Supporting Information

Probing Substrate Binding inside a Paramagnetic Cavity: A NMR Spectroscopy Toolbox for Combined Experimental and Theoretical Investigation

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Instrumentation

UV-vis spectra were recorded on an Agilent Cary8454 UV-vis spectrometer. ^{1}H NMR spectra were recorded on a JEOL 500 MHz instrument. The spectra for paramagnetic molecules were recorded over a 100-kHz bandwidth with 64 K data points and a 5-ms 90° pulse. The residual ^{1}H resonances of the solvents were used as a secondary reference. Electron paramagnetic resonance (EPR) spectra were obtained by using a Bruker EMX EPR spectrometer.

X-ray Structure Solution and Refinement

Single-crystal X-ray data were collected at 100 K on a Bruker SMART APEX CCD diffractometer equipped with a CRYO Industries' low-temperature apparatus, and intensity data were collected using graphite monochromated MoKα radiation (λ = 0.71073 Å). The data integration and reduction were processed with SAINT software.[1] An absorption correction was applied.[2] The structure was solved by the direct method using SHELXS-97 and was refined on F2 by the full matrix least-squares technique using the SHELXL-2018 program package.[3] Non hydrogen atoms were refined anisotropically. In the refinement, hydrogens were treated as riding atoms using SHELXL default parameters.

Computational Details

All geometry optimizations were carried out using the package *Gaussian 09*, Revision B.01[3] using unrestricted density functional method B97D in gas-phase and with solvent correction.[4] The basis set was LANL2DZ including for Fe, Br and 6-31G** for C, H, N, F, O atoms. The self-consistent reaction field method was applied in all the optimizations to consider the solvent effect (chloroform). Frequency calculations were also carried out on all optimized structures to ensure that there were zero imaginary frequencies. Energies were taken from the Gaussian frequencies and contain zero point corrections at 298.15 K and 1 atm. All the TD-DFT calculations were performed at the ω-B97XD level.[5] Visualization of the molecular orbitals and the corresponding diagrams were done using the *Chemcraft* software.[6] The electrostatic potentials were mapped onto the van der Waals surface with a data range from −0.02 (red) to +0.02 (blue) calculated at the B97D level of theory by taking coordinates directly from the crystal structures of the respective complexes, and were plotted by using VMD software version 1.9.2.[7] DFT calculations to investigate the ^{19}F NMR spectra of *exo-exo* and *exo-endo* dimers were employed within the ADF program.[8,9] Spin-unrestricted density functional calculations were executed for all complexes in this study. The spin state adopted in the DFT calculations is assigned as $S = 10$ ($S_{Fe1} = +5/2$, $S_{Fe2} = +5/2$). Molecular geometries were attained by optimising the X-ray crystal structures, utilizing BP86_D3 in conjunction with TZ2P (triple-ζ plus double polarization function) basis set for all atoms.[10,11] The spin density, NMR parameters, and free energy calculations were conducted adopting ZORA-scalar-BP86/TZ2P (COSMO/CH_2Cl_2) level of theory. The calculation of hyperfine coupling A-tensors is implemented by the CPL code of the Amsterdam Density Functional program as a second derivative property. This involves incorporating spin-orbit coupling and nuclear magnetic field perturbations within the two-component relativistic zeroth-order regular approximation (ZORA). An all-electron basis set for the Fluorine nucleus is used to accurately evaluate the spin-polarization density at the nucleus.[12] The orbital (or diamagnetic) shift in Eq. (1) of the text is determined by calculating the disparity between the chemical shielding of a reference compound and the orbital-induced effect on the chemical shielding of the compound under investigation, $\delta_{orb} = \sigma_{ref} - \sigma_{orb}$. This shift can also be assessed using the diamagnetic analog. In our investigation, $CFCl_3$ (160 ppm) served as the reference compound, and the Zn porphyrin dimer was employed to calculate the orbital shift.[13]

