistic hyperfine coupling tensor can be separated into the isotropic Fermi contact term, and the anisotropic dipolar coupling term. There are other terms arising from spin-orbit coupling (SOC) which can be separated into the isotropic pseudocontact (PC) term, the anisotropic symmetric and anti-symmetric contributions.

Since solution based experimental measurements only report the isotropic contributions, by removing the anisotropic and anti-symmetric terms equation S2 can be reduced to (omitting K for simplicity)

$$\sigma^{iso} = \sigma^{iso}_{orb} - \frac{S(S+1)}{3k_BT}\frac{2\pi\mu_B}{g_N\mu_N}\left[g_{iso}A_{FC} + g_eA_{PC} + \frac{1}{3}Tr(\Delta\tilde{g}\cdot A_{SD})\right] \quad \text{(S3)}$$

where A_{FC} is the isotropic Fermi contact hyperfine coupling constant, A_{PC} is the isotropic pseudocontact hyperfine coupling constant, and the remaining isotropic term is taken from the tensor product between the g-tensor and the spin-dipolar hyperfine coupling tensor (since A_{SD} is symmetric, the transpose idempotent).

For isotropic systems 3*d* metal systems,[15-17] the Fermi contact term is presumed to massively dominate the pseudocontact and spin-dipolar contributions and thus these spin-orbit and anisotropic contributions are neglected. The pseudocontact term δ_{PC} has previously been shown[15, 16, 18, 19] to be negligibly small in Co- and Fe-containing systems similar to those studied here. Thus the computed absolute chemical shift becomes

$$\sigma^{iso} = \sigma^{iso}_{orb} - \frac{S(S+1)}{3k_BT}\frac{2\pi\mu_B}{\gamma}g_{iso}A_{FC} \quad \text{(S4)}$$

where γ is the gyromagnetic ratio for nucleus K, g_{iso} is the isotropic *g*-factor, μ_B is the Bohr magneton, $A_{iso}$is the isotropic hyperfine coupling constant for nucleus K in frequency units (multiply by $\hbar$ if the HFC is in energy units), S is the electronic total spin, k_B is Boltzmann's constant, and T is temperature. Since σ_{iso} is an absolute chemical shielding, the observable chemical shift becomes

$$\delta = \sigma_{ref} - \sigma_{iso} \quad \text{(S5)}$$

where σ_{ref} is the chemical shift of a reference compound, typically tetramethylsilane (TMS).

^{1}H chemical shifts δ_{orb}, referenced to tetramethylsilane (TMS), were computed at the B3LYP level of DFT employing the all-electron 6-311+G basis set[20, 21] for the metal atoms and the EPR-II basis[22] for C, N, H, O and the 6-311+G(2df) basis[23, 24] for S. The isotropic chemical shielding constants were computed using the SMD continuum solvation model with a water solvent.[25] At this level of theory, σ_{TMS} = 31.9449. We chose to use the B3LYP functional based on previously demonstrated good NMR and EPR performance for metal-containing systems like those studied here,[18] although we do *not* consider electronic energies computed from this level of

theory as Swart has shown B3LYP to do poorly for the prediction of spin-state-energy splitting in iron coordination compounds.[26]

While the costly pseudocontact spin-orbit correction to the hyperfine tensor can be neglected, inclusion of the spin-orbit correction to the *g*-tensor is critical. Hyperfine coupling constants and the *g*-tensor were computed using the DFT level of theory in gas phase within the spin orbit mean field approximation SOMF(1X).[27]

D. Zero Field Splitting

The extension for systems with S > ½ using the zero-field splitting interaction is neglected in this work; discussion of why we neglect this follows. The prior formalism is derived for the S = ½ spin state, and extensions for systems having S > ½ involve incorporation of the zero field splitting (ZFS) phenomenon. Several methods have been derived to account for ZFS effects on paramagnetic shifts,[28-30] and this work has examined the effect from the extended formulation for the Kurland and McGarvey [28, 29]

$$\sigma_{con}^{iso} = \frac{2\pi S(S+1)}{\gamma \quad 3kT}\mu_B\left[1 + \lambda_{KMcG}^{(1)} + \lambda_{KMcG}^{(2)}\right]g_{iso}A_{FC} \qquad \text{(S6)}$$

where σ_{con}^{iso} is the ZFS corrected isotropic contact shielding, the first order ZFS correction term $\lambda_{KMcG}^{(1)}$ is given in from Hrobarik *et al.*[29] equation 39 , and the second order ZFS correction term $\lambda_{KMcG}^{(2)}$ is spin dependent and selected from Hrobarik *et al.*[29] equations 40(a-d) according to the S quantum number. The magnetic anisotropy was computed using the coupled-perturbed spin orbit correction method of Neese.[31] The ZFS correction to paramagnetic chemical shifts was examined for a computed ZFS parameter of quintet Fe^{II}, D = -3.65 cm^{-1}, and found to change σ_{con}^{iso} by 0.02%. Since this method is known to underestimate the D value,[32, 33] additional estimates for the upper limit of the ZFS correction were performed with larger D values. For the Fe^{II} quintet, a D = -45 cm^{-1} yields a change in σ_{con}^{iso} by -0.87%. Given the small magnitude of this correction and the expense of computing D, the ZFS correction will be neglected.

II. Computational Results

A. Correlation Between Experiment and Predicted ^{1}H NMR

A linear regression is made between the predicted chemical shifts of $[Co(\mathbf{1})_3]^{1-}$ to the ^{1}H NMR spectra of the full cage (depicted in Figure S1). For this regression, the experimental assignments are swapped for the ^{1}H pairs (pyr-3 with pyr-5) and (phe-2 with phe-2′). We note that the pyr-6 ^{1}H is a strong outlier with regard to experimental measurements, and the deviation for this point from fit is over 1.7σ.

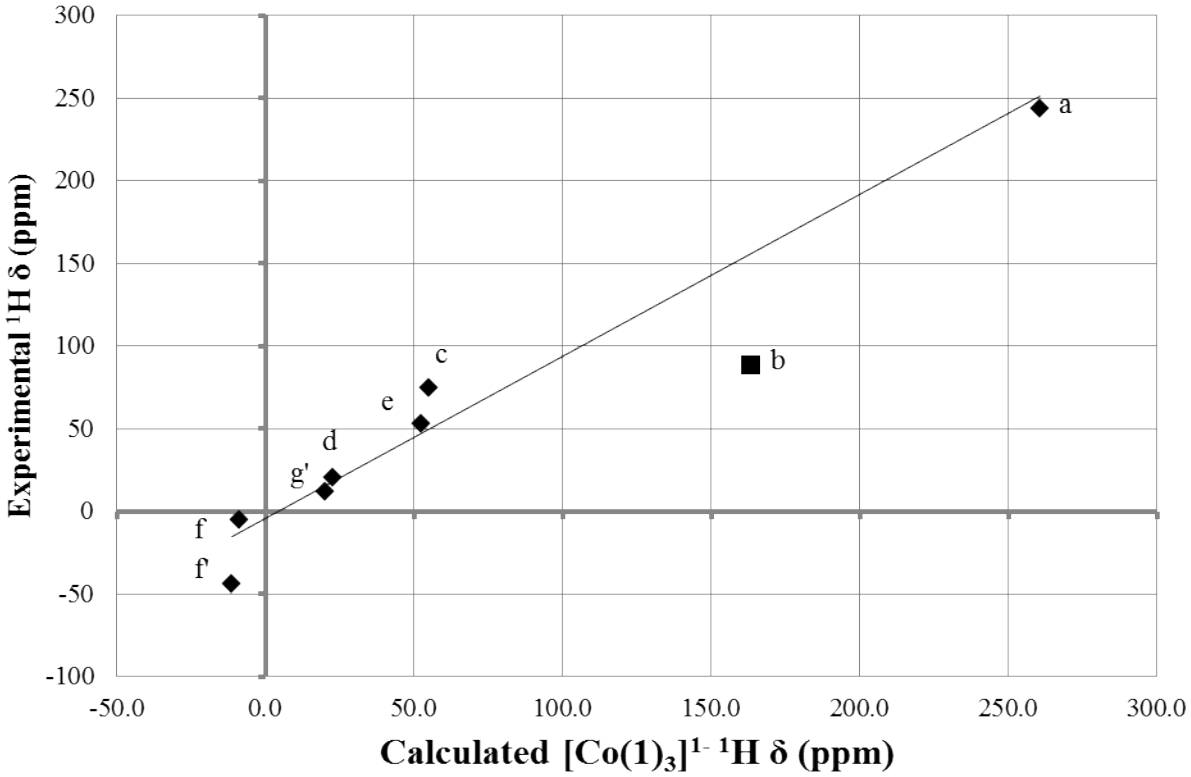


Figure S1. Correlation between calculated δ (ppm) for $[Co(\mathbf{1})_3]^{1-}$ and experimental δ (ppm) for **A**. Linear fit is also shown, the pyr-6 proton is excluded from the fit. $[Co(1)_3]^{1-}$ protons, labeled according to Scheme 1, included in the fit are represented by diamonds, and H_b is represented by squares. With an $R^2 = 0.9697$, the line of best fit equation is

$$\delta_{exp} = 0.979(\delta_{pred}) - 4.024 \qquad \text{(S7)}$$

B. Results for $[Co(2)_3]^{2+}$

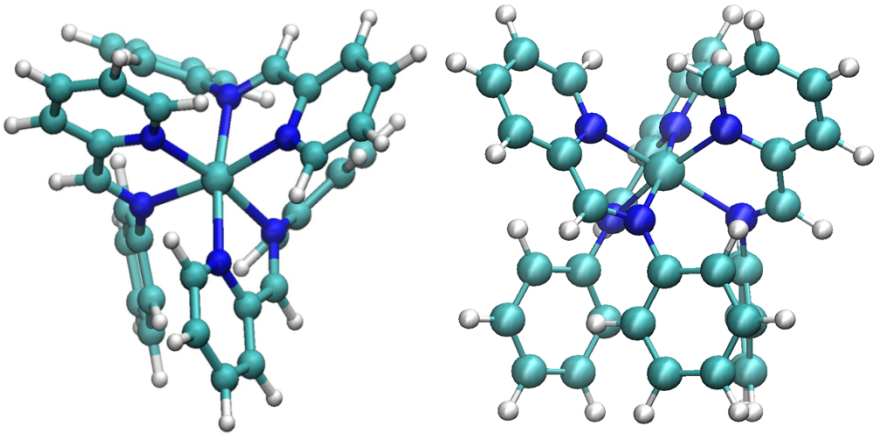
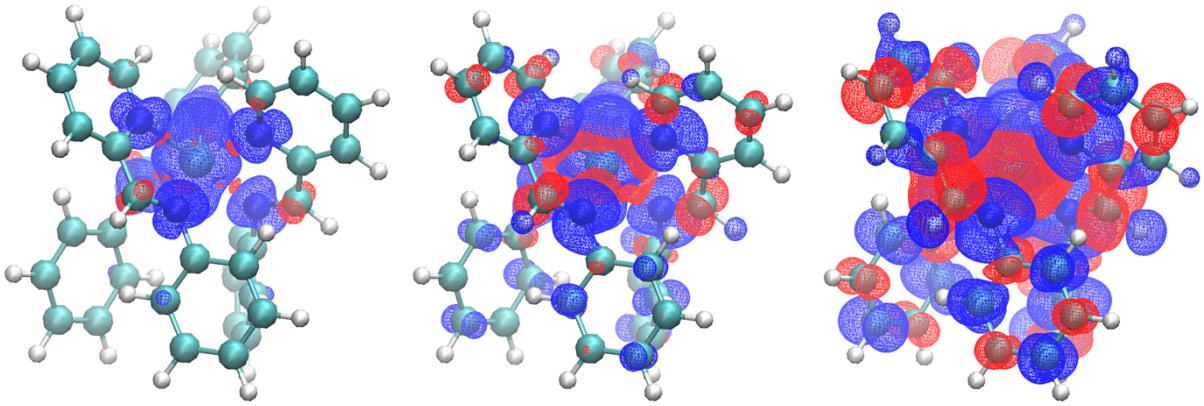


Figure S2. Optimized structure for $[Co(\mathbf{2})_3]^{2+}$ in the quartet spin state shown in two orientations.

It is also instructive to examine the chemical effects of the substituents, so we expand the study to the unsubstituted **2** ligand. The optimized structure for the high-spin quartet state of $[Co(\mathbf{2})_3]^{2+}$ (Figure 3) has Co–N bond lengths of 2.177 and 2.129 Å averaged over the 3 equivalent bonds to the imine and pyridine nitrogen atoms, respectively. The unsubstituted model is predicted to have longer metal – N bond lengths by approximate 0.1 Å. At the M06-L level, the low-spin doublet state is computed to be 5.8 kcal/mol higher in enthalpy than the quartet state. The standard deviation of the ^{1}H chemical shifts between equivalent protons of $[Co(\mathbf{2})_3]^{2+}$ was small, having percent deviations equal to or less than 1.7%, 1.7% and 6.7% for imine, pyridyl and phenyl protons respectively.

The degree to which spin is localized in the vicinity of the individual protons is obviously directly reported by the measured and predicted chemical shift values, but it is instructive to examine the overall spin density of $[Co(\mathbf{2})_3]^{2+}$ (see Figure S3 for the electronic spin density at different isosurface values). Figure S3a demonstrates that most of the excess spin density is concentrated on the metal center and nitrogen atoms. A spin density surface rendered with a smaller spin density threshold highlights the localized spin density on the imine and pyr-6

protons (see Figure S3b). A further expansion of the isosurface results in the appearance of spin density on pyr-3 and pyr-5 (see Figure S3c).



a) b) c)

Figure S3. Total spin density plots of $[Co(\mathbf{2})_3]^{2+}$ for S=3/2 with an isosurface values of a) 0.001, b) 0.0004, and c) 0.0001. Here the blue surface corresponds to positive spin density and red to negative spin density.

C. MCSCF Exploration on $[Fe(2)_3]^{2+}$

Complete active space self-consistent field (CASSCF) calculations on the $[Fe(\mathbf{2})_3]^{2+}$ ground state singlet structure demonstrate that this system is largely single configurational at all accessible spin states. Results from the complete active space second order perturbation theory (CASPT2) spin splitting on the ground state $[Fe(\mathbf{2})_3]^{2+}$ structure are presented in Table S1. An active space of ten electrons in twelve orbitals (10/12) was selected, with orbitals shown as linear combinations of atomic orbitals in Figure S4 for the singlet state and are angled out of the plane.

Table S1.

	CASSCF Rel. E (kcal mol^{-1})	Config. Weight	CASPT2 Rel. E (kcal mol^{-1})
singlet	0.0	92%	0.0
triplet	27.9	93%	29.6
quintet	20.0	98%	27.7

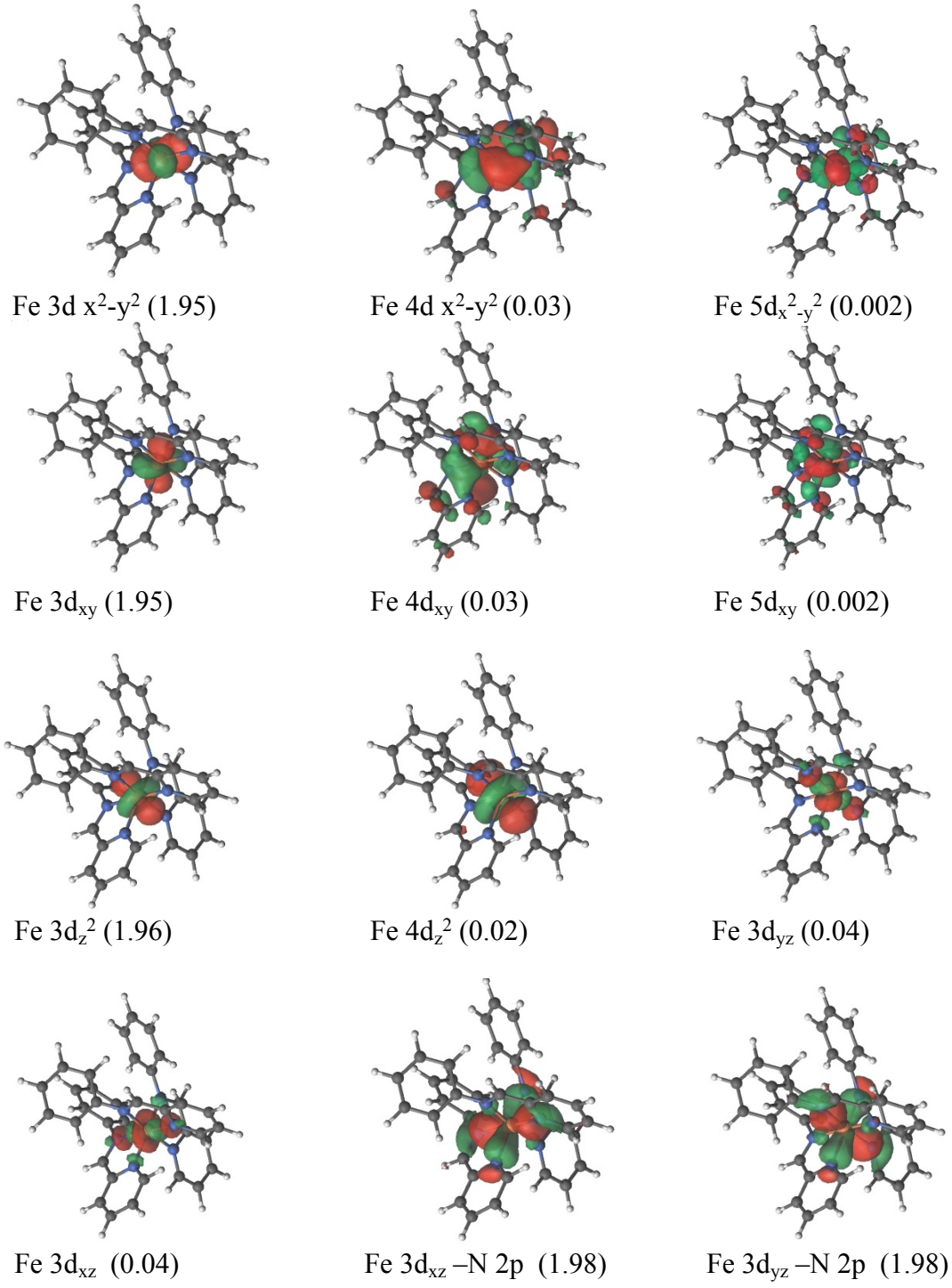


Figure S4. Active space orbitals and occupations for the singlet state from CASSCF/PT2 calculations on the $[Fe(\mathbf{2})_3]^{2+}$ singlet ground state structure.

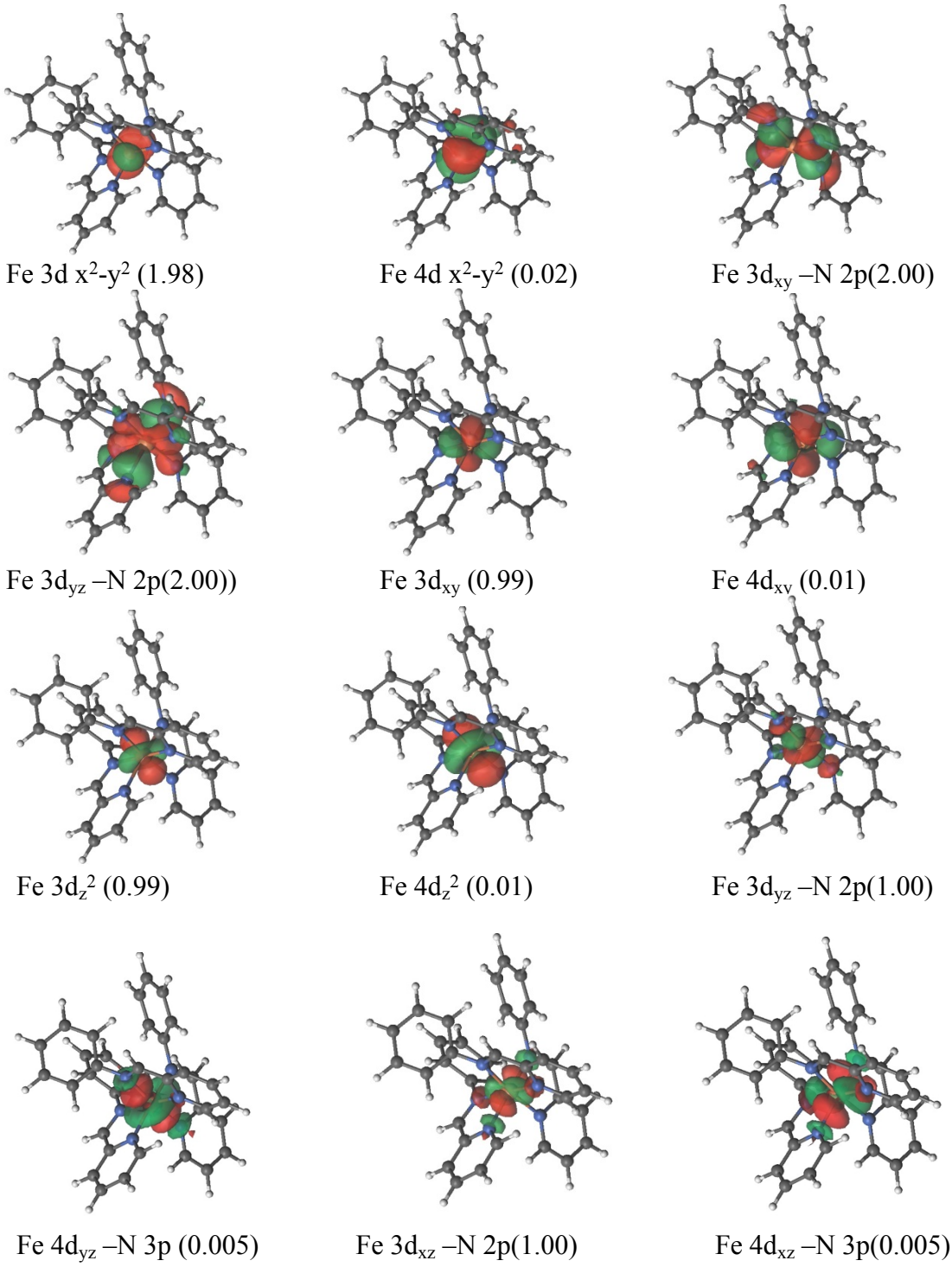


Figure S5. Active space orbitals and occupation for the quintet electronic configuration from CASSCF/PT2 calculations on the $[Fe(\mathbf{2})_3]^{2+}$ singlet ground state structure.

D. Computed Properties for the 2D Potential Energy Surface

Table S2. 2D potential energy surface and ^{1}H NMR for Fe–N bond variations in $[Fe(\mathbf{2})_3]^{2+}$.

					H_a (Imine C)			H_b (Py-6)			H_c (Py-5)			H_d (Py-4)		
X [a]	Y [b]	ΔH [c,d]	ΔG [c,d]	g_{iso}	δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]
2.00	2.00	30.6	27.1	2.029	395.0	24.9	1.806	247.8	21.5	1.105	119.5	23.8	0.518	46.9	23.4	0.178
2.00	2.05	23.1	20.1	2.029	368.4	24.4	1.680	247.0	22.1	1.104	111.7	23.8	0.482	44.0	23.3	0.164
2.00	2.10	20.3	17.2	2.034	317.9	24.6	1.442	246.8	21.2	1.096	100.0	23.8	0.427	43.6	23.4	0.163
2.05	2.00	24.4	21.2	2.031	397.3	24.9	1.815	230.6	21.5	1.024	112.9	23.8	0.487	39.3	23.4	0.143
2.05	2.05	19.1	15.8	2.034	355.0	24.8	1.615	228.8	21.3	1.013	103.4	23.8	0.442	39.4	23.4	0.143
2.05	2.10	13.3	9.9	2.033	327.1	24.2	1.483	226.4	21.9	1.005	95.8	23.8	0.407	36.2	23.2	0.128
2.05	2.15	12.4	8.9	2.038	270.8	24.1	1.219	226.5	21.6	1.002	82.8	23.7	0.346	35.2	23.3	0.123
2.10	2.00	18.6	15.5	2.030	416.8	24.3	1.904	215.3	22.3	0.957	111.2	23.8	0.480	30.9	23.2	0.103
2.10	2.05	13.3	10.0	2.033	369.9	24.2	1.683	211.1	22.1	0.935	101.1	23.8	0.432	30.8	23.2	0.103
2.10	2.10	9.9	6.3	2.035	328.4	24.0	1.487	207.8	22.0	0.918	91.7	23.8	0.388	30.0	23.2	0.099
2.10	2.15	10.1	6.6	2.041	277.9	24.3	1.251	206.9	21.2	0.908	81.6	23.7	0.340	28.8	23.3	0.093
2.10	2.20	8.5	4.4	2.043	242.7	24.1	1.129	201.0	21.1	0.918	68.5	23.6	0.304	22.2	23.3	0.084
2.15	2.05	11.7	8.6	2.034	347.9	23.8	1.578	200.0	22.4	0.884	94.5	23.8	0.401	29.5	23.3	0.097
2.15	2.10	8.3	5.1	2.037	307.5	23.6	1.387	195.0	22.4	0.860	86.8	23.8	0.365	28.2	23.3	0.091
2.15	2.15	6.1	3.3	2.038	270.9	23.0	1.215	193.9	22.8	0.857	78.1	23.9	0.325	28.4	23.2	0.091
2.15	2.20	8.1	4.7	2.045	249.8	24.0	1.117	191.3	21.3	0.835	68.6	23.7	0.278	23.9	23.3	0.070
2.20	2.10	6.7	3.8	2.037	298.9	23.1	1.345	185.1	23.2	0.818	79.8	23.9	0.333	26.2	23.2	0.081
2.20	2.15	7.8	3.7	2.044	279.3	24.0	1.254	174.8	21.7	0.760	72.7	23.7	0.298	21.5	23.2	0.059
2.20	2.20	3.9	1.0	2.041	271.8	23.4	1.218	171.0	22.8	0.749	67.5	23.8	0.275	15.4	23.2	0.031

[a] X is the bond coordinate N_{py}–Fe in Å. [b] Y is the bond coordinate N_{im}–Fe in Å. [c] Computed in kcal/mol for mononuclear cage corner model $Fe(\mathbf{2})_3^{2+}$. [d] Zero of energy is unconstrained singlet geometry. [e] Computed according to equation 2, and then scaled according to the linear regression in S7. [f] Values are averaged for equivalent protons by symmetry.

Table S2. Continued.

H_e (Py-4)			H_f (Phe-2)			$H_{f'}$ (Phe-2')			H_g (Phe-3)			$H_{g'}$ (Phe-3')			H_h (Phe-4)		
δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]	δ [e]	σ_{orb} [f]	A_{FC} [f]
100.2	23.9	0.429	-13.3	25.5	-0.092	-21.9	26.0	-0.130	21.9	24.0	0.065	31.1	23.9	0.107	-18.8	23.8	-0.126
103.1	23.7	0.441	-12.0	26.1	-0.083	-13.1	24.7	-0.095	24.0	24.2	0.076	30.0	23.7	0.102	-9.2	23.9	-0.081
94.2	23.9	0.400	-13.7	25.4	-0.094	-21.4	26.0	-0.127	20.3	24.0	0.057	29.6	23.9	0.100	-16.8	23.8	-0.116
91.4	23.9	0.388	-13.1	25.5	-0.091	-23.5	26.0	-0.137	21.3	24.0	0.062	31.1	23.9	0.107	-20.3	23.8	-0.133
87.8	23.9	0.370	-13.0	25.5	-0.091	-22.0	25.9	-0.130	20.5	24.0	0.058	30.2	23.9	0.103	-17.5	23.8	-0.119
90.6	23.7	0.382	-11.4	26.2	-0.080	-11.8	24.6	-0.089	22.3	24.2	0.068	28.1	23.7	0.092	-7.5	23.8	-0.073
82.2	23.7	0.343	-10.0	25.3	-0.077	-18.6	26.1	-0.114	18.3	24.0	0.048	27.1	24.0	0.089	-12.5	23.8	-0.096
89.6	23.6	0.378	-13.8	26.0	-0.092	-13.7	24.6	-0.098	23.5	24.2	0.073	31.0	23.8	0.106	-11.7	23.8	-0.092
86.3	23.6	0.362	-12.8	26.2	-0.086	-12.1	24.5	-0.091	22.6	24.2	0.069	29.1	23.7	0.097	-9.5	23.8	-0.082
83.3	23.6	0.348	-11.8	26.2	-0.082	-10.6	24.5	-0.084	21.4	24.2	0.063	27.4	23.7	0.089	-7.7	23.8	-0.073
75.6	23.8	0.312	-9.7	25.5	-0.075	-20.7	26.0	-0.123	17.4	23.9	0.044	28.3	23.9	0.094	-13.9	23.8	-0.102
68.5	23.7	0.304	-13.1	25.4	-0.073	-22.9	26.1	-0.116	12.6	23.9	0.041	23.0	23.9	0.091	-15.9	23.8	-0.094
73.0	23.6	0.300	-8.7	25.5	-0.070	-7.0	24.3	-0.068	22.1	24.0	0.066	25.6	23.9	0.082	-7.3	23.8	-0.072
71.1	23.6	0.291	-5.4	25.5	-0.055	-5.9	24.3	-0.063	20.8	24.0	0.060	24.3	24.0	0.076	-5.1	23.9	-0.061
67.8	23.4	0.275	9.1	25.1	0.010	-3.5	24.5	-0.051	18.9	24.0	0.051	21.8	24.2	0.065	-0.7	24.0	-0.040
65.8	23.7	0.266	-7.0	25.4	-0.062	-18.5	26.1	-0.112	16.1	24.0	0.037	27.0	24.0	0.088	-11.3	23.8	-0.090
62.8	23.4	0.251	9.3	25.0	0.011	-4.3	24.7	-0.053	19.4	24.0	0.053	21.9	24.2	0.066	-2.7	24.0	-0.049
63.8	23.6	0.257	-8.4	25.3	-0.070	-17.2	25.8	-0.108	17.3	23.9	0.043	25.5	24.0	0.081	-10.3	23.8	-0.085
65.3	23.5	0.263	-7.6	26.1	-0.063	-6.5	25.3	-0.061	18.8	24.5	0.052	23.8	23.9	0.073	-4.1	24.0	-0.056

[a] X is the bond coordinate N_{py}–Fe in Å. [b] Y is the bond coordinate N_{im}–Fe in Å. [c] Computed in kcal/mol for mononuclear cage corner model Fe(**2**)$_3^{2+}$. [d] Zero of energy is unconstrained singlet geometry. [e] Computed according to equation 2, and then scaled according to the linear regression in S7. [f] Values are averaged for equivalent protons by symmetry.

E. Computed Properties for Ground State Models

Table S3. Computed spin state separations and ^{1}H NMR for $[Co(1)_3]^{1-}$, $[Co(2)_3]^{2+}$, and $[Fe(2)_3]^{2+}$. Chemical shifts for low-spin Co^{II} species were not computed.

						H_a (Imine C)			H_b (Py-6)			H_c (Py-5)			H_d (Py-4)		
		S	ΔH_{SCO}[a]	ΔG_{SCO}[a]	g_{iso}	δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]
$[Fe(2)_3]^{2+}$		0	0.0	0.0	0.000	9.4			8.2			8.2			8.9		
		1	16.8	14.4	2.055	68.2	22.8	0.891	61.5	24.1	0.815	23.8	23.9	0.281	21.1	23.1	0.232
	Q_1	2	7.7	4.2	2.043	244.5	23.7	1.135	175.9	21.9	0.803	63.5	23.7	0.280	18.2	23.2	0.065
	Q_2	2	4.0	1.3	2.041	247.4	22.9	1.146	167.2	23.1	0.769	65.3	23.9	0.291	16.6	23.2	0.057
	Q_3	2	3.7	0.9	2.042	259.4	23.5	1.206	167.0	22.9	0.766	62.0	23.8	0.274	10.1	23.2	0.026
$[Co(1)_3]^{1-}$		1/2	8.6	10.3													
		3/2	0.0	0.0	2.098	251.3	22.5	1.791	155.8	24.2	1.108	50.0	23.8	0.335	15.8	23.0	0.080
$[Co(2)_3]^{2+}$		1/2	5.8	7.7													
		3/2	0.0	0.0	2.098	247.0	22.5	1.779	172.9	24.7	1.250	56.6	23.8	0.388	19.8	22.9	0.111

[a] Computed in kcal/mol for mononuclear cage corner. Zero of energy is unconstrained lowest energy spin state. [b] Computed according to equation 2, and then scaled according to the linear regression in S7 (with the exception of the diamagnetic Fe^{II} species). [c] Values are averaged for equivalent protons by symmetry.

Table S3. Continued.

H_e (Py-3)			H_f (Phe-2)			$H_{f'}$ (Phe-2')			H_g (Phe-3)			$H_{g'}$ (Phe-3')			H_h (Phe-4)		
δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]	δ[b]	σ_{orb}[c]	A_{FC}[c]
9.0			6.6			4.6			7.8			7.6			8.0		
17.0	23.0	0.173	-3.8	24.9	-0.095	-5.7	27.4	-0.086	6.5	24.1	0.040	7.9	24.5	0.065	-2.4	24.1	-0.085
59.8	23.5	0.262	-10.9	25.4	-0.063	-21.9	26.2	-0.111	12.2	24.0	0.040	21.3	24.1	0.083	-14.4	23.9	-0.087
56.4	23.4	0.246	9.4	25.1	0.032	-7.8	24.7	-0.051	13.7	24.0	0.047	16.2	24.3	0.060	-4.6	24.1	-0.039
61.4	23.5	0.270	-10.8	26.0	-0.060	-10.2	25.3	-0.060	14.4	24.5	0.052	19.1	23.9	0.072	-7.9	24.1	-0.055
47.5	23.0	0.311	-12.8	24.5	-0.117	-15.4	26.4	-0.122	[d]	[d]	[d]	18.3	24.4	0.109	-10.8	23.9	-0.107
52.0	22.8	0.346	-12.8	24.4	-0.119	-25.4	27.8	-0.187	11.6	24.0	0.058	23.4	24.7	0.149	-15.8	24.2	-0.143

[a] Computed in kcal/mol for mononuclear cage corner. Zero of energy is unconstrained lowest energy spin state. [b] Computed according to equation 2, and then scaled according to the linear regression in S7 (with the exception of the diamagnetic Fe^{II} species). [c] Values are averaged for equivalent protons by symmetry. [d] Position is occupied by sulfonate substituent.

III. Experimental NMR Results

A. ^{1}H VT NMR experiments

All reagents and solvents were purchased from commercial sources and used as supplied. 4,4'-diaminobiphenyl-2,2'-disulfonic acid was purchased from TCI Europe having a nominal content of water of 30% at maximum; its elemental analysis was in agreement with a 14% water content. The tetramethylammonium salt of cage **B** was prepared according to the previously reported method.[34] NMR spectra were recorded using a Bruker AVC-500-BB. δ_H values are reported relative to the internal standard *t*BuOH (δ_H = 1.24 ppm).

General procedure for the preparation of the cage solutions. A J-Young NMR tube was loaded with cage **3** dissolved in D_2O (2.0×10^{-3} M, 0.400 mL). Either no guest, pure guest or a D_2O solution of the guest was added, the tube was then sealed under nitrogen and kept at 50 °C for equilibration.

Protocol for VT NMR experiments. The J-Young NMR tube, containing the solution of cage **B** or its host-guest complex with one of the guests shown in Table S4, was inserted in the NMR spectrometer. The sample was locked and shimmed. A ^{1}H NMR spectrum was acquired to check the full encapsulation of the guest. Then a variable temperature NMR experiment was performed on the sample using an automated ramp, which consisted of going from 278 K to 358 K in steps of 10 K. After each temperature was reached, 3 minutes for the equilibration of the sample were allowed and a ^{1}H NMR spectrum was acquired. In Figure S6 a stacked plot for the variable temperature NMR experiment performed on $C_6H_{12}\subset$**B** is shown as representative example of the VT NMR studies for all the host-guest complexes. For these host-guest complexes the chemical shift of the imine proton at the various temperatures is reported in Table S4.