Estimation of g_{xx}, g_{yy} *and* g_{zz}

In the context of high-spin iron, the $g_{//}$ value represents the actual g_{zz} value, showing a slight deviation from the expected g_e = 2.00232 of a free spin due to spin-orbital coupling. Meanwhile, the experimental g_{xx} and g_{yy} values serve as effective *g* values, influenced by the zero-field effect and potential spin-admixed contributions between sextet and quartet spin states. While simulations can estimate the g_{xx} and g_{yy} values, it's important to note that these effective *g* values, derived from the 77K EPR data, may not perfectly correspond to those obtained at room temperature in a solution (if detectable). Therefore, in addition to conducting several possible NMR dipolar shift hypotheses to speculate on the actual *g* values of the complexes in solution, our subsequent analysis will also use the EPR g_{zz} value as a guide to systematically explore the changes in g_{xx} and g_{yy} values to produce a more comprehensive understanding of the impact of dipolar transitions. Thus, it is evaluated through the data regarding the *ortho*-fluorine (*exo*-phenol) of **2b**. Herein, based on the EPR data (refer to the Supplementary Information) indicating g_{zz} = 1.99, the dipolar shift of *ortho*-F is determined by $\delta_{dip}^{MC} = \delta_{obs}(experiment) - \delta_{orb}(DFT) - \delta_{con}(DFT)$, and subsequently applied in Eq. (3) in the text, utilizing the experimental ^{19}F NMR chemical shift of −14.6 ppm, DFT-calculated averaged orbital and contact shift, −136 and 99.1 ppm to obtain $\delta_{dip}^{MC} = 21.9\ ppm$. When setting *S* = 10, g_{zz} = 1.99, and considering the geometric factors of *o*-F for *exo*-phenol in **2b**, Eq. (2) simplifies to:

$$21.9 = 3.4841 \times \left[\left(2 \times 1.99^2 - g_{xx}^2 - g_{yy}^2\right) \times \frac{(3\,cos^2\,\theta - 1)}{r^3} + \left(g_{xx}^2 - g_{yy}^2\right) \times 3 \times \frac{sin^2\theta cos2\phi}{r^3}\right]$$

Here, the averaged $\frac{(3\,cos^2\,\theta - 1)}{r^3}$ and $\frac{sin^2\theta cos2\phi}{r^3}$ terms are evaluated to be 8.37 and 4.34, respectively, as indicated in Table S3. Examining the plotted relationship between metal-centered dipolar shifts and g_{yy} values for various g_{xx} values ranging from 1.95 to 2.15 with a 0.05 interval reveals numerous possibilities for *g* factors, as shown in Figure S17. However, when specifying g_{xx} = 2.10 and g_{yy} = 1.94, the calculated isotropic g value, (g_{xx} + g_{yy} + g_{zz})/3, is 2.01 very close to the spin-only value of 2.0023 for high-spin (*S* = 5/2) Fe^{3+} complexes under weak crystal fields.[14]

Experimental Section:

Materials:

1,2-Bis[μ-oxo iron(III)-5-(2,3,7,8,12,13,17,18-octaethylporphyrinyl)]-pyrrole was prepared by using previously reported methods.[15] Reagents and solvents were purchased from commercial sources and were purified by using standard procedures before use.

Synthesis of 2a:

100 mg of **1** (0.075 mmol) was dissolved in dichloromethane (50 mL) and 2,4,6-trinitrophenol, HTNP (37.8 mg, 0.165 mmol) was added. The mixture was stirred for 10 min, and during the progress of the reaction, the green solution changed to brown. It was then evaporated to complete dryness. The solid thus obtained was dissolved in a minimum volume of dichloromethane and carefully layered with *n*-hexane. After 7-8 d, a dark-brown crystalline solid was formed that was then collected by filtration, washed well with the mother liquor, and dried under vacuum. Yield: 100 mg (75%). ^{1}H NMR ($CDCl_3$, 298 K): δ = −46.0, −49.3, −59.5, −63.3 (*meso-H*); 5.8, 6.2(4) 6.5(3) (C*H*$_3$); 1.4 (C*H*$_3$-py); 2.8 (C*H*$_2$-py); 28.6, 33.2, 37.2, 38.2, 38.8, 39.2, 39.6, 40.6, 44.5, 45.8, 46.5, 48.2, 49.6, 50.0, 50.4, 52.0 (C*H*$_2$); 67.3, 118.2 (C*H*$_2$(b)); 59.2, 69.1 (m_t-*H*) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 355 (1.2×10^5), 380 (1.3×10^5), 513 (1.4×10^4), 550 (1.0×10^3), 643 nm (5.5×10^3).

Same synthetic protocol that of **2a** has been followed for the synthesis of other phenolato species (**2b**-**2i**).