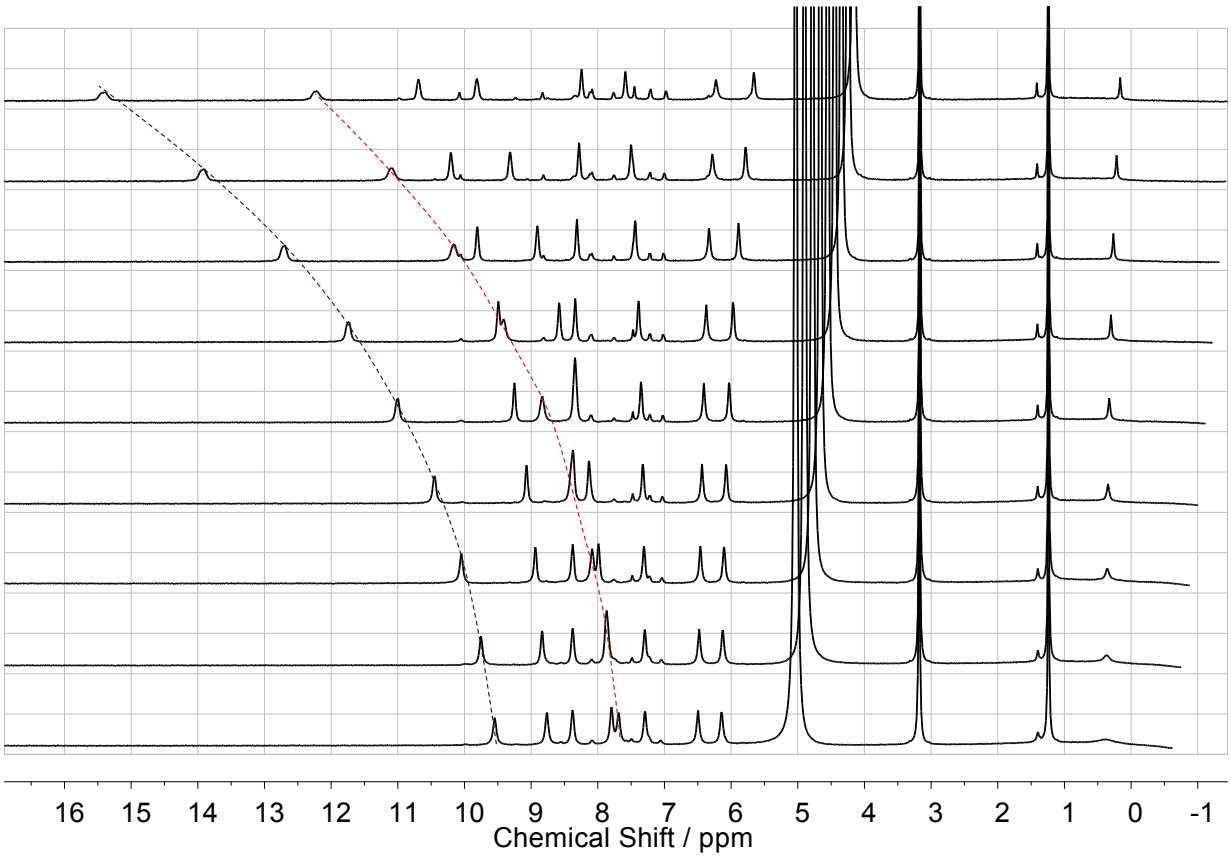


Figure S6. Stacked plot of ^{1}H NMR spectra for C_6H_{12}⊂**B** in D_2O acquired at various temperatures going from 278 K to 358 K with steps of 10 K. Lines are drawn to guide the eye on the change of chemical shift of the imine proton (depicted in blue) and py-6 proton (depicted in red).

Table S4. Chemical shift (ppm) of the imine proton measured by VT NMR experiments in D_2O for cage **B** and its host guest complexes at various temperatures (K).

	δ_{imine} (ppm)								
Guest	**278 K**	**288 K**	**298 K**	**308 K**	**318 K**	**328 K**	**338 K**	**348 K**	**358 K**
methylcyclopentane	11.42	12.31	13.36	14.62	16.11	17.79	19.53	21.49	n/a[a]
Cyclopentane	9.71	9.97	10.32	10.79	11.41	12.19	13.18	14.39	15.83
Cyclohexane	9.55	9.75	10.05	10.45	11.00	11.73	12.69	13.91	15.40
CH_2Cl_2	9.31	9.41	9.55	9.75	10.02	10.40	10.90	11.55	12.38
$CHCl_3$	9.44	9.60	9.82	10.13	10.56	11.15	11.91	12.91	14.10
CCl_4	9.54	9.76	10.07	10.51	11.10	11.81	12.89	14.17	15.69
fluorobenzene	9.96	10.35	10.87	11.56	12.45	13.57	14.93	16.55	n/a[a]
1,2-difluorobenzene	10.27	10.81	11.52	12.44	13.59	15.02	16.67	18.53	n/a[a]
1,4-difluorobenzene	10.72	11.40	12.26	13.32	14.61	16.12	17.80	19.62	n/a[a]
benzene	9.64	9.90	10.25	10.73	11.38	12.21	13.18	14.50	16.06
THF	9.43	9.58	9.78	10.07	10.46	11.00	11.72	12.63	13.61
acetone	9.55	9.75	10.02	10.38	10.86	11.49	12.29	13.30	14.51
pyridine	9.63	9.89	10.25	10.73	11.35	12.17	13.22	14.47	15.92
1,4-dioxane	9.58	9.80	10.10	10.49	11.02	11.70	12.59	13.67	14.97
1,3,5-trioxane	9.29	9.37	9.50	9.68	9.95	10.34	10.88	11.62	12.59
Empty	9.21	9.26	9.32	9.42	9.56	9.76	10.05	10.46	11.00

[a] Data not available since at this temperature the host-guest complex was no longer present.

B. Fitting ^{1}H VT NMR

The experimental ^{1}H VT NMR data were fit using equation 1. δ_{LS}, the low-spin chemical shift, and *C/T,* the chemical shift of the high-spin state, were kept as fixed parameters. The low-spin chemical shift was fixed at the value of 9.2 ppm measured experimentally, and the high-spin chemical shift was supplied by theoretical predictions and fixed at 259.4 ppm. Fitting was performed with the Origin 8.6 software package.[35] All fits had an adjusted $R^2 > 0.998$ and F values $> 5.5 \times 10^4$. Errors introduced by the fit to the enthalpy are less than 0.1 kcal mol^{-1} for all fits and errors introduced to the entropy by the fit are less than 0.1 cal mol^{-1} K^{-1}.

C. Relation of SCO behavior with static guest properties

No correlation was found between the enthalpies of spin crossover and any of the static guest properties tested (Table S5).

Guest	H (kcal mol^{-1})	S (cal mol^{-1} K^{-1})	δ_{LS} (ppm)	V (Å^3)	Ω	V/Ω (Å^3)	μ (Debye)	logP	Abraham acidity	Abraham basicity
Solvent	8.8	14.9	9.2	--	--	--	--	--	--	--
Cyclohexane	7.0	12.2	9.2	112	0.040	2762.6	0.00	3.44	0.0	0.00
Cyclopentane	6.3	10.3	9.2	95	0.038	2496.5	0.00	3.00	0.0	0.00
methylcyclopentane	4.6	7.3	9.2	113	0.072	1572.1	0.00	3.37	0.0	0.00
THF	7.0	11.6	9.2	86	0.040	2128.3	1.75	0.46	0.0	0.48
benzene	6.6	11.2	9.2	99	0.063	1587.2	0.00	2.13	0.0	0.14
fluorobenzene	6.1	10.6	9.2	104	0.089	1161.6	1.60	2.73	0.0	0.10
1,2-difluorobenzene	5.8	10.1	9.2	109	0.069	1563.8	2.46	2.40[a]	--	--
1,4-difluorobenzene	5.1	8.5	9.2	109	0.127	856.1	0.00	2.20[a]	--	--
pyridine	6.5	11.0	9.2	93	0.063	1484.5	2.22	0.65	0.0	0.52
1,4-dioxane	6.6	10.8	9.2	94	0.042	2215.7	0.00	-0.27	0.0	0.64
1,3,5-trioxane	8.4	14.8	9.2	84	0.044	1919.9	2.08	-0.43	0.0	--
acetone	6.6	10.7	9.2	73	0.053	1364.2	2.88	-0.24	0.0	0.49
CH_2Cl_2	7.6	12.4	9.2	61	0.187	325.7	1.60	1.25	--	--
$CHCl_3$	7.3	12.5	9.2	75	0.056	1336.6	1.04	1.97	0.2	0.02
CCl_4	7.1	12.4	9.2	89	0.000	--	0.00	2.84	--	--

Table S5. Spin crossover enthalpies and entropies of the iron cage, **B**, with encapsulated guests. Shown are static guest properties. V is the volume of the guest molecule computed by the enclosed van der Waals surface. Ω is an asphericity parameter, see Smulders *et al.* ,[36] μ is the molecular dipole moment of the guest molecule from the *CRC Handbook of Chemistry and Physics*,[37] logP is the octanol-water partitioning coefficient from the *CRC Handbook of Chemistry and Physics*,[37] and the Abraham acidity and basicity are from the Minnesota Solvent Database. [a] Data obtained from PUBCHEM database.[38, 39]

IV. Structures

Doublet $[Co(1)_3]^{1-}$

N	1.729560	0.373170	2.602542
N	0.976285	1.440113	0.346101
N	-1.801111	0.148731	0.314437
N	0.814123	-1.523782	0.515314
N	-1.073454	1.677851	2.339906
N	-0.740773	-1.261889	2.576229
C	2.086328	-0.219144	3.759214
H	1.344099	-0.870657	4.223253
C	3.338243	-0.017274	4.348773
H	3.577216	-0.520712	5.284735
C	4.260609	0.826308	3.730054
H	5.243004	0.996198	4.170431
C	3.904667	1.451362	2.533821
H	4.591973	2.117478	2.011367
C	2.638917	1.204693	2.000359
C	2.166631	1.777713	0.757709
H	2.793516	2.477433	0.195018
C	0.515541	1.971692	-0.908825
C	-0.567510	2.854222	-0.923776
H	-1.020787	3.184233	0.010893
C	-1.042624	3.327667	-2.151027
C	-0.447167	2.932381	-3.353862
C	0.648301	2.063216	-3.321255
H	1.126665	1.752776	-4.251420
C	1.136071	1.583253	-2.104985
H	1.994078	0.912860	-2.073836
C	-2.456517	-2.360514	-3.024870
C	3.095487	-1.411971	-3.040241
C	-2.519766	-2.875321	-1.725275
C	3.650888	-1.000304	-1.824055
C	-2.337127	-2.046801	-0.612720
H	-2.398275	-2.449646	0.398993
C	2.912211	-1.063863	-0.638256
H	3.350302	-0.749723	0.309840
C	-2.094511	-0.682668	-0.810355
C	1.602620	-1.553242	-0.676482
C	-2.050548	-0.150008	-2.108139
H	-1.873527	0.916241	-2.243512
C	1.041686	-1.994164	-1.885189
H	0.023733	-2.383830	-1.892385
C	-2.227844	-0.991959	-3.206650
H	-2.182709	-0.576918	-4.214992
C	1.789472	-1.915225	-3.060344
H	1.347741	-2.245679	-4.001789
C	-2.676164	1.016777	0.706614
H	-3.661849	1.126377	0.237479
C	0.414753	-2.645692	1.034704
H	0.697772	-3.626506	0.635122
C	-2.320641	1.888098	1.822490
C	-0.424111	-2.550949	2.211726
C	-3.175143	2.877282	2.310735
H	-4.161265	3.006848	1.863351
C	-0.887969	-3.657027	2.922971
H	-0.612495	-4.658112	2.590588
C	-2.738947	3.684991	3.362489
H	-3.384828	4.465824	3.763954
C	-1.694449	-3.455663	4.043015
H	-2.070617	-4.304854	4.612960
C	-1.464415	3.476213	3.888088
H	-1.085561	4.084924	4.708235
C	-2.007371	-2.149799	4.417485
H	-2.630397	-1.945275	5.287026
C	-0.661661	2.464284	3.353896
H	0.336655	2.266086	3.747458
C	-1.515842	-1.079019	3.668346
H	-1.741606	-0.049894	3.943691
H	-0.839337	3.296721	-4.303323
H	3.676308	-1.337992	-3.959439
Co	0.010902	0.138375	1.437379
S	5.320907	-0.343488	-1.736387
S	-2.455806	4.437982	-2.135404
O	-1.952460	5.721325	-1.573427
O	-2.904066	4.549576	-3.546829
O	-3.448765	3.775036	-1.246174
O	5.777563	-0.187458	-3.141187
O	5.183881	0.947558	-1.007889
O	6.105069	-1.351330	-0.971008
S	-2.827447	-4.623023	-1.441744
O	-1.819225	-5.035606	-0.427768
O	-4.223260	-4.706846	-0.927913
O	-2.648848	-5.287049	-2.758200
H	-2.580732	-3.022145	-3.882012

Quartet $[Co(1)_3]^{1-}$

N 1.014286 2.156369 1.238284
N -0.738536 1.597002 -0.682077
N -1.759239 -1.068667 0.687833
N 1.569476 -0.446027 0.670473
N -2.222366 1.176717 1.990148
N 0.207140 -0.614299 2.942857
C 1.903468 2.426842 2.215065
H 1.761657 1.895081 3.157559
C 2.955572 3.331688 2.047849
H 3.644342 3.513029 2.872038
C 3.106201 3.984312 0.824190
H 3.921316 4.690518 0.666260
C 2.195715 3.713246 -0.197446
H 2.272619 4.195107 -1.172753
C 1.169947 2.795664 0.039445
C 0.188263 2.455089 -0.978669
H 0.241201 2.963700 -1.950531
C -1.698651 1.257339 -1.683127
C -3.053252 1.279699 -1.325395
H -3.347283 1.641414 -0.341292
C -4.018751 0.892905 -2.254984
C -3.650562 0.485377 -3.543727
C -2.298793 0.489290 -3.899926
H -2.003238 0.185715 -4.905140
C -1.320600 0.874278 -2.980497
H -0.266095 0.867568 -3.257737
C -0.447543 -3.950014 -2.091156
C 3.643946 0.754335 -2.795830
C 0.206329 -3.777290 -0.861830
C 4.203799 0.974234 -1.528664
C -0.274248 -2.867999 0.074625
H 0.219068 -2.752513 1.036587
C 3.556946 0.528927 -0.377461
H 3.976826 0.728604 0.609429
C -1.412476 -2.105338 -0.218805
C 2.314106 -0.115760 -0.493991
C -2.093789 -2.288575 -1.432032
H -2.975004 -1.684791 -1.655882
C 1.738332 -0.328372 -1.754564
H 0.766965 -0.821758 -1.826909
C -1.603872 -3.211384 -2.360167
H -2.122245 -3.344049 -3.310982
C 2.418394 0.090707 -2.900656
H 1.981685 -0.086942 -3.884368
C -2.995760 -0.851733 1.010468
H -3.817484 -1.517909 0.718432
C 2.173662 -1.025217 1.660768
H 3.210817 -1.381010 1.602401
C -3.285983 0.332804 1.806744
C 1.432923 -1.220796 2.897903
C -4.557450 0.612197 2.309271
H -5.376554 -0.084121 2.126968
C 1.937015 -1.974266 3.959982
H 2.921249 -2.435644 3.873135
C -4.750118 1.787873 3.037907
H -5.732629 2.030933 3.442406
C 1.161336 -2.120594 5.110321
H 1.529235 -2.703751 5.954458
C -3.666884 2.642373 3.239364
H -3.776294 3.568967 3.801187
C -0.090334 -1.508681 5.159564
H -0.726594 -1.596728 6.039038
C -2.422072 2.303603 2.700803
H -1.551909 2.949548 2.831049
C -0.532448 -0.767605 4.060298
H -1.504422 -0.272035 4.072850
H -4.410818 0.177564 -4.262271
H 4.154691 1.106975 -3.693322
Co -0.362239 0.495269 1.184534
S 5.740512 1.897798 -1.392096
S -5.737679 0.836761 -1.734949
O -5.882599 1.900172 -0.706744
O -6.545658 1.074634 -2.959179
O -5.921634 -0.533099 -1.175880
O 6.740250 1.135844 -2.188137
O 5.443452 3.235057 -1.976247
O 6.057778 1.949040 0.058668
S 1.750198 -4.627033 -0.515125
O 2.784084 -3.852063 -1.257091
O 1.927616 -4.557195 0.959683
O 1.585442 -6.011988 -1.030915
H -0.058536 -4.651972 -2.830034

Doublet $[Co(2)_3]^{2+}$

N	-1.694714	-0.169638	-1.785985
N	0.380772	-1.508677	-0.952373
N	0.072379	-0.156799	1.685564
N	0.325361	1.589816	-0.779728
N	-2.009720	-1.472867	0.838340
N	-1.924914	1.597263	0.623334
C	-2.809768	0.496817	-2.158989
H	-3.254750	1.158925	-1.417433
C	-3.373016	0.348746	-3.427179
H	-4.272896	0.909167	-3.676600
C	-2.775606	-0.508554	-4.350656
H	-3.196350	-0.633923	-5.348049
C	-1.627970	-1.205483	-3.974289
H	-1.125569	-1.889075	-4.658847
C	-1.112212	-1.025734	-2.691360
C	0.065061	-1.710873	-2.195891
H	0.628310	-2.377958	-2.859646
C	1.559213	-2.126134	-0.428376
C	1.446663	-3.041933	0.628662
H	0.460527	-3.337329	0.987681
C	2.603650	-3.586398	1.189799
C	3.867159	-3.202429	0.722355
C	3.970697	-2.292540	-0.334935
H	4.950994	-1.993184	-0.710464
C	2.820218	-1.762210	-0.922851
H	2.888360	-1.056739	-1.751364
C	3.514115	2.052269	2.781489
C	4.045734	1.226976	-2.751395
C	2.256630	2.668934	2.773617
C	2.858886	0.930793	-3.433338
C	1.116079	1.944879	2.419317
H	0.133672	2.416523	2.434659
C	1.623251	1.061753	-2.795004
H	0.697619	0.843521	-3.328177
C	1.240155	0.589850	2.083083
C	1.578096	1.516917	-1.468273
C	2.490056	-0.041457	2.115090
H	2.565659	-1.102422	1.880405
C	2.761210	1.844700	-0.790565
H	2.706540	2.215563	0.233340
C	3.625624	0.697067	2.457566
H	4.598910	0.203375	2.474152
C	3.991882	1.686553	-1.431371
H	4.910557	1.930877	-0.894565
C	-0.413874	-1.032977	2.518464
H	0.027611	-1.195656	3.507716
C	-0.131098	2.751247	-0.436376
H	0.379373	3.688948	-0.690875
C	-1.578769	-1.786027	2.102170
C	-1.378084	2.810926	0.318381
C	-2.212819	-2.741461	2.896723
H	-1.827777	-2.958066	3.893363
C	-1.958995	4.015621	0.716789
H	-1.482422	4.959408	0.449524
C	-3.333825	-3.399843	2.388856
H	-3.850535	-4.150276	2.986808
C	-3.140629	3.980703	1.458151
H	-3.615172	4.905756	1.785320
C	-3.778529	-3.080959	1.106069
H	-4.651028	-3.570700	0.675435
C	-3.700736	2.743276	1.773426
H	-4.621447	2.672103	2.351175
C	-3.093203	-2.116845	0.361063
H	-3.416798	-1.847752	-0.645338
C	-3.066587	1.575760	1.338889
H	-3.482084	0.591545	1.562143
H	4.766927	-3.616558	1.179140
H	4.401696	2.626720	3.049841
H	5.007648	1.106893	-3.251564
H	2.517460	-4.309844	2.001931
H	2.160018	3.720332	3.047964
H	2.892743	0.593123	-4.470302
Co	-0.801256	-0.049947	-0.057633

Quartet $[Co(2)_3]^{2+}$

N	1.880446	1.921163	0.004403
N	-0.256815	1.201394	1.417899
N	-0.189256	-1.819921	0.340670
N	-0.236706	0.636567	-1.743895
N	1.955863	-0.893340	1.617228
N	1.930156	-0.905325	-1.615487
C	3.026412	2.238952	-0.629925
H	3.515962	1.429822	-1.175881
C	3.564754	3.528284	-0.599158
H	4.494239	3.736877	-1.127397
C	2.895077	4.528514	0.105296
H	3.288551	5.544545	0.137900
C	1.711418	4.208783	0.772049
H	1.157993	4.957857	1.339273
C	1.238227	2.897380	0.711988
C	0.031563	2.465464	1.406779
H	-0.576316	3.218491	1.926265
C	-1.466023	0.784406	2.058993
C	-1.408425	-0.170733	3.085752
H	-0.441390	-0.533148	3.435514
C	-2.592055	-0.614892	3.678568
C	-3.831563	-0.137681	3.233186
C	-3.882147	0.812439	2.207900
H	-4.843143	1.192763	1.856503
C	-2.703343	1.285930	1.628126
H	-2.731524	2.030185	0.831642
C	-3.773974	-2.834034	-1.659069
C	-3.893616	2.748319	-1.533388
C	-2.540937	-2.964379	-2.310674
C	-2.678833	3.424138	-1.359996
C	-1.354158	-2.637441	-1.651112
H	-0.392389	-2.747044	-2.152686
C	-1.467002	2.733892	-1.438457
H	-0.519518	3.258292	-1.310008
C	-1.401610	-2.205338	-0.316688
C	-1.472512	1.359899	-1.723943
C	-2.631799	-2.098125	0.348527
H	-2.652124	-1.765845	1.386395
C	-2.685254	0.684074	-1.926437
H	-2.672975	-0.382039	-2.153984
C	-3.814537	-2.399673	-0.330265
H	-4.770164	-2.297091	0.187494
C	-3.892178	1.378380	-1.816170
H	-4.833064	0.842522	-1.956207
C	0.167699	-2.457411	1.410912
H	-0.388132	-3.319726	1.802616
C	0.098550	0.016215	-2.831523
H	-0.486559	0.085662	-3.758133
C	1.385735	-2.039110	2.094803
C	1.322433	-0.775768	-2.832663
C	1.938100	-2.764518	3.151110
H	1.440118	-3.668676	3.502619
C	1.836035	-1.362964	-3.989692
H	1.310681	-1.239697	-4.937262
C	3.127643	-2.315673	3.726940
H	3.583325	-2.866694	4.549693
C	3.021520	-2.094549	-3.904223
H	3.445334	-2.563458	-4.792290
C	3.721600	-1.155863	3.230447
H	4.651832	-0.774982	3.650045
C	3.652906	-2.214568	-2.666825
H	4.581071	-2.774346	-2.559013
C	3.106375	-0.470619	2.179244
H	3.537432	0.444985	1.769729
C	3.077983	-1.608392	-1.546867
H	3.538776	-1.687296	-0.560606
H	-4.752906	-0.502847	3.688607
H	-4.698119	-3.074538	-2.186279
H	-4.836585	3.290693	-1.452080
H	-2.545872	-1.342453	4.490283
H	-2.501469	-3.319301	-3.341590
H	-2.673338	4.496196	-1.157078
Co	0.910373	0.026166	0.005146

Singlet $[Fe(2)_3]^{2+}$ Ground State

Fe	-0.764124	-0.001016	-0.000394
N	-1.831823	1.550618	-0.638440
N	0.263034	0.449272	-1.640332
N	0.263464	-1.645165	0.427175
N	0.260755	1.194314	1.210314
N	-1.832626	-1.329296	-1.025877
N	-1.833116	-0.225790	1.661957
C	-2.931413	2.090669	-0.065753
H	-3.284797	1.624954	0.853628
C	-3.596283	3.186596	-0.617345
H	-4.478365	3.580839	-0.114672
C	-3.123448	3.757541	-1.799304
H	-3.628695	4.613972	-2.244983
C	-1.989745	3.212540	-2.400833
H	-1.579726	3.624370	-3.323084
C	-1.367378	2.116489	-1.803843
C	-0.182778	1.469020	-2.319387
H	0.300303	1.826748	-3.234310
C	1.458624	-0.204492	-2.104173
C	1.380125	-1.486278	-2.666068
H	0.409754	-1.959779	-2.815532
C	2.553175	-2.131839	-3.064357
C	3.797352	-1.512912	-2.890962
C	3.864233	-0.228074	-2.343521
H	4.827844	0.268860	-2.217625
C	2.696287	0.434955	-1.958529
H	2.736960	1.442920	-1.546708
C	3.787914	-1.756734	2.765514
C	3.780594	3.280712	0.135106
C	2.542288	-1.585506	3.382084
C	2.533418	3.730457	-0.315943
C	1.372801	-1.559095	2.618611
H	0.400769	-1.443789	3.098215
C	1.365286	3.054320	0.044099
H	0.391739	3.411590	-0.291978
C	1.456381	-1.721315	1.228844
C	1.452198	1.928869	0.875180
C	2.695242	-1.926404	0.608300
H	2.739667	-2.079631	-0.469638
C	2.692697	1.491953	1.356993
H	2.739204	0.632520	2.025367
C	3.859716	-1.933038	1.380284
H	4.824554	-2.081614	0.892101
C	3.855591	2.165790	0.975615
H	4.821908	1.816405	1.343676
C	-0.177486	-2.741931	-0.122965
H	0.308599	-3.712154	0.021329
C	-0.185091	1.271148	2.433041
H	0.296622	1.885763	3.200334
C	-1.362790	-2.619867	-0.940101
C	-1.368240	0.498909	2.735582
C	-1.982984	-3.685431	-1.592092
H	-1.568168	-4.688581	-1.492957
C	-1.989620	0.466940	3.983676
H	-1.578540	1.058889	4.801520
C	-3.121444	-3.439123	-2.358287
H	-3.625996	-4.253376	-2.877735
C	-3.123831	-0.325730	4.154491
H	-3.628667	-0.368899	5.119222
C	-3.600649	-2.131869	-2.447091
H	-4.487149	-1.895089	-3.033827
C	-3.597721	-1.061912	3.068174
H	-4.480548	-1.693481	3.157438
C	-2.937333	-1.105614	-1.773181
H	-3.295995	-0.078061	-1.823205
C	-2.933851	-0.990533	1.842764
H	-3.288706	-1.551963	0.979234
H	4.710016	-2.028718	-3.192106
H	4.697942	-1.763035	3.366795
H	4.689532	3.806036	-0.160824
H	2.493042	-3.124312	-3.513283
H	2.478116	-1.471770	4.465163
H	2.467173	4.613861	-0.952626

Triplet $[Fe(2)_3]^{2+}$ Ground State

Fe	0.786237	-0.038755	0.056175
N	1.995790	-1.345128	-1.089367
N	-0.057177	0.118482	-1.723699
N	-0.313541	1.509570	1.052092
N	-0.340163	-1.709693	0.717447
N	1.888183	1.744690	-0.376634
N	1.670776	-0.438892	1.771873
C	3.083969	-2.050987	-0.718194
H	3.412800	-1.929662	0.315570
C	3.761130	-2.895743	-1.599436
H	4.635742	-3.444491	-1.252462
C	3.303056	-3.024639	-2.912373
H	3.813971	-3.682183	-3.615566
C	2.182745	-2.298172	-3.312630
H	1.793905	-2.365131	-4.328874
C	1.555590	-1.464761	-2.383501
C	0.398296	-0.651427	-2.677216
H	-0.059837	-0.670802	-3.671399
C	-1.225594	0.919089	-1.991066
C	-1.106785	2.311819	-2.094890
H	-0.125881	2.783555	-2.036643
C	-2.251782	3.081163	-2.313384
C	-3.508083	2.470376	-2.414799
C	-3.615086	1.079477	-2.320682
H	-4.588223	0.593224	-2.410416
C	-2.475124	0.297854	-2.116657
H	-2.544010	-0.787875	-2.058462
C	-4.018913	0.737792	2.927799
C	-3.866745	-3.053793	-1.175607
C	-2.824760	0.340501	3.542834
C	-2.614451	-3.368348	-1.718997
C	-1.594270	0.604666	2.937168
H	-0.662808	0.300183	3.415877
C	-1.442699	-2.943613	-1.088956
H	-0.465052	-3.184246	-1.508222
C	-1.561712	1.299110	1.718112
C	-1.530015	-2.221354	0.111019
C	-2.752428	1.723786	1.110873
H	-2.707317	2.270212	0.168055
C	-2.780046	-1.923241	0.672979
H	-2.827294	-1.359726	1.605475
C	-3.977786	1.429652	1.712912
H	-4.902611	1.749171	1.228820
C	-3.945197	-2.332048	0.020000
H	-4.916725	-2.085188	0.452315
C	0.122564	2.717677	0.882521
H	-0.395033	3.598924	1.281719
C	0.015363	-2.134542	1.893591
H	-0.510584	-2.935351	2.427325
C	1.354729	2.897551	0.128236
C	1.173251	-1.505200	2.490017
C	1.931904	4.148661	-0.094536
H	1.467056	5.039922	0.327976
C	1.743124	-1.911355	3.697404
H	1.310749	-2.757196	4.232012
C	3.093867	4.227371	-0.862168
H	3.564527	5.191439	-1.054799
C	2.852861	-1.229096	4.191509
H	3.315762	-1.531743	5.130390
C	3.640314	3.052633	-1.379911
H	4.545050	3.071131	-1.986197
C	3.358670	-0.151765	3.461998
H	4.224160	0.409172	3.812003
C	3.012699	1.833282	-1.115685
H	3.415925	0.894152	-1.499176
C	2.748344	0.217640	2.264936
H	3.122299	1.054463	1.675857
H	-4.398952	3.078853	-2.575658
H	-4.976909	0.512711	3.398425
H	-4.777453	-3.374725	-1.682982
H	-2.159704	4.163979	-2.408818
H	-2.849974	-0.183990	4.499198
H	-2.548824	-3.944461	-2.643189

Quintet Q_1 $[Fe(2)_3]^{2+}$

Fe	-0.868732	0.152988	-0.121950
N	-2.142790	-0.946128	-1.494922
N	0.015746	-1.878376	-0.239181
N	0.366826	0.706454	1.596379
N	0.410555	1.230030	-1.525628
N	-1.994993	-0.543032	1.579072
N	-1.686203	2.175016	-0.192123
C	-3.231763	-0.456007	-2.122467
H	-3.477724	0.587478	-1.916622
C	-4.009290	-1.230404	-2.987086
H	-4.878686	-0.788269	-3.471359
C	-3.656071	-2.560541	-3.210386
H	-4.245397	-3.188519	-3.878735
C	-2.533449	-3.079770	-2.562785
H	-2.222235	-4.114591	-2.708403
C	-1.799792	-2.250580	-1.714428
C	-0.609860	-2.710993	-1.006848
H	-0.287457	-3.751314	-1.146419
C	1.196331	-2.329935	0.443431
C	1.117380	-2.736052	1.783694
H	0.149386	-2.770702	2.285563
C	2.284390	-3.113976	2.454570
C	3.523285	-3.076431	1.803089
C	3.591051	-2.670833	0.466357
H	4.549948	-2.642727	-0.054894
C	2.431417	-2.298081	-0.217378
H	2.474021	-1.985396	-1.259860
C	4.241225	2.384733	1.344213
C	3.751827	-0.654967	-3.280310
C	3.112036	3.189808	1.147441
C	2.451750	-1.068112	-3.600050
C	1.829625	2.644207	1.239728
H	0.947844	3.270796	1.101184
C	1.349879	-0.441190	-3.016204
H	0.333903	-0.766589	-3.242672
C	1.678055	1.285743	1.556189
C	1.552609	0.637694	-2.141005
C	2.804359	0.483828	1.787451
H	2.667673	-0.565207	2.050361
C	2.851834	1.068904	-1.832338
H	2.992665	1.896061	-1.135114
C	4.082732	1.033014	1.666298
H	4.955825	0.398357	1.830425
C	3.947385	0.407931	-2.391664
H	4.957834	0.728178	-2.131082
C	-0.041608	0.206851	2.726441
H	0.553099	0.272517	3.646483
C	0.262213	2.518748	-1.525704
H	0.956278	3.197098	-2.039352
C	-1.345210	-0.429092	2.780688
C	-0.904219	3.081174	-0.855105
C	-1.902764	-0.887482	3.977367
H	-1.342422	-0.779716	4.906376
C	-1.208358	4.442444	-0.896426
H	-0.547823	5.127603	-1.428573
C	-3.169399	-1.467600	3.956155
H	-3.627754	-1.829871	4.875912
C	-2.361865	4.895646	-0.253984
H	-2.623913	5.953395	-0.272071
C	-3.839894	-1.574735	2.736332
H	-4.832543	-2.018495	2.675476
C	-3.170629	3.972942	0.408634
H	-4.080713	4.285551	0.918979
C	-3.222610	-1.108262	1.575913
H	-3.719277	-1.182740	0.607510
C	-2.798739	2.625995	0.421792
H	-3.400287	1.875850	0.938813
H	4.429881	-3.366766	2.335622
H	5.240087	2.813632	1.253120
H	4.609763	-1.164678	-3.720886
H	2.222701	-3.441302	3.493610
H	3.229297	4.250348	0.919129
H	2.295886	-1.893113	-4.296682

Quintet Q_2 $[Fe(2)_3]^{2+}$

Fe	-0.605361	-0.147059	-0.194830
N	-1.890913	1.667762	-0.517040
N	0.517644	1.148612	-1.534566
N	0.053321	-2.216551	0.129447
N	0.361079	0.909771	1.421268
N	-1.833731	-1.349100	-1.559035
N	-1.946676	-0.377038	1.498264
C	-3.139340	1.925480	-0.066986
H	-3.657742	1.101657	0.426045
C	-3.769073	3.161374	-0.222483
H	-4.777927	3.301180	0.163642
C	-3.093096	4.195745	-0.871221
H	-3.557162	5.173737	-0.998494
C	-1.814981	3.947731	-1.364156
H	-1.249542	4.715878	-1.892736
C	-1.247529	2.681355	-1.180980
C	0.054120	2.352432	-1.714083
H	0.591721	3.121716	-2.280913
C	1.814678	0.794806	-1.999623
C	2.078581	-0.577308	-2.149790
H	1.272982	-1.290273	-1.965507
C	3.346520	-1.010221	-2.534527
C	4.361746	-0.077188	-2.771501
C	4.099446	1.291367	-2.625808
H	4.894164	2.019787	-2.794214
C	2.834985	1.733034	-2.240522
H	2.659251	2.796920	-2.077925
C	3.372838	-3.144538	2.558101
C	4.181838	2.669950	1.087690
C	2.259408	-2.491117	3.100344
C	3.067582	3.483766	1.323916
C	1.156787	-2.196854	2.298879
H	0.287216	-1.686352	2.710922
C	1.796048	2.919640	1.453953
H	0.917096	3.543633	1.628308
C	1.158643	-2.584094	0.949571
C	1.642208	1.530141	1.329750
C	2.265759	-3.254490	0.403663
H	2.261494	-3.528218	-0.653062
C	2.752676	0.713142	1.061667
H	2.612907	-0.362656	0.949039
C	3.372807	-3.523221	1.211256
H	4.240198	-4.029128	0.784598
C	4.020881	1.285105	0.961534
H	4.884484	0.646100	0.768826
C	-0.491888	-3.103684	-0.642444
H	-0.197208	-4.161264	-0.632005
C	-0.400878	1.169296	2.445715
H	-0.095398	1.837946	3.260180
C	-1.565562	-2.690417	-1.539259
C	-1.675411	0.480160	2.534341
C	-2.278059	-3.605924	-2.313558
H	-2.025488	-4.665501	-2.266671
C	-2.550125	0.638863	3.613688
H	-2.294914	1.333995	4.414015
C	-3.310426	-3.140606	-3.130771
H	-3.884926	-3.835389	-3.743341
C	-3.730554	-0.100934	3.643577
H	-4.429484	0.009048	4.472718
C	-3.592755	-1.776577	-3.147781
H	-4.389531	-1.372151	-3.770462
C	-4.001136	-0.985687	2.597008
H	-4.909984	-1.585727	2.586247
C	-2.834205	-0.914831	-2.349954
H	-3.022264	0.159559	-2.344535
C	-3.090940	-1.091284	1.544300
H	-3.279845	-1.760562	0.702708
H	5.357726	-0.414206	-3.061803
H	4.240171	-3.356758	3.184552
H	5.172999	3.115639	0.992405
H	3.543288	-2.077322	-2.647975
H	2.251968	-2.203255	4.152547
H	3.188529	4.564840	1.409085