Synthesis of 2b:

Yield: 98 mg (78%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −38.8, −41.2, −46.0, −51.0 (*meso-H*); 4.2(2), 4.8, 5.4(3), 6.3(2) (C*H*$_3$); 1.4 (C*H*$_3$-py); 2.8 (C*H*$_2$-py); 31.0(2), 33.3(2), 36.3(3), 37.9(2), 42.9, 44.6(2), 46.3(2), 54.3(2) (C*H*$_2$); 84.8, 89.6 (C*H*$_2$(b)); ^{19}F NMR (C_6D_6, 298 K): δ = 29.7 (*p*-F_{exo}), −14.6 (*o*-F_{exo}), −210.2 (*m*-F_{exo}), −226.5 (*m*-F_{endo}), −218.3, 18.7 (*o*-F_{endo}) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 367 (1.2×10^5), 372 (1.1×10^5), 394 (9.3×10^3), 504 (1.3×10^4), 584 (1.0×10^4), 628 (7.3×10^3).

Synthesis of 2c:

Yield: 99 mg (83%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −37.3, −41.1, −46.7, −49.9 (*meso-H*); 3.5, 4.1, 4.8, 5.2(3), 5.8, 6.4 (C*H*$_3$); 1.6 (C*H*$_3$-py); 2.9 (C*H*$_2$-py); 31.2(2), 32.7(2), 34.4, 35.7(2), 37.3(2), 38.1, 41.8, 42.6, 44.2(2), 44.7, 46.5(C*H*$_2$); 77.5, 97.9 (C*H*$_2$(b)); 52.4, 62.3 (m_t-*H*) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 363 (1.3×10^5), 395 (1.1×10^5), 508 (1.9×10^4), 541 (1.2×10^4), 627 nm (8.0×10^3).

Synthesis of 2d:

Yield: 104 mg (85%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −36.9, −43.8, −49.2, −57.9 (*meso-H*); 4.9, 5.2, 5.5(3), 6.0(3) (C*H*$_3$); 1.4 (C*H*$_3$-py); 3.0 (C*H*$_2$-py); 27.7, 28.4, 30.9, 33.8, 36.1(2), 37.2(2), 40.8, 42.2(3), 43.8, 55.9(2), 57.4 (C*H*$_2$); 82.1, 95.1 (C*H*$_2$(b)); ^{19}F NMR ($CDCl_3$, 298 K): δ = −29.2 (*o-F*$_{exo}$); −171.7 (*o-F*$_{endo}$) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 349 (1.0×10^5), 390 (1.4×10^5), 572 (0.6×10^3), 599 (0.3×10^3).

Synthesis of 2e:

Yield: 107 mg (86%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −38.9, −43.7, −51.1, −56.9 (*meso-H*); 5.2(3), 5.4(3), 6.2(2) (C*H*$_3$); 1.3 (C*H*$_3$-py); 3.1 (C*H*$_2$-py); 26.9, 32.3(2), 34.2, 34.9(2), 36.5(2), 37.6(2), 41.8(3), 43.5, 56.9(2) (C*H*$_2$); 81.7, 98.3 (C*H*$_2$(b)); 54.1, 56.3 (m_t-*H*) ppm; ^{19}F NMR ($CDCl_3$, 298 K): δ = 55.2 (*p-F*$_{exo}$), −32.9 (*o-F*$_{exo}$); −170.1 (*o-F*$_{endo}$) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 369 (6.0×10^4), 397 (5.0×10^4), 510 (0.7×10^3), 544 (0.5×10^3), 630 (0.3×10^3).

Synthesis of 2f:

Yield: 93 mg (72%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −45.2(2) (*meso-H*); 4.6, 6.5, 7.1, 7.3 (C*H*$_3$); 1.4 (C*H*$_3$-py); 2.8 (C*H*$_2$-py); 24.1, 27.3, 30.2(2), 31.9, 32.9, 34.3, 37.4 (C*H*$_2$); 102.0 (C*H*$_2$(b)); −62.1 (*o-H*); 40.4 (m_t-*H*) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 350 (6.4×10^4), 402 (1.1×10^5), 492 (2.0×10^4), 534 (1.7×10^4), 610 (1.5×10^4).