Quintet Q_3 $[Fe(2)_3]^{2+}$

Fe	-0.161818	0.799526	-0.342191
N	1.525518	0.972886	-1.771070
N	-0.268781	-1.027249	-1.618821
N	-1.521207	-0.064209	1.160860
N	1.627200	0.491841	0.899183
N	-2.130995	1.467104	-0.914005
N	0.048060	2.648204	0.816963
C	2.417443	1.979932	-1.857755
H	2.147261	2.906936	-1.348731
C	3.625625	1.859948	-2.549189
H	4.307740	2.708032	-2.592923
C	3.941281	0.646748	-3.161257
H	4.883231	0.521311	-3.695295
C	3.030767	-0.406575	-3.076326
H	3.234546	-1.374008	-3.536704
C	1.835738	-0.210776	-2.379874
C	0.836861	-1.262900	-2.260940
H	1.044318	-2.224475	-2.750040
C	-1.199622	-2.099730	-1.464300
C	-2.570372	-1.831561	-1.609346
H	-2.895919	-0.838088	-1.916589
C	-3.501570	-2.851628	-1.411054
C	-3.077337	-4.138749	-1.059236
C	-1.711039	-4.407772	-0.925284
H	-1.373376	-5.408857	-0.652246
C	-0.770811	-3.396927	-1.129226
H	0.293665	-3.600352	-1.002354
C	-0.272026	-3.065666	3.850825
C	4.218585	-2.734932	0.086349
C	0.225954	-1.762639	3.972904
C	4.734352	-1.435453	0.156169
C	-0.203865	-0.758244	3.105326
H	0.177265	0.257985	3.196334
C	3.898444	-0.362486	0.464795
H	4.287226	0.657218	0.478326
C	-1.156197	-1.057200	2.118834
C	2.530765	-0.589784	0.701524
C	-1.687713	-2.353628	2.017826
H	-2.424270	-2.571469	1.242545
C	2.010993	-1.893288	0.628230
H	0.947619	-2.058402	0.810315
C	-1.232252	-3.356283	2.876034
H	-1.628208	-4.368733	2.777902
C	2.859196	-2.960578	0.331385
H	2.454343	-3.972599	0.281906
C	-2.787015	0.161791	0.962120
H	-3.575836	-0.290830	1.576269
C	2.016965	1.533104	1.575897
H	2.968481	1.560166	2.122167
C	-3.165988	1.044260	-0.127139
C	1.152209	2.692156	1.632383
C	-4.490203	1.394406	-0.398730
H	-5.286866	1.033569	0.252278
C	1.429520	3.779339	2.467541
H	2.324769	3.761896	3.089747
C	-4.763777	2.194530	-1.507997
H	-5.789788	2.479114	-1.741340
C	0.551584	4.859884	2.489825
H	0.742808	5.717578	3.134621
C	-3.707926	2.619522	-2.316305
H	-3.883023	3.239789	-3.194085
C	-0.577303	4.819548	1.670365
H	-1.291775	5.641609	1.653257
C	-2.406512	2.239023	-1.985346
H	-1.548510	2.552418	-2.583438
C	-0.791440	3.708192	0.854203
H	-1.662434	3.661784	0.200439
H	-3.809670	-4.929971	-0.893656
H	0.085790	-3.851388	4.517599
H	4.874400	-3.569677	-0.164326
H	-4.564730	-2.639995	-1.535904
H	0.958745	-1.527917	4.746318
H	5.791020	-1.253856	-0.046623

Quintet $[Fe(2)_3]^{2+}$ X=2.00, Y=2.00

Fe	-0.760034	0.099991	-0.025170
N	-1.953448	-0.417975	-1.544206
N	0.150036	-1.575978	-0.627584
N	0.366571	0.308010	1.614186
N	0.281409	1.389970	-1.143809
N	-1.845820	-0.983398	1.258315
N	-1.759514	1.782979	0.385428
C	-2.995939	0.272572	-2.063486
H	-3.183721	1.260464	-1.640398
C	-3.806100	-0.236299	-3.077646
H	-4.633679	0.362502	-3.455395
C	-3.549035	-1.512482	-3.584009
H	-4.176195	-1.935555	-4.368638
C	-2.473992	-2.236715	-3.072092
H	-2.229683	-3.232797	-3.441834
C	-1.692941	-1.663478	-2.068101
C	-0.517099	-2.286144	-1.498395
H	-0.218743	-3.293363	-1.808620
C	1.331881	-2.185292	-0.068814
C	1.227179	-2.980571	1.081404
H	0.245069	-3.194220	1.505686
C	2.385589	-3.507090	1.659956
C	3.639947	-3.251512	1.093543
C	3.731638	-2.477866	-0.068082
H	4.703268	-2.287740	-0.528081
C	2.582095	-1.939169	-0.651163
H	2.647255	-1.344565	-1.561113
C	4.104647	2.281940	1.900372
C	3.674698	0.316232	-3.422404
C	2.923787	3.028116	1.805913
C	2.397810	-0.107838	-3.812158
C	1.686027	2.386197	1.721961
H	0.766203	2.969237	1.669823
C	1.275096	0.252381	-3.065070
H	0.279505	-0.078278	-3.362130
C	1.630405	0.984508	1.752711
C	1.433125	1.072698	-1.937498
C	2.807159	0.234789	1.889987
H	2.747105	-0.852405	1.943982
C	2.705807	1.522153	-1.555663
H	2.811606	2.156677	-0.674950
C	4.041255	0.885594	1.947166
H	4.954733	0.294533	2.035825
C	3.824348	1.129034	-2.294022
H	4.815890	1.464076	-1.984572
C	-0.027066	-0.402500	2.642230
H	0.537978	-0.453577	3.579608
C	-0.017789	2.641764	-0.959651
H	0.544251	3.469192	-1.410287
C	-1.264128	-1.124723	2.500550
C	-1.183891	2.917087	-0.134649
C	-1.821254	-1.906242	3.516917
H	-1.304463	-1.983001	4.474004
C	-1.673994	4.198204	0.103421
H	-1.165965	5.059857	-0.330267
C	-3.021598	-2.567729	3.280421
H	-3.478694	-3.184240	4.053968
C	-2.816532	4.343969	0.893570
H	-3.227853	5.332971	1.094204
C	-3.629934	-2.421588	2.029821
H	-4.574297	-2.914888	1.802961
C	-3.418238	3.201225	1.416449
H	-4.313075	3.267687	2.033800
C	-3.022225	-1.632649	1.056596
H	-3.490979	-1.500097	0.080649
C	-2.863280	1.946798	1.147705
H	-3.316108	1.039430	1.549136
H	4.540330	-3.663464	1.551112
H	5.068850	2.789552	1.949264
H	4.549730	0.014181	-3.999278
H	2.304272	-4.127383	2.553945
H	2.963486	4.118432	1.798415
H	2.275414	-0.730517	-4.699455

Quintet $[Fe(2)_3]^{2+}$ X=2.00, Y=2.05

Fe	-0.727661	-0.247868	-0.085451
N	-1.644045	0.949811	-1.399008
N	0.706046	-0.138674	-1.546692
N	0.410542	-1.448428	1.125324
N	-0.254688	1.531529	0.815804
N	-1.348857	-2.056303	-0.671874
N	-2.227361	-0.117094	1.231228
C	-2.900068	1.457627	-1.348167
H	-3.594010	0.965576	-0.664608
C	-3.310378	2.538486	-2.127116
H	-4.335260	2.897976	-2.044038
C	-2.402514	3.142889	-3.000722
H	-2.700144	3.995476	-3.610624
C	-1.110000	2.629770	-3.081588
H	-0.365069	3.059654	-3.752034
C	-0.765366	1.539215	-2.280883
C	0.528953	0.893318	-2.329610
H	1.283056	1.242500	-3.046204
C	1.947485	-0.848324	-1.641890
C	1.912788	-2.250491	-1.715373
H	0.955811	-2.767255	-1.776734
C	3.106146	-2.972082	-1.770220
C	4.337376	-2.307011	-1.735549
C	4.369481	-0.909728	-1.681070
H	5.324727	-0.382668	-1.667164
C	3.181885	-0.177324	-1.646141
H	3.205035	0.911458	-1.603652
C	3.632217	-0.043491	3.463602
C	2.677801	4.302070	-0.441762
C	2.322964	0.354212	3.761071
C	1.321893	4.642604	-0.505983
C	1.250763	-0.124922	3.007695
H	0.229793	0.180814	3.233427
C	0.351133	3.739113	-0.073868
H	-0.711829	3.981747	-0.141653
C	1.492075	-1.030086	1.962776
C	0.739587	2.479102	0.415333
C	2.799067	-1.458814	1.680783
H	2.970332	-2.158615	0.861242
C	2.095743	2.125841	0.459731
H	2.387520	1.141537	0.826674
C	3.866122	-0.951475	2.425700
H	4.883699	-1.268600	2.190961
C	3.059594	3.046713	0.044424
H	4.115783	2.776891	0.096626
C	0.194415	-2.726035	0.989910
H	0.737203	-3.493202	1.554631
C	-1.203871	1.981153	1.599676
H	-1.189610	2.989606	2.027790
C	-0.814218	-3.116412	0.017359
C	-2.288846	1.087652	1.902933
C	-1.174544	-4.435348	-0.248692
H	-0.727004	-5.244734	0.328203
C	-3.316612	1.409400	2.794977
H	-3.304656	2.379593	3.292275
C	-2.098986	-4.688927	-1.264290
H	-2.395888	-5.712072	-1.494357
C	-4.328174	0.483871	3.026324
H	-5.142354	0.709902	3.714416
C	-2.630834	-3.616958	-1.981052
H	-3.348882	-3.775907	-2.784109
C	-4.275729	-0.742402	2.356820
H	-5.045507	-1.498274	2.506671
C	-2.238648	-2.317697	-1.653229
H	-2.643270	-1.451153	-2.179583
C	-3.225407	-1.004579	1.480827
H	-3.177419	-1.955642	0.951085
H	5.267536	-2.876030	-1.761861
H	4.467746	0.352295	4.042458
H	3.435356	5.010938	-0.778353
H	3.072205	-4.060153	-1.842714
H	2.135112	1.047585	4.582210
H	1.017962	5.613860	-0.899167

Quintet $[Fe(2)_3]^{2+}$ X=2.00, Y=2.10

Fe	-0.874488	-0.100551	0.018817
N	-2.008531	0.485048	1.558587
N	0.142433	1.632746	0.627888
N	0.369662	-0.326370	-1.657721
N	0.287746	-1.405422	1.183290
N	-1.866156	0.993254	-1.330246
N	-1.774653	-1.846443	-0.358050
C	-3.081128	-0.169071	2.062922
H	-3.329129	-1.125902	1.600754
C	-3.846309	0.340046	3.111714
H	-4.700287	-0.227572	3.478543
C	-3.509316	1.576019	3.665599
H	-4.097150	1.998826	4.480157
C	-2.405606	2.263227	3.161048
H	-2.103330	3.228865	3.566832
C	-1.673436	1.694176	2.119647
C	-0.482472	2.301814	1.551969
H	-0.149124	3.280631	1.916264
C	1.329362	2.221079	0.066368
C	1.240052	2.976963	-1.111499
H	0.263471	3.181731	-1.552285
C	2.406728	3.478353	-1.695596
C	3.655282	3.230905	-1.112586
C	3.732471	2.492488	0.072765
H	4.699360	2.306084	0.544377
C	2.573646	1.985580	0.665818
H	2.625276	1.418029	1.593741
C	4.107216	-2.303497	-1.855901
C	3.724450	-0.295606	3.376334
C	2.922523	-3.046976	-1.788347
C	2.454117	0.123573	3.792367
C	1.684891	-2.402009	-1.732776
H	0.761721	-2.981158	-1.698050
C	1.316657	-0.245569	3.072129
H	0.327086	0.084426	3.389146
C	1.632878	-1.000054	-1.768293
C	1.451877	-1.072772	1.946155
C	2.814718	-0.253099	-1.875927
H	2.757933	0.834593	-1.926601
C	2.719281	-1.517184	1.539846
H	2.809043	-2.155931	0.660433
C	4.048405	-0.906873	-1.902787
H	4.965481	-0.318110	-1.967006
C	3.852686	-1.112515	2.248246
H	4.838609	-1.442384	1.915598
C	-0.003074	0.407113	-2.671862
H	0.579351	0.479512	-3.598200
C	0.016385	-2.657011	0.971381
H	0.606556	-3.481262	1.392347
C	-1.247021	1.129332	-2.553572
C	-1.158975	-2.956766	0.164854
C	-1.776743	1.908763	-3.585531
H	-1.233673	1.984294	-4.528074
C	-1.626115	-4.251012	-0.051285
H	-1.089742	-5.096672	0.379664
C	-2.985181	2.568888	-3.385790
H	-3.420360	3.182180	-4.174404
C	-2.782170	-4.431806	-0.813510
H	-3.173699	-5.432588	-0.994551
C	-3.628846	2.426961	-2.152636
H	-4.578726	2.921615	-1.953654
C	-3.425225	-3.309895	-1.333793
H	-4.331774	-3.405214	-1.929822
C	-3.046722	1.643304	-1.159787
H	-3.534092	1.517955	-0.191921
C	-2.893132	-2.041273	-1.092553
H	-3.371486	-1.146507	-1.493762
H	4.562129	3.620318	-1.577043
H	5.070978	-2.813645	-1.881700
H	4.610605	0.014640	3.931581
H	2.336908	4.070962	-2.609158
H	2.959835	-4.137386	-1.778168
H	2.348490	0.750734	4.678693

Quintet $[Fe(2)_3]^{2+}$ X=2.05, Y=2.00

Fe	-0.723816	0.049235	-0.063438
N	-1.788239	1.801198	-0.054896
N	0.320255	1.103246	-1.404595
N	0.167671	-1.728596	-0.274528
N	0.304126	0.616715	1.555714
N	-1.910909	-0.807556	-1.498270
N	-1.908982	-0.727140	1.418173
C	-2.919873	2.121186	0.610033
H	-3.402548	1.314711	1.163550
C	-3.464827	3.408057	0.599559
H	-4.382355	3.604308	1.152765
C	-2.824989	4.419388	-0.115737
H	-3.227967	5.431677	-0.133119
C	-1.655024	4.110195	-0.811063
H	-1.116912	4.864235	-1.386192
C	-1.174241	2.802935	-0.767020
C	0.018275	2.368460	-1.471608
H	0.607075	3.093219	-2.047555
C	1.511742	0.656045	-2.067054
C	1.420780	-0.373773	-3.015441
H	0.445864	-0.781385	-3.283876
C	2.584148	-0.844583	-3.627520
C	3.833635	-0.318169	-3.275350
C	3.915846	0.703513	-2.323570
H	4.885532	1.118746	-2.043325
C	2.757288	1.203513	-1.725928
H	2.809800	2.000984	-0.983318
C	3.621400	-2.940244	1.856026
C	4.000548	2.683221	1.462287
C	2.359806	-3.027392	2.456994
C	2.802062	3.378391	1.260456
C	1.212451	-2.649126	1.754235
H	0.225619	-2.728221	2.212449
C	1.577673	2.706727	1.307470
H	0.642367	3.249841	1.165826
C	1.335726	-2.185533	0.436546
C	1.556284	1.329952	1.575223
C	2.592534	-2.110811	-0.177700
H	2.669828	-1.767554	-1.208495
C	2.749684	0.636067	1.815656
H	2.716036	-0.426439	2.055364
C	3.731915	-2.489223	0.536830
H	4.709572	-2.428862	0.055171
C	3.969213	1.314141	1.746263
H	4.896758	0.766127	1.922672
C	-0.436258	-2.592138	-1.042433
H	-0.103935	-3.630177	-1.155186
C	-0.173214	0.221292	2.708673
H	0.325966	0.434920	3.660403
C	-1.590817	-2.112070	-1.779412
C	-1.413033	-0.515075	2.685367
C	-2.291188	-2.873949	-2.713956
H	-2.002269	-3.909876	-2.892218
C	-2.054547	-0.982087	3.836629
H	-1.610654	-0.786339	4.813241
C	-3.347205	-2.281407	-3.407235
H	-3.911241	-2.851675	-4.145286
C	-3.246436	-1.688209	3.706896
H	-3.767772	-2.063814	4.587080
C	-3.666899	-0.949448	-3.141599
H	-4.483402	-0.451362	-3.662423
C	-3.762465	-1.903136	2.425192
H	-4.695027	-2.446450	2.278270
C	-2.933317	-0.249283	-2.181698
H	-3.170404	0.787924	-1.940930
C	-3.074287	-1.413428	1.317262
H	-3.465160	-1.562820	0.309767
H	4.739748	-0.703362	-3.744675
H	4.512901	-3.231864	2.412791
H	4.953519	3.211320	1.410120
H	2.514568	-1.632371	-4.379086
H	2.264761	-3.396422	3.479426
H	2.817150	4.451782	1.065361

Quintet $[Fe(2)_3]^{2+}$ X=2.05, Y=2.05

Fe	-0.780830	0.102329	-0.025647
N	-1.769072	1.852225	0.378881
N	0.300046	1.426456	-1.157717
N	0.129674	-1.623188	-0.655050
N	0.369290	0.281088	1.661899
N	-2.001510	-0.447614	-1.577996
N	-1.878294	-1.004317	1.305726
C	-2.880376	2.035511	1.122880
H	-3.353530	1.135503	1.518096
C	-3.414768	3.301255	1.380387
H	-4.316865	3.388750	1.984368
C	-2.780581	4.429412	0.863577
H	-3.174311	5.427234	1.055908
C	-1.630059	4.259331	0.090063
H	-1.100211	5.110451	-0.338236
C	-1.160856	2.967691	-0.138193
C	0.012040	2.676661	-0.950586
H	0.592611	3.503778	-1.378678
C	1.466318	1.109152	-1.928662
C	1.331973	0.300136	-3.067365
H	0.343273	-0.027563	-3.389203
C	2.470623	-0.055448	-3.792774
C	3.739875	0.359443	-3.369544
C	3.866346	1.158188	-2.228409
H	4.851513	1.484758	-1.890478
C	2.732088	1.548649	-1.513234
H	2.820216	2.173017	-0.623465
C	3.634218	-3.275227	1.053938
C	4.111276	2.243772	1.920104
C	2.384428	-3.527894	1.632044
C	2.929343	2.991767	1.855515
C	1.220521	-3.008145	1.058596
H	0.242605	-3.215156	1.495677
C	1.690460	2.351083	1.780301
H	0.768404	2.932115	1.746509
C	1.314534	-2.228641	-0.103162
C	1.635488	0.949199	1.793527
C	2.559875	-1.986019	-0.697175
H	2.614336	-1.400591	-1.613676
C	2.813517	0.196547	1.897642
H	2.753222	-0.891561	1.932742
C	3.715795	-2.512389	-0.115429
H	4.683699	-2.321794	-0.583189
C	4.048603	0.846727	1.944255
H	4.963647	0.254662	2.006461
C	-0.512762	-2.289011	-1.572654
H	-0.194340	-3.274410	-1.931403
C	-0.029103	-0.444543	2.673844
H	0.538831	-0.517518	3.608698
C	-1.697485	-1.666224	-2.133377
C	-1.277762	-1.154158	2.535497
C	-2.453699	-2.230596	-3.160997
H	-2.174889	-3.204905	-3.562920
C	-1.828635	-1.934926	3.555945
H	-1.300251	-2.022007	4.505813
C	-3.551790	-1.526770	-3.654175
H	-4.159288	-1.944533	-4.456930
C	-3.040039	-2.582362	3.333636
H	-3.492071	-3.197273	4.111515
C	-3.858225	-0.280776	-3.104485
H	-4.707082	0.299447	-3.463533
C	-3.665072	-2.425896	2.093053
H	-4.616917	-2.909881	1.877761
C	-3.067426	0.222312	-2.070961
H	-3.289456	1.187659	-1.613528
C	-3.061406	-1.639288	1.114328
H	-3.535690	-1.500408	0.141906
H	4.626745	0.060198	-3.929644
H	4.538868	-3.679775	1.509702
H	5.076276	2.750548	1.961656
H	2.366386	-0.668429	-4.689133
H	2.311515	-4.138664	2.533290
H	2.969728	4.082077	1.862820

Quintet $[Fe(2)_3]^{2+}$ X=2.05, Y=2.10

Fe	-0.736360	-0.271239	-0.106662
N	-1.342370	-2.139007	-0.695283
N	0.417800	-1.512915	1.132734
N	-0.308661	1.551486	0.844400
N	0.764126	-0.100322	-1.566062
N	-2.296421	-0.133773	1.215937
N	-1.618047	0.987365	-1.463421
C	-2.254562	-2.412793	-1.651064
H	-2.695003	-1.551407	-2.157351
C	-2.625887	-3.718987	-1.977102
H	-3.364440	-3.890099	-2.758692
C	-2.044071	-4.781755	-1.286459
H	-2.320684	-5.810603	-1.516572
C	-1.097497	-4.512263	-0.295586
H	-0.615150	-5.315008	0.262277
C	-0.764862	-3.186477	-0.025122
C	0.245768	-2.788598	0.945351
H	0.820999	-3.557772	1.475094
C	1.487379	-1.073822	1.970275
C	1.218975	-0.168210	3.008684
H	0.189500	0.118364	3.221814
C	2.274559	0.337299	3.767901
C	3.594473	-0.032024	3.480201
C	3.856008	-0.937015	2.446171
H	4.882370	-1.229006	2.217013
C	2.805786	-1.472053	1.696846
H	2.999058	-2.167260	0.878291
C	2.630762	4.342242	-0.344045
C	4.404518	-2.253370	-1.679103
C	1.275963	4.687594	-0.405925
C	3.176306	-2.921273	-1.752793
C	0.301106	3.778672	0.005171
H	-0.760859	4.025055	-0.065060
C	1.980711	-2.202411	-1.722513
H	1.025097	-2.718787	-1.809167
C	0.684400	2.508152	0.470764
C	2.010280	-0.800582	-1.637143
C	2.039786	2.149698	0.509934
H	2.326701	1.155691	0.854614
C	3.242312	-0.126441	-1.600584
H	3.261677	0.961967	-1.546001
C	3.007661	3.075902	0.116948
H	4.062908	2.801719	0.165813
C	4.431939	-0.856561	-1.609714
H	5.385531	-0.328279	-1.563748
C	-1.283116	1.975046	1.607003
H	-1.294084	2.979493	2.045888
C	0.593203	0.948605	-2.323923
H	1.361194	1.321953	-3.013710
C	-2.369133	1.069324	1.883918
C	-0.707214	1.589813	-2.298484
C	-3.413427	1.386694	2.758354
H	-3.415119	2.356463	3.256587
C	-1.023624	2.699067	-3.085859
H	-0.256946	3.142117	-3.722367
C	-4.425511	0.456472	2.972176
H	-5.251471	0.679617	3.647172
C	-2.316890	3.215107	-3.034195
H	-2.591877	4.081751	-3.634969
C	-4.358541	-0.769128	2.303986
H	-5.127608	-1.528021	2.441798
C	-3.253902	2.598417	-2.201414
H	-4.278530	2.962926	-2.140592
C	-3.292309	-1.025840	1.444416
H	-3.226824	-1.977009	0.916208
C	-2.870815	1.498782	-1.433995
H	-3.583294	0.995576	-0.777520
H	4.417001	0.385270	4.062545
H	3.391324	5.055468	-0.664270
H	5.336454	-2.820045	-1.685608
H	2.066080	1.030538	4.584134
H	0.976019	5.666801	-0.782117
H	3.147142	-4.008815	-1.834911

Quintet $[Fe(2)_3]^{2+}$ X=2.05, Y=2.15

Fe	-0.894070	0.156581	-0.036753
N	-1.886990	-0.929632	1.390395
N	0.405263	0.357945	1.665607
N	0.323554	1.448757	-1.230310
N	0.110110	-1.706900	-0.634344
N	-1.739673	1.990947	0.313327
N	-2.077593	-0.539040	-1.559214
C	-3.085886	-1.550397	1.258981
H	-3.594570	-1.426822	0.301631
C	-3.660262	-2.306241	2.278709
H	-4.626976	-2.780250	2.113803
C	-2.985670	-2.445600	3.494763
H	-3.413875	-3.035403	4.304911
C	-1.755061	-1.814323	3.651379
H	-1.189171	-1.890464	4.580311
C	-1.234366	-1.064145	2.593357
C	0.034822	-0.375797	2.677407
H	0.635994	-0.472836	3.589941
C	1.689265	0.991131	1.744865
C	1.782466	2.390312	1.687123
H	0.875566	2.994805	1.657493
C	3.039795	2.997800	1.714790
C	4.202359	2.219352	1.774583
C	4.102606	0.825866	1.841254
H	5.002739	0.210749	1.898102
C	2.849462	0.209633	1.843186
H	2.760081	-0.875350	1.906906
C	3.717457	0.194493	-3.408384
C	3.592174	-3.318449	1.145881
C	2.436009	-0.227102	-3.786057
C	2.337462	-3.544636	1.724123
C	1.315130	0.186573	-3.064521
H	0.316624	-0.147922	-3.346743
C	1.179919	-3.040486	1.124402
H	0.197173	-3.224508	1.561076
C	1.477191	1.062416	-1.979281
C	1.285266	-2.301157	-0.062856
C	2.757018	1.502795	-1.608076
H	2.868891	2.170582	-0.752993
C	2.536308	-2.081185	-0.654105
H	2.599045	-1.523191	-1.587053
C	3.873915	1.053515	-2.315351
H	4.869498	1.380652	-2.010005
C	3.685183	-2.594690	-0.047645
H	4.657475	-2.424267	-0.514049
C	0.110073	2.708907	-0.998343
H	0.744979	3.508306	-1.402602
C	-0.570742	-2.388820	-1.499945
H	-0.286342	-3.395433	-1.831471
C	-1.061194	3.063247	-0.207627
C	-1.769636	-1.777381	-2.060952
C	-1.476567	4.379547	-0.010807
H	-0.894840	5.197992	-0.435562
C	-2.541690	-2.393424	-3.044574
H	-2.261601	-3.381973	-3.409004
C	-2.641527	4.617360	0.720686
H	-2.992392	5.636120	0.884106
C	-3.660658	-1.725562	-3.544535
H	-4.279792	-2.187232	-4.313568
C	-3.348108	3.529989	1.234149
H	-4.264074	3.672468	1.805902
C	-3.973026	-0.462050	-3.043884
H	-4.838639	0.090381	-3.406460
C	-2.866169	2.237555	1.017746
H	-3.386993	1.364682	1.415382
C	-3.164628	0.095392	-2.052359
H	-3.387535	1.075799	-1.627956
H	5.181515	2.700034	1.777484
H	4.590999	-0.149349	-3.963855
H	4.491834	-3.711581	1.621062
H	3.110542	4.086274	1.688133
H	2.309274	-0.891574	-4.641915
H	2.255562	-4.122937	2.645859

Quintet $[Fe(2)_3]^{2+}$ X=2.10, Y=2.00

Fe	-0.594342	-0.207669	-0.071852
N	-2.232815	-0.144377	1.239991
N	-0.240847	1.507374	0.894131
N	0.735018	-0.036038	-1.556191
N	0.375997	-1.552390	1.046350
N	-1.627937	1.059889	-1.388720
N	-1.391851	-2.010376	-0.795564
C	-3.244376	-1.024741	1.434316
H	-3.199114	-1.956621	0.871005
C	-4.308745	-0.780930	2.301105
H	-5.091825	-1.530429	2.408785
C	-4.355598	0.419587	3.015013
H	-5.178936	0.631148	3.696991
C	-3.328187	1.339802	2.836627
H	-3.313863	2.291075	3.369088
C	-2.289576	1.034700	1.949701
C	-1.192526	1.928103	1.692722
H	-1.167615	2.915362	2.166492
C	0.770632	2.459356	0.545351
C	0.404876	3.749456	0.122996
H	-0.653470	4.014295	0.065682
C	1.393242	4.657378	-0.257358
C	2.742594	4.289398	-0.209345
C	3.100919	3.002211	0.206278
H	4.151718	2.710171	0.242830
C	2.119689	2.077800	0.569983
H	2.392431	1.068923	0.881426
C	4.344052	-2.225336	-1.874248
C	3.644045	-0.417553	3.468300
C	3.107385	-2.880341	-1.899132
C	2.355891	0.045128	3.763353
C	1.921268	-2.151864	-1.796167
H	0.958576	-2.659463	-1.842114
C	1.269795	-0.342257	2.977973
H	0.264752	0.014562	3.201297
C	1.971042	-0.752744	-1.688572
C	1.474965	-1.221266	1.903284
C	3.209086	-0.089984	-1.697910
H	3.240516	0.997202	-1.626941
C	2.759328	-1.711932	1.619537
H	2.901709	-2.388128	0.775270
C	4.389461	-0.830621	-1.778461
H	5.349228	-0.311911	-1.769287
C	3.841669	-1.295828	2.397522
H	4.843019	-1.661228	2.163506
C	0.548584	1.013967	-2.314351
H	1.298224	1.371853	-3.031238
C	0.100929	-2.813468	0.850060
H	0.605537	-3.625395	1.386190
C	-0.739581	1.672991	-2.238858
C	-0.926135	-3.116314	-0.132247
C	-1.065559	2.804566	-2.989690
H	-0.315888	3.252545	-3.642766
C	-1.388171	-4.402092	-0.410749
H	-0.991927	-5.252642	0.144268
C	-2.348803	3.336850	-2.877556
H	-2.632815	4.222227	-3.446053
C	-2.356773	-4.566681	-1.403193
H	-2.738780	-5.559891	-1.639139
C	-3.264146	2.711603	-2.028046
H	-4.281208	3.087298	-1.922945
C	-2.825632	-3.445335	-2.087565
H	-3.576902	-3.536089	-2.870859
C	-2.870255	1.584308	-1.304728
H	-3.568897	1.069163	-0.642790
C	-2.321637	-2.185151	-1.754603
H	-2.669011	-1.281852	-2.259143
H	3.513757	5.001836	-0.504912
H	5.268863	-2.800130	-1.937827
H	4.492113	-0.094868	4.073678
H	1.108018	5.653896	-0.597807
H	3.063273	-3.965721	-2.000395
H	2.195958	0.717040	4.607840

Quintet $[Fe(2)_3]^{2+}$ X=2.10, Y=2.05

Fe	-0.637957	0.238586	0.086626
N	-1.363929	2.085250	0.773881
N	0.405587	1.567554	-1.074334
N	-0.281287	-1.527490	-0.891158
N	0.754561	0.033880	1.577005
N	-2.267066	0.156685	-1.235951
N	-1.634430	-1.037435	1.423707
C	-2.283359	2.298737	1.735740
H	-2.671726	1.410046	2.236703
C	-2.724294	3.579976	2.076875
H	-3.467240	3.703186	2.863564
C	-2.205272	4.680365	1.395073
H	-2.537606	5.689876	1.636875
C	-1.249031	4.473693	0.398503
H	-0.813827	5.306764	-0.153706
C	-0.847351	3.169510	0.113588
C	0.170877	2.832875	-0.869781
H	0.701398	3.632964	-1.399638
C	1.486747	1.195796	-1.933118
C	1.245995	0.305126	-2.990903
H	0.228458	-0.025463	-3.197589
C	2.312434	-0.127787	-3.779274
C	3.616643	0.299955	-3.502460
C	3.850303	1.189047	-2.448048
H	4.864576	1.526424	-2.227983
C	2.788043	1.651386	-1.668177
H	2.959651	2.336341	-0.836546
C	2.680783	-4.326181	0.221246
C	4.405030	2.160062	1.820336
C	1.328792	-4.683774	0.274295
C	3.180347	2.837008	1.855715
C	0.346428	-3.771067	-0.109981
H	-0.713754	-4.027208	-0.047086
C	1.980775	2.127993	1.778417
H	1.027291	2.652375	1.831328
C	0.720418	-2.485924	-0.540898
C	2.003816	0.726781	1.686855
C	2.072614	-2.114786	-0.569994
H	2.352101	-1.109615	-0.887374
C	3.230746	0.042873	1.684791
H	3.242849	-1.045302	1.623017
C	3.047717	-3.044168	-0.202907
H	4.100622	-2.760188	-0.243165
C	4.424766	0.763747	1.739430
H	5.375288	0.228485	1.720801
C	-1.251076	-1.938798	-1.669006
H	-1.251444	-2.931947	-2.132115
C	0.558925	-1.019824	2.324545
H	1.309728	-1.398485	3.029825
C	-2.340981	-1.032764	-1.925105
C	-0.740591	-1.659956	2.260595
C	-3.391696	-1.338638	-2.796935
H	-3.394678	-2.298308	-3.314292
C	-1.069818	-2.789409	3.013429
H	-0.316533	-3.246621	3.655877
C	-4.409765	-0.408649	-2.981390
H	-5.241522	-0.621798	-3.652602
C	-2.359763	-3.308263	2.917502
H	-2.645259	-4.191513	3.488587
C	-4.342654	0.803116	-2.288681
H	-5.117213	1.560426	-2.402936
C	-3.279618	-2.672940	2.080325
H	-4.301386	-3.038749	1.987011
C	-3.268108	1.047389	-1.434709
H	-3.202361	1.987150	-0.886449
C	-2.883128	-1.549504	1.353191
H	-3.583632	-1.026967	0.699005
H	4.449140	-0.058937	-4.109084
H	3.447223	-5.042398	0.519992
H	5.340422	2.719416	1.863366
H	2.124582	-0.808693	-4.610771
H	1.036902	-5.675767	0.622265
H	3.156613	3.924149	1.944274

Quintet $[Fe(2)_3]^{2+}$ X=2.10, Y=2.10

Fe	-0.669981	-0.283886	-0.098151
N	-1.633835	0.979894	-1.470532
N	0.797089	-0.031515	-1.579394
N	0.475252	-1.564450	1.109706
N	-0.394962	1.550337	0.886595
N	-1.265605	-2.189598	-0.749044
N	-2.308347	-0.238466	1.214695
C	-2.896456	1.459813	-1.428172
H	-3.596400	0.921787	-0.785861
C	-3.305070	2.570655	-2.167342
H	-4.337337	2.911247	-2.097710
C	-2.382263	3.227539	-2.984401
H	-2.676596	4.102441	-3.563812
C	-1.077291	2.742218	-3.048591
H	-0.321355	3.218448	-3.673838
C	-0.735995	1.622422	-2.286651
C	0.584058	1.020262	-2.322123
H	1.337384	1.428731	-3.008191
C	2.071246	-0.680134	-1.654914
C	2.096633	-2.081314	-1.748478
H	1.161618	-2.634358	-1.831544
C	3.319158	-2.752451	-1.790672
C	4.520273	-2.037136	-1.718889
C	4.493088	-0.641040	-1.635907
H	5.425565	-0.076489	-1.588752
C	3.275778	0.042135	-1.615119
H	3.253001	1.130101	-1.549989
C	3.597657	-0.058797	3.511803
C	2.449871	4.463911	-0.232252
C	2.270172	0.303945	3.770844
C	1.085833	4.775686	-0.263041
C	1.234036	-0.209739	2.990772
H	0.198605	0.071687	3.180857
C	0.140046	3.826735	0.125154
H	-0.928151	4.049399	0.076095
C	1.529142	-1.117765	1.961542
C	0.562158	2.550217	0.537682
C	2.855368	-1.508763	1.716391
H	3.069769	-2.205347	0.904380
C	1.926995	2.225626	0.542585
H	2.245044	1.226636	0.843179
C	3.886082	-0.965081	2.485852
H	4.918914	-1.250989	2.279561
C	2.865471	3.190719	0.172902
H	3.927880	2.942286	0.195657
C	0.330975	-2.837884	0.886259
H	0.920335	-3.607273	1.399999
C	-1.397618	1.912502	1.643072
H	-1.461603	2.906945	2.100132
C	-0.670056	-3.235509	-0.094180
C	-2.446926	0.954517	1.887479
C	-0.984379	-4.563382	-0.379432
H	-0.487673	-5.365823	0.166227
C	-3.526896	1.222602	2.735334
H	-3.582969	2.187335	3.240172
C	-1.933910	-4.834564	-1.366906
H	-2.197468	-5.864462	-1.607557
C	-4.506455	0.250790	2.912774
H	-5.359275	0.434532	3.566018
C	-2.536482	-3.772063	-2.039650
H	-3.278584	-3.944284	-2.817673
C	-4.373213	-0.964608	2.236762
H	-5.114753	-1.754844	2.346806
C	-2.179966	-2.464440	-1.700847
H	-2.635067	-1.603164	-2.194274
C	-3.272887	-1.170733	1.405984
H	-3.152660	-2.113629	0.872483
H	5.473660	-2.566695	-1.735536
H	4.405593	0.364708	4.109864
H	3.187358	5.208536	-0.534420
H	3.332176	-3.839660	-1.880850
H	2.040739	0.998312	4.580427
H	0.755541	5.760168	-0.597858