Synthesis of 2g:

Yield: 104 mg (70%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −54.1, −59.1 (*meso-H*); 4.7, 4.9, 5.8, 6.0 (C*H*$_3$); 1.4 (C*H*$_3$-py); 2.8 (C*H*$_2$-py); 30.0, 34.9(2), 39.3, 40.9, 42.4, 46.4, 50.8 (C*H*$_2$); 74.2 (C*H*$_2$(b)); 70.4 (*m*$_t$-*H*) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 398 (1.3×10^5), 511 (2.2×10^4), 575 (1.4×10^4), 644 (7.5×10^3).

Synthesis of 2h:

Yield: 94 mg (79%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −47.0(2) (*meso-H*); 4.9, 5.8, 6.4(2) (C*H*$_3$); 1.4 (C*H*$_3$-py); 2.8 (C*H*$_2$-py); 28.2, 29.4, 32.4, 33.5, 37.1, 38.6, 40.6, 47.4 (C*H*$_2$); 54.2 ppm (C*H*$_2$(b)); −107.0 (*o*-*H*); 68.2, 78.9 (*m*$_t$-*H*); −2.9 (*o*-C*H*$_3$); −22.2 (*o*-C*H*$_2$); ^{19}F NMR ($CDCl_3$, 298 K): δ = 97.1 (*p*-*F*$_{exo}$) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 355 (6.7×10^4), 391 (1.1×10^5), 505 (1.2×10^3), 543 (0.9×10^3), 614 (0.7×10^3).

Synthesis of 2i:

Yield: 84 mg (72%); ^{1}H NMR ($CDCl_3$, 298 K): δ = −47.5(2) (*meso-H*); 6.3(2), 6.6(2) (C*H*$_3$); 1.4 (C*H*$_3$-py); 2.8 (C*H*$_2$-py); 27.7, 31.9, 34.4(2), 36.1, 39.2(2), 47.9 (C*H*$_2$); 81.8 (C*H*$_2$(b)); −89.0 (*o*-*H*), −26.4 (*p*-*H*), −30.2 (*m*$_t$-C*H*$_3$) ppm; UV-vis (chloroform) [λ_{max}, nm (ε, $M^{-1}\,cm^{-1}$)]: 336 (7.2×10^4), 389 (1.0×10^5), 565 (9.5×10^3).

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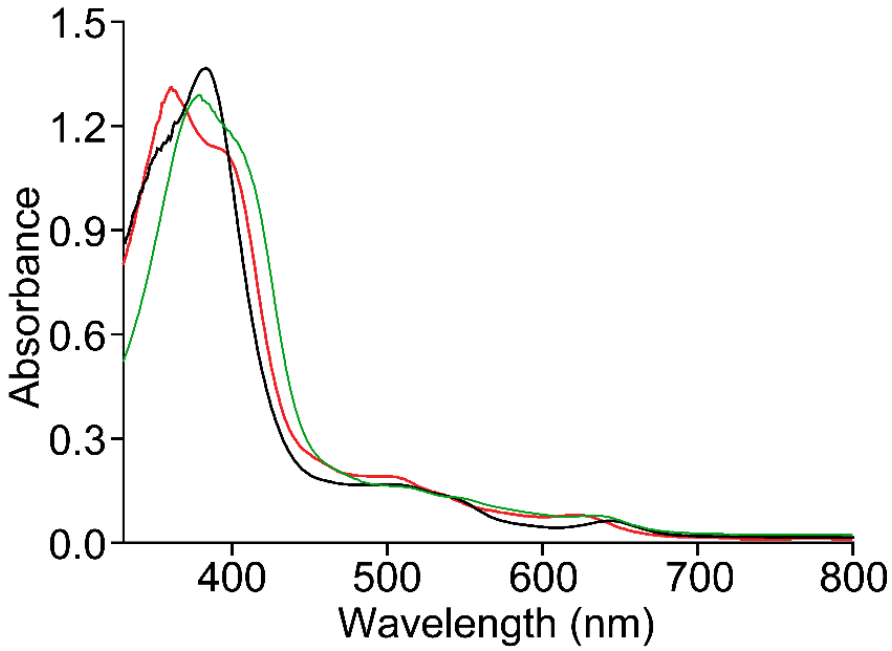


Figure S1. UV-vis spectra of **2a** (black trace), **2e** (green trace) and **2c** (red trace) in $CHCl_3$ at 298 K.