Quintet $[Fe(2)_3]^{2+}$ X=2.10, Y=2.15

Fe	-0.866102	0.065027	-0.072901
N	-1.959214	-0.536708	1.616054
N	0.303301	0.845861	1.553561
N	0.331653	1.010457	-1.587620
N	0.133332	-1.838363	-0.094235
N	-1.800442	1.929586	-0.318964
N	-2.024288	-1.060800	-1.414887
C	-3.137539	-1.203087	1.638397
H	-3.589496	-1.420842	0.669491
C	-3.755034	-1.601077	2.823224
H	-4.701812	-2.137748	2.780920
C	-3.146661	-1.305414	4.045680
H	-3.609041	-1.608616	4.984882
C	-1.937045	-0.615113	4.042543
H	-1.424457	-0.360251	4.970666
C	-1.369984	-0.241585	2.820939
C	-0.114944	0.477130	2.730591
H	0.437198	0.704293	3.651154
C	1.572956	1.507391	1.464023
C	1.635393	2.833711	1.010425
H	0.714791	3.380954	0.804489
C	2.879209	3.452607	0.865042
C	4.058099	2.750601	1.146091
C	3.987795	1.430776	1.603404
H	4.900352	0.877700	1.834600
C	2.748509	0.810115	1.775966
H	2.682200	-0.213810	2.144352
C	3.818820	-0.748242	-3.193224
C	3.657001	-2.706279	2.079958
C	2.554280	-1.250995	-3.526599
C	2.412617	-2.715154	2.722513
C	1.400937	-0.667093	-2.999516
H	0.414039	-1.058627	-3.247870
C	1.243594	-2.445750	2.006421
H	0.272486	-2.456485	2.502348
C	1.515712	0.453605	-2.162313
C	1.323174	-2.185905	0.630171
C	2.778612	0.974680	-1.842054
H	2.852134	1.838247	-1.179727
C	2.562804	-2.195466	-0.023404
H	2.607256	-2.001997	-1.094791
C	3.926502	0.360829	-2.347604
H	4.908064	0.755418	-2.078626
C	3.726466	-2.448155	0.707379
H	4.690196	-2.445427	0.194448
C	0.090620	2.278838	-1.725357
H	0.726323	2.945919	-2.322647
C	-0.394429	-2.719105	-0.885762
H	0.011155	-3.730904	-1.010801
C	-1.104060	2.822391	-1.091353
C	-1.591508	-2.342499	-1.628374
C	-1.513280	4.144860	-1.261856
H	-0.916647	4.819275	-1.876774
C	-2.245147	-3.212897	-2.499266
H	-1.865567	-4.225625	-2.636412
C	-2.687713	4.573161	-0.641003
H	-3.032174	5.600345	-0.759325
C	-3.378474	-2.762911	-3.179125
H	-3.907378	-3.423662	-3.865847
C	-3.410632	3.663975	0.130766
H	-4.334008	3.956963	0.628653
C	-3.821820	-1.458504	-2.965289
H	-4.702874	-1.071504	-3.475023
C	-2.935875	2.358169	0.272291
H	-3.471946	1.625008	0.877614
C	-3.122391	-0.639132	-2.076364
H	-3.443336	0.384925	-1.878673
H	5.026734	3.234875	1.015234
H	4.716698	-1.222810	-3.591229
H	4.566721	-2.905337	2.647877
H	2.926298	4.489379	0.528313
H	2.465645	-2.109786	-4.193492
H	2.349314	-2.931673	3.790081

Quintet $[Fe(2)_3]^{2+}$ X=2.10, Y=2.20

Fe	0.952168	0.110226	0.034765
N	1.958823	-0.806031	-1.564192
N	-0.327254	0.554258	-1.698993
N	-0.326345	1.295019	1.377029
N	-0.117321	-1.776111	0.406146
N	1.802105	2.029310	-0.034850
N	2.076517	-0.802255	1.555627
C	3.148640	-1.448133	-1.502069
H	3.660765	-1.424855	-0.538656
C	3.705042	-2.107644	-2.596958
H	4.666920	-2.607452	-2.490576
C	3.015321	-2.119265	-3.811686
H	3.426552	-2.633547	-4.680110
C	1.791158	-1.459544	-3.894506
H	1.217987	-1.439017	-4.821886
C	1.290794	-0.809297	-2.763225
C	0.029765	-0.092167	-2.770772
H	-0.576173	-0.096792	-3.685934
C	-1.599794	1.213355	-1.702579
C	-1.662510	2.600417	-1.498309
H	-0.742197	3.179783	-1.418297
C	-2.906438	3.232802	-1.441554
C	-4.086761	2.488528	-1.562979
C	-4.017907	1.107678	-1.773248
H	-4.931705	0.519202	-1.876469
C	-2.778588	0.469191	-1.857595
H	-2.715178	-0.605094	-2.031181
C	-3.763863	-0.175427	3.338800
C	-3.671613	-3.056899	-1.500053
C	-2.487457	-0.601073	3.729455
C	-2.437951	-3.184621	-2.150378
C	-1.351608	-0.116098	3.078766
H	-0.354991	-0.447434	3.373067
C	-1.259161	-2.777391	-1.520201
H	-0.295380	-2.885584	-2.018983
C	-1.495023	0.833576	2.055071
C	-1.318037	-2.253157	-0.220233
C	-2.769661	1.278742	1.673400
H	-2.865034	2.009095	0.868673
C	-2.546599	-2.143779	0.444806
H	-2.573419	-1.749982	1.460092
C	-3.900429	0.759921	2.307467
H	-4.891602	1.092794	1.993634
C	-3.720292	-2.539605	-0.201603
H	-4.675340	-2.444367	0.318762
C	-0.118467	2.571506	1.272472
H	-0.775503	3.322490	1.731356
C	0.408148	-2.497260	1.346631
H	-0.012546	-3.459709	1.664987
C	1.072997	3.022627	0.563073
C	1.620091	-2.014685	1.997842
C	1.456796	4.362620	0.515679
H	0.834950	5.119027	0.995253
C	2.269208	-2.729016	3.004381
H	1.870539	-3.691640	3.325112
C	2.641328	4.703098	-0.139975
H	2.966864	5.742063	-0.187367
C	3.421741	-2.191501	3.580275
H	3.946738	-2.731132	4.368400
C	3.399419	3.691856	-0.730122
H	4.331799	3.914907	-1.247011
C	3.889593	-0.957111	3.131083
H	4.786576	-0.505449	3.552037
C	2.946331	2.372531	-0.663792
H	3.503386	1.556060	-1.127516
C	3.194387	-0.294775	2.117519
H	3.533417	0.668958	1.733882
H	-5.055242	2.986385	-1.499368
H	-4.648283	-0.573434	3.837986
H	-4.588835	-3.366555	-2.002635
H	-2.952827	4.313590	-1.299340
H	-2.375802	-1.323006	4.539835
H	-2.390087	-3.604535	-3.156294

Quintet $[Fe(2)_3]^{2+}$ X=2.15, Y=2.05

Fe	-0.565726	-0.174226	-0.125126
N	-1.707391	1.460191	-0.929450
N	0.663898	0.517734	-1.612310
N	0.091400	-1.982586	0.582347
N	0.154460	1.214858	1.199366
N	-1.736317	-1.575961	-1.257836
N	-2.071708	-0.151494	1.409152
C	-2.933996	1.927909	-0.601497
H	-3.542453	1.289495	0.039911
C	-3.433290	3.146407	-1.062769
H	-4.430714	3.464010	-0.761292
C	-2.648299	3.935238	-1.906146
H	-3.013227	4.894494	-2.272682
C	-1.392801	3.464123	-2.279178
H	-0.744810	4.032205	-2.947380
C	-0.955496	2.231174	-1.782832
C	0.317388	1.660646	-2.146974
H	0.941072	2.179969	-2.883644
C	1.940849	-0.026021	-1.956257
C	2.074192	-1.420250	-2.044509
H	1.202132	-2.057802	-1.903522
C	3.313566	-1.981063	-2.357035
C	4.426232	-1.160387	-2.567609
C	4.293492	0.230301	-2.473543
H	5.160810	0.875141	-2.623029
C	3.058302	0.800813	-2.172179
H	2.964858	1.881886	-2.058204
C	3.376466	-2.251540	3.222350
C	3.755139	3.365105	0.679568
C	2.237999	-1.522390	3.584877
C	2.531912	4.045886	0.670951
C	1.144691	-1.446456	2.721894
H	0.254542	-0.885583	3.002698
C	1.336824	3.347453	0.852040
H	0.375455	3.865138	0.839870
C	1.184766	-2.125727	1.494229
C	1.367767	1.953644	1.026242
C	2.312311	-2.882944	1.137683
H	2.331999	-3.401041	0.177884
C	2.588320	1.261956	0.994913
H	2.600744	0.176394	1.101419
C	3.408215	-2.933653	2.001530
H	4.291554	-3.506824	1.715938
C	3.778646	1.976126	0.844854
H	4.728424	1.439014	0.840584
C	-0.438353	-3.053499	0.068143
H	-0.141346	-4.065951	0.368175
C	-0.686311	1.639987	2.108372
H	-0.471029	2.496274	2.757920
C	-1.483040	-2.881342	-0.930978
C	-1.919518	0.907251	2.272013
C	-2.176441	-3.947629	-1.500446
H	-1.936714	-4.969819	-1.207102
C	-2.877891	1.232231	3.238338
H	-2.708311	2.085645	3.895574
C	-3.176241	-3.673850	-2.437254
H	-3.738382	-4.486779	-2.896556
C	-4.028608	0.456006	3.335505
H	-4.793028	0.689688	4.076343
C	-3.441639	-2.348097	-2.771877
H	-4.213381	-2.093342	-3.496746
C	-4.185531	-0.628481	2.467415
H	-5.069924	-1.262570	2.513299
C	-2.701625	-1.328499	-2.163395
H	-2.880343	-0.280161	-2.405944
C	-3.194264	-0.896669	1.523323
H	-3.299837	-1.731888	0.829334
H	5.396178	-1.602139	-2.799509
H	4.236405	-2.290759	3.892238
H	4.687514	3.915783	0.548153
H	3.408219	-3.064996	-2.436345
H	2.202043	-1.004172	4.544118
H	2.507618	5.126821	0.524326

Quintet $[Fe(2)_3]^{2+}$ X=2.15, Y=2.10

Fe	-0.603314	0.180054	0.136565
N	-1.720162	-1.475746	0.931947
N	0.657923	-0.549416	1.648645
N	0.085027	2.030153	-0.580024
N	0.174626	-1.230025	-1.210951
N	-1.759239	1.602953	1.257891
N	-2.073443	0.129509	-1.431451
C	-2.948214	-1.936471	0.597878
H	-3.551770	-1.291364	-0.041459
C	-3.453604	-3.156495	1.047837
H	-4.451607	-3.467326	0.741303
C	-2.672874	-3.955875	1.884925
H	-3.041769	-4.917047	2.242393
C	-1.415794	-3.492904	2.263114
H	-0.770990	-4.069972	2.926752
C	-0.972176	-2.257104	1.779764
C	0.304597	-1.700246	2.155950
H	0.923732	-2.241480	2.880994
C	1.938591	-0.016390	1.984073
C	2.084750	1.378683	2.040108
H	1.216084	2.018246	1.885417
C	3.330061	1.936006	2.333767
C	4.436498	1.110303	2.558217
C	4.291565	-0.281036	2.495802
H	5.154704	-0.929509	2.653748
C	3.050607	-0.847748	2.211667
H	2.950236	-1.930072	2.116121
C	3.389359	2.308680	-3.190877
C	3.802229	-3.330912	-0.694407
C	2.261181	1.564925	-3.556108
C	2.590593	-4.032057	-0.708365
C	1.162069	1.485434	-2.701029
H	0.279859	0.911908	-2.981696
C	1.385528	-3.350606	-0.887390
H	0.433070	-3.884388	-0.893046
C	1.184612	2.176905	-1.479589
C	1.394246	-1.953484	-1.036026
C	2.303445	2.945720	-1.119264
H	2.312187	3.468249	-0.161562
C	2.602924	-1.242096	-0.980152
H	2.596836	-0.154333	-1.065691
C	3.405640	2.999682	-1.974612
H	4.282063	3.581848	-1.685936
C	3.803873	-1.938806	-0.833717
H	4.744590	-1.386406	-0.811910
C	-0.442997	3.091446	-0.048131
H	-0.141283	4.109136	-0.326082
C	-0.662033	-1.654222	-2.120960
H	-0.441865	-2.505734	-2.775921
C	-1.495081	2.908867	0.942840
C	-1.902151	-0.929523	-2.289555
C	-2.185000	3.973691	1.519721
H	-1.936503	4.997064	1.238010
C	-2.849850	-1.264535	-3.262454
H	-2.667593	-2.117499	-3.916894
C	-3.191640	3.698555	2.448557
H	-3.749817	4.511292	2.913032
C	-4.006937	-0.498681	-3.371573
H	-4.762523	-0.741223	-4.118605
C	-3.468749	2.371660	2.769217
H	-4.245863	2.115355	3.487761
C	-4.181440	0.586574	-2.508421
H	-5.070820	1.212816	-2.563958
C	-2.732296	1.353405	2.155258
H	-2.918125	0.303979	2.387368
C	-3.201070	0.865156	-1.555900
H	-3.318095	1.700112	-0.863431
H	5.411553	1.548647	2.774751
H	4.254057	2.351104	-3.854408
H	4.742633	-3.868379	-0.565469
H	3.435354	3.020586	2.386360
H	2.238605	1.037669	-4.510819
H	2.583344	-5.115699	-0.581209

Quintet $[Fe(2)_3]^{2+}$ X=2.15, Y=2.15

Fe	-0.625770	0.118078	0.211471
N	-1.765043	-1.673667	0.548771
N	0.617691	-1.048211	1.521483
N	-0.045559	2.159412	-0.133608
N	0.353108	-0.913966	-1.400648
N	-1.888188	1.237567	1.543991
N	-1.964640	0.330706	-1.457215
C	-3.009710	-1.987851	0.116167
H	-3.571717	-1.188827	-0.368148
C	-3.581988	-3.248953	0.279636
H	-4.589785	-3.430914	-0.091359
C	-2.853346	-4.255813	0.915876
H	-3.273021	-5.253159	1.046295
C	-1.581837	-3.952670	1.392238
H	-0.975762	-4.694997	1.912556
C	-1.072052	-2.662723	1.205702
C	0.215599	-2.272693	1.722970
H	0.793901	-3.009133	2.292019
C	1.902413	-0.632058	1.974352
C	2.124614	0.750708	2.096227
H	1.303141	1.442201	1.902829
C	3.380514	1.229776	2.466843
C	4.425942	0.335542	2.718997
C	4.205458	-1.043079	2.604025
H	5.022050	-1.743601	2.785696
C	2.954403	-1.530822	2.232571
H	2.813578	-2.602990	2.093853
C	3.203256	3.180508	-2.622549
C	4.193911	-2.641099	-1.104946
C	2.118816	2.458361	-3.135011
C	3.082705	-3.464918	-1.320523
C	1.038087	2.135346	-2.315020
H	0.190980	1.572837	-2.704988
C	1.805549	-2.911272	-1.437429
H	0.929598	-3.543655	-1.595842
C	1.032118	2.560610	-0.977255
C	1.642041	-1.521907	-1.320501
C	2.107371	3.303931	-0.463141
H	2.096648	3.612448	0.583810
C	2.749643	-0.695297	-1.071527
H	2.603074	0.379328	-0.957116
C	3.193566	3.601796	-1.288453
H	4.037647	4.163347	-0.885323
C	4.023753	-1.256934	-0.985883
H	4.884421	-0.609986	-0.807042
C	-0.634872	3.041923	0.612132
H	-0.397491	4.112802	0.569313
C	-0.415279	-1.199309	-2.414271
H	-0.109172	-1.874214	-3.223091
C	-1.679153	2.590940	1.523670
C	-1.695486	-0.523939	-2.497258
C	-2.420666	3.475617	2.305292
H	-2.214712	4.544958	2.253839
C	-2.572457	-0.686002	-3.574418
H	-2.316326	-1.380471	-4.375027
C	-3.420316	2.966726	3.137109
H	-4.016802	3.636611	3.756340
C	-3.754138	0.050887	-3.602115
H	-4.455347	-0.060861	-4.429058
C	-3.640560	1.591592	3.159680
H	-4.409251	1.152771	3.794171
C	-4.021989	0.936983	-2.555579
H	-4.930929	1.536878	-2.543355
C	-2.856267	0.762299	2.352344
H	-2.998008	-0.318881	2.352920
C	-3.110381	1.044625	-1.504960
H	-3.301263	1.715796	-0.665834
H	5.411498	0.710187	2.998288
H	4.054954	3.414413	-3.262566
H	5.189644	-3.078587	-1.020032
H	3.543830	2.304743	2.556604
H	2.116885	2.138758	-4.178013
H	3.210575	-4.545694	-1.399343

Quintet $[Fe(2)_3]^{2+}$ X=2.15, Y=2.20

Fe	-0.921342	0.077296	0.083395
N	-1.884638	-1.433997	1.268585
N	0.357397	-0.110919	1.864200
N	0.235968	1.705620	-0.839123
N	0.187668	-1.510876	-0.959236
N	-1.917239	1.875790	0.710103
N	-2.072896	-0.283551	-1.694588
C	-3.061637	-2.041064	1.010278
H	-3.619706	-1.666282	0.150827
C	-3.551003	-3.093297	1.787188
H	-4.509484	-3.545923	1.536448
C	-2.796345	-3.551613	2.867113
H	-3.151432	-4.377865	3.482869
C	-1.576703	-2.934322	3.146485
H	-0.954192	-3.258372	3.981052
C	-1.154458	-1.876237	2.339754
C	0.089286	-1.157395	2.584610
H	0.744553	-1.501236	3.396171
C	1.591920	0.579231	2.065601
C	1.568635	1.966167	2.280516
H	0.612466	2.484722	2.359038
C	2.771676	2.659656	2.425427
C	3.995237	1.984637	2.323339
C	4.011778	0.603595	2.101256
H	4.960726	0.070270	2.018886
C	2.814077	-0.105365	1.986604
H	2.815503	-1.182439	1.814343
C	3.688512	1.150721	-3.211364
C	3.869997	-3.191681	0.286121
C	2.419855	0.856397	-3.728102
C	2.668329	-3.619164	0.864241
C	1.278009	1.039218	-2.945347
H	0.287617	0.810656	-3.340503
C	1.449667	-3.076888	0.448077
H	0.511837	-3.419339	0.886742
C	1.408310	1.553612	-1.646361
C	1.434440	-2.111067	-0.569516
C	2.672992	1.868648	-1.129850
H	2.755418	2.263496	-0.116894
C	2.632233	-1.697514	-1.168242
H	2.604216	-0.961680	-1.970805
C	3.810453	1.653077	-1.911805
H	4.794852	1.884439	-1.500546
C	3.846553	-2.232242	-0.730953
H	4.776079	-1.898163	-1.196178
C	-0.101046	2.896397	-0.454707
H	0.452233	3.797984	-0.748945
C	-0.300617	-1.824456	-2.121942
H	0.187622	-2.546462	-2.789035
C	-1.295621	3.045156	0.370962
C	-1.553102	-1.224226	-2.544660
C	-1.780571	4.287537	0.776649
H	-1.252153	5.195133	0.483842
C	-2.189645	-1.588834	-3.733889
H	-1.731995	-2.339942	-4.378339
C	-2.942776	4.339843	1.549452
H	-3.343486	5.299180	1.876622
C	-3.401268	-0.986276	-4.066053
H	-3.919019	-1.255877	-4.986519
C	-3.580837	3.149290	1.892938
H	-4.490778	3.148380	2.491105
C	-3.939797	-0.034925	-3.197469
H	-4.886023	0.457222	-3.418582
C	-3.038125	1.937713	1.456946
H	-3.508755	0.983612	1.701631
C	-3.251420	0.289540	-2.028531
H	-3.643959	1.029507	-1.329073
H	4.931930	2.535773	2.417127
H	4.577380	0.989375	-3.822669
H	4.818625	-3.611027	0.623804
H	2.753902	3.734483	2.611903
H	2.318316	0.474856	-4.745224
H	2.676837	-4.381844	1.644461

Quintet $[Fe(2)_3]^{2+}$ X=2.20, Y=2.10

Fe	0.544635	0.106798	-0.208434
N	1.753827	-1.714266	-0.455635
N	-0.621989	-1.109216	-1.461550
N	0.096005	2.140290	0.062937
N	-0.369965	-0.821109	1.438532
N	1.917487	1.134154	-1.586632
N	1.965353	0.388218	1.447286
C	2.991584	-2.016935	0.000066
H	3.539925	-1.213714	0.492250
C	3.576522	-3.274717	-0.148495
H	4.578569	-3.447783	0.241942
C	2.867727	-4.288562	-0.795511
H	3.298090	-5.282571	-0.916356
C	1.601922	-3.997495	-1.294257
H	1.010777	-4.746460	-1.822074
C	1.079568	-2.710530	-1.118236
C	-0.202519	-2.331139	-1.654030
H	-0.768097	-3.069769	-2.232760
C	-1.909194	-0.724088	-1.940820
C	-2.140448	0.645958	-2.151144
H	-1.324303	1.356013	-2.007339
C	-3.399974	1.089818	-2.552744
C	-4.438069	0.173155	-2.748410
C	-4.207492	-1.193428	-2.544957
H	-5.018250	-1.910682	-2.681985
C	-2.953122	-1.646108	-2.140889
H	-2.802666	-2.705241	-1.929713
C	-3.224738	3.337743	2.377637
C	-4.230565	-2.523346	1.239182
C	-2.159110	2.654482	2.975490
C	-3.125971	-3.345521	1.491361
C	-1.051738	2.272489	2.218005
H	-0.220129	1.741282	2.678606
C	-1.843650	-2.798081	1.576583
H	-0.972795	-3.429333	1.764634
C	-1.001815	2.600304	0.854408
C	-1.668162	-1.417815	1.391387
C	-2.057763	3.305544	0.253741
H	-2.011464	3.537915	-0.811675
C	-2.769344	-0.593873	1.107972
H	-2.614945	0.473102	0.943871
C	-3.170179	3.662482	1.018085
H	-3.998344	4.194139	0.547086
C	-4.048609	-1.148170	1.052308
H	-4.904297	-0.503100	0.844947
C	0.716205	2.988983	-0.699324
H	0.500728	4.064966	-0.683729
C	0.390358	-1.064463	2.471546
H	0.066916	-1.692463	3.310537
C	1.757568	2.493038	-1.588472
C	1.680418	-0.407796	2.527386
C	2.541883	3.341509	-2.369004
H	2.372145	4.417908	-2.335619
C	2.551784	-0.530820	3.615178
H	2.282799	-1.180413	4.448616
C	3.537846	2.785464	-3.174736
H	4.168276	3.424896	-3.792606
C	3.744622	0.188137	3.609840
H	4.441454	0.108371	4.444227
C	3.710494	1.403264	-3.172478
H	4.475647	0.929195	-3.785558
C	4.028902	1.016555	2.521251
H	4.946497	1.601981	2.482309
C	2.882469	0.613220	-2.368032
H	2.986124	-0.472254	-2.350842
C	3.121521	1.084370	1.462940
H	3.326833	1.709192	0.592114
H	-5.425946	0.521324	-3.052737
H	-4.096563	3.616297	2.970953
H	-5.230365	-2.955543	1.178310
H	-3.570793	2.155433	-2.712966
H	-2.192089	2.412136	4.038625
H	-3.262866	-4.419826	1.624680

Quintet $[Fe(2)_3]^{2+}$ X=2.20, Y=2.15

Fe	0.765127	0.194544	0.044664
N	1.959881	-0.948515	-1.406373
N	-0.410781	0.229835	-1.755079
N	-0.403162	1.569512	1.214049
N	-0.030807	-1.676405	0.743390
N	1.651428	2.165458	-0.367138
N	2.156302	-0.437731	1.627037
C	3.186387	-1.493945	-1.250327
H	3.688116	-1.299352	-0.301075
C	3.799863	-2.264996	-2.238361
H	4.791533	-2.678280	-2.058775
C	3.128530	-2.495584	-3.440717
H	3.584848	-3.097653	-4.226297
C	1.863536	-1.940511	-3.619180
H	1.300739	-2.090860	-4.540918
C	1.308683	-1.170902	-2.592117
C	0.004570	-0.550129	-2.712210
H	-0.588251	-0.731897	-3.617487
C	-1.726263	0.786062	-1.859396
C	-1.895630	2.177157	-1.791025
H	-1.023020	2.828252	-1.730665
C	-3.182393	2.716816	-1.844758
C	-4.299380	1.877243	-1.938082
C	-4.123807	0.491307	-2.007702
H	-4.988535	-0.170332	-2.085194
C	-2.839965	-0.057365	-1.984341
H	-2.690442	-1.136563	-2.041055
C	-3.719033	0.246313	3.465967
C	-3.458788	-3.489700	-0.953274
C	-2.419203	-0.132602	3.825482
C	-2.192509	-3.729820	-1.499641
C	-1.324637	0.306015	3.078858
H	-0.310930	0.001673	3.341351
C	-1.054239	-3.153021	-0.928996
H	-0.063034	-3.344122	-1.342977
C	-1.533359	1.164401	1.987707
C	-1.190996	-2.328053	0.197194
C	-2.831869	1.559778	1.631475
H	-2.978214	2.210122	0.768179
C	-2.454601	-2.084317	0.750785
H	-2.543051	-1.456174	1.635801
C	-3.921360	1.086244	2.365434
H	-4.932172	1.377650	2.074982
C	-3.583510	-2.673151	0.175373
H	-4.565414	-2.488500	0.615361
C	-0.229639	2.826516	0.939870
H	-0.885633	3.614397	1.333603
C	0.686793	-2.317807	1.612622
H	0.431274	-3.325146	1.964173
C	0.913133	3.209070	0.118552
C	1.884774	-1.675741	2.139771
C	1.242315	4.540515	-0.137215
H	0.617676	5.339402	0.263447
C	2.701430	-2.278777	3.097136
H	2.448178	-3.268982	3.476729
C	2.377876	4.818280	-0.901030
H	2.658936	5.849236	-1.115451
C	3.832685	-1.595300	3.545750
H	4.487344	-2.044551	4.292588
C	3.144886	3.757230	-1.379975
H	4.041396	3.932488	-1.973113
C	4.114093	-0.334384	3.020286
H	4.991180	0.226356	3.340408
C	2.749139	2.446945	-1.094799
H	3.316984	1.589121	-1.459966
C	3.256356	0.209406	2.060921
H	3.448447	1.187692	1.617036
H	-5.303110	2.303734	-1.961627
H	-4.572030	-0.116982	4.040609
H	-4.343078	-3.942783	-1.403433
H	-3.312759	3.799626	-1.811378
H	-2.257653	-0.784461	4.685197
H	-2.085864	-4.375492	-2.372761

Quintet $[Fe(2)_3]^{2+}$ X=2.20, Y=2.20

Fe	-0.155352	0.778028	-0.331221
N	1.509963	0.996747	-1.752306
N	-0.249289	-1.023240	-1.592335
N	-1.539917	-0.086672	1.142215
N	1.641532	0.503962	0.907179
N	-2.161583	1.456937	-0.926987
N	0.018255	2.629773	0.841218
C	2.378143	2.023943	-1.849522
H	2.092457	2.945429	-1.338937
C	3.580616	1.929244	-2.553914
H	4.243201	2.792136	-2.606648
C	3.917029	0.722225	-3.168137
H	4.855665	0.617881	-3.712421
C	3.032190	-0.351395	-3.072006
H	3.252377	-1.314429	-3.533936
C	1.839716	-0.180573	-2.364116
C	0.858818	-1.246392	-2.238342
H	1.074663	-2.205513	-2.727758
C	-1.166440	-2.110806	-1.448626
C	-2.539756	-1.864148	-1.604899
H	-2.879421	-0.874147	-1.907935
C	-3.455604	-2.901312	-1.423296
C	-3.013305	-4.183982	-1.077802
C	-1.644026	-4.431252	-0.932871
H	-1.292041	-5.428704	-0.664772
C	-0.719086	-3.403202	-1.119821
H	0.347430	-3.590303	-0.985330
C	-0.268100	-3.077819	3.833328
C	4.274815	-2.681129	0.070113
C	0.219179	-1.770647	3.954663
C	4.771971	-1.374369	0.139681
C	-0.218511	-0.770710	3.085930
H	0.153738	0.248834	3.176031
C	3.922937	-0.314530	0.457813
H	4.296768	0.710748	0.470901
C	-1.167938	-1.078414	2.099240
C	2.560709	-0.562862	0.703963
C	-1.688417	-2.379179	1.998582
H	-2.422314	-2.604058	1.222705
C	2.059585	-1.873803	0.631634
H	0.999825	-2.054339	0.820803
C	-1.225072	-3.377255	2.857977
H	-1.612364	-4.393088	2.760319
C	2.921005	-2.927694	0.325309
H	2.530706	-3.945422	0.276057
C	-2.805901	0.128956	0.939155
H	-3.592610	-0.334416	1.548140
C	2.015003	1.550885	1.584133
H	2.968200	1.594833	2.126377
C	-3.191927	1.016459	-0.145436
C	1.128871	2.693592	1.646640
C	-4.519529	1.355861	-0.412871
H	-5.312887	0.980403	0.233949
C	1.394906	3.786814	2.477783
H	2.296114	3.785792	3.091550
C	-4.800729	2.166277	-1.513350
H	-5.829449	2.443773	-1.743395
C	0.498432	4.851744	2.507050
H	0.680268	5.713238	3.149498
C	-3.749119	2.610798	-2.315708
H	-3.929672	3.240132	-3.185926
C	-0.636265	4.791613	1.696973
H	-1.364603	5.601481	1.685075
C	-2.443731	2.237638	-1.988509
H	-1.588419	2.565719	-2.582535
C	-0.837960	3.676090	0.883369
H	-1.712013	3.615458	0.235168
H	-3.733852	-4.988701	-0.925985
H	0.095818	-3.860023	4.500949
H	4.940853	-3.505366	-0.188197
H	-4.520859	-2.706403	-1.556990
H	0.949543	-1.529298	4.728339
H	5.824276	-1.176922	-0.070870

V. References.

1. Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101.
2. Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157-167.
3. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
4. M. Dolg, U. Wedig, H. Stoll and H. Preuss, *J. Chem. Phys.*, 1987, **86**, 866-872.
5. J. M. L. Martin and A. Sundermann, *J. Chem. Phys.*, 2001, **114**, 3408-3420.
6. R. E. Easton, D. J. Giesen, A. Welch, C. J. Cramer and D. G. Truhlar, *Theor. Chim. Acta*, 1996, **93**, 281-301.
7. R. F. Ribeiro, A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2011, **115**, 14556-14562.
8. C. J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, John Wiley & Sons, Chichester, 2004.
9. F. Aquilante, L. De Vico, N. Ferre, G. Ghigo, P. A. Malmqvist, P. Neogrady, T. B. Pedersen, M. Pitonak, M. Reiher, B. O. Roos, L. Serrano-Andres, M. Urban, V. Veryazov and R. Lindh, *J. Comput. Chem.*, 2010, **31**, 224-247.
10. V. Veryazov, P.-O. Widmark and B. r. O. Roos, *Theor. Chem. Acc.*, 2004, **111**, 345-351.
11. B. O. Roos, R. Lindh, P.-Å. Malmqvist, V. Veryazov and P.-O. Widmark, *J. Phys. Chem. A*, 2005, **109**, 6575-6579.
12. N. Forsberg and P.-Å. Malmqvist, *Chem. Phys. Lett.*, 1997, **274**, 196-204.
13. F. Aquilante, R. Lindh and T. B. Pedersen, *J. Chem. Phys.*, 2007, **127**, 114107.
14. S. Moon and S. Patchkovskii, *First-Principles Calculations of Paramagnetic NMR Shifts*, Wiley-VCH, 2004.
15. G. Kervern, G. Pintacuda, Y. Zhang, E. Oldfield, C. Roukoss, E. Kuntz, E. Herdtweck, J. M. Basset, S. Cadars, A. Lesage, C. Coperet and L. Emsley, *J. Am. Chem. Soc.*, 2006, **128**, 13545-13552.
16. J. Mao, Y. Zhang and E. Oldfield, *J. Am. Chem. Soc.*, 2002, **124**, 13911-13920.
17. M. Kruck, D. C. Sauer, M. Enders, H. Wadepohl and L. H. Gade, *Dalton Trans.*, 2011, **40**, 10406-10415.
18. F. Rastrelli and A. Bagno, *Chem. Eur. J.*, 2009, **15**, 7990-8004.
19. Y. Zhang, H. Sun and E. Oldfield, *J. Am. Chem. Soc.*, 2005, **127**, 3652-3653.
20. A. J. H. Wachters, *J. Chem. Phys.*, 1970, **52**, 1033.
21. P. J. Hay, *J. Chem. Phys.*, 1977, **66**, 4377.
22. V. Barone, in *Recent Advances in Density Functional Methods, Part I*, ed. D. P. Chong, World Scientific Publ. Co., Singapore, 1996.
23. A. D. McLean and G. S. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639.
24. R. Krishnan, J. S. Binkley, R. Seeger and J. A. Pople, *J. Chem. Phys.*, 1980, **72**, 650.
25. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.
26. M. Swart, *J. Chem. Theory Comput.*, 2008, **4**, 2057-2066.
27. F. Neese, *J. Chem. Phys.*, 2005, **122**, 34107.
28. R. J. Kurland and B. R. McGarvey, *J. Magn. Reson.*, 1970, **2**, 286-301.
29. P. Hrobarik, R. Reviakine, A. V. Arbuznikov, O. L. Malkina, V. G. Malkin, F. H. Kohler and M. Kaupp, *J. Chem. Phys.*, 2007, **126**, 024107.
30. T. O. Pennanen and J. Vaara, *Phys. Rev. Lett.*, 2008, **100**, 133002.
31. F. Neese, *J. Chem. Phys.*, 2007, **127**, 164112.
32. A. Kubica, J. Kowalewski, D. Kruk and M. Odelius, *J. Chem. Phys.*, 2013, **138**, 064304.

33. C. Duboc, D. Ganyushin, K. Sivalingam, M. N. Collomb and F. Neese, *J. Phys. Chem. A*, 2010, **114**, 10750-10758.
34. P. Mal, D. Schultz, K. Beyeh, K. Rissanen and J. R. Nitschke, *Angew. Chem. Int. Ed.*, 2008, **47**, 8297-8301.
35. in *Origin Lab 8.2*, OriginLab Corportation, Northhampton, MA.
36. M. M. Smulders, S. Zarra and J. R. Nitschke, *J. Am. Chem. Soc.*, 2013, **135**, 7039-7046.
37. in *CRC Handbook of Chemistry and Physics*, ed. W. M. Haynes, CRC Press, Boca Raton, FL, 2012.
38. National Center for Biotechnology Information, PubChem Compound Database; CID=9706, http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=9706, Accessed January 31, 2014.
39. National Center for Biotechnology Information, PubChem Compound Database; CID=10892, http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?cid=10892, Accessed January 31, 2014.