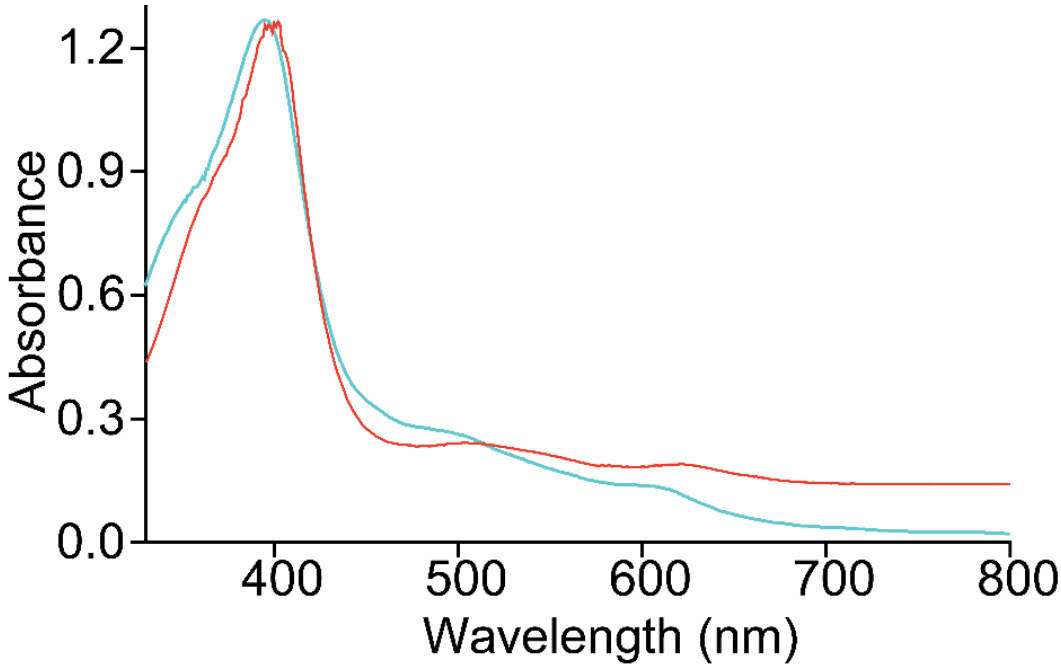


Figure S2. UV-vis spectra of **2i** (blue trace) and **2h** (red trace) in $CHCl_3$ at 298 K.

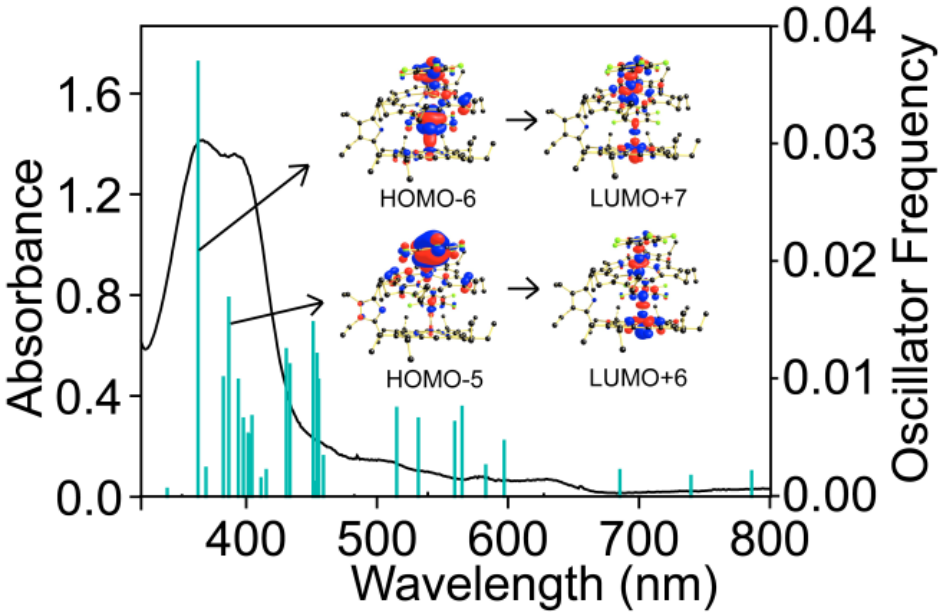


Figure S3. Absorption spectra (curved line, left axis) in CH_2Cl_2 and oscillator strengths (vertical line, right axis) of **2b** obtained from TD-DFT calculations at the ω-B97XD/6-31G**/LANL2DZ level of theory.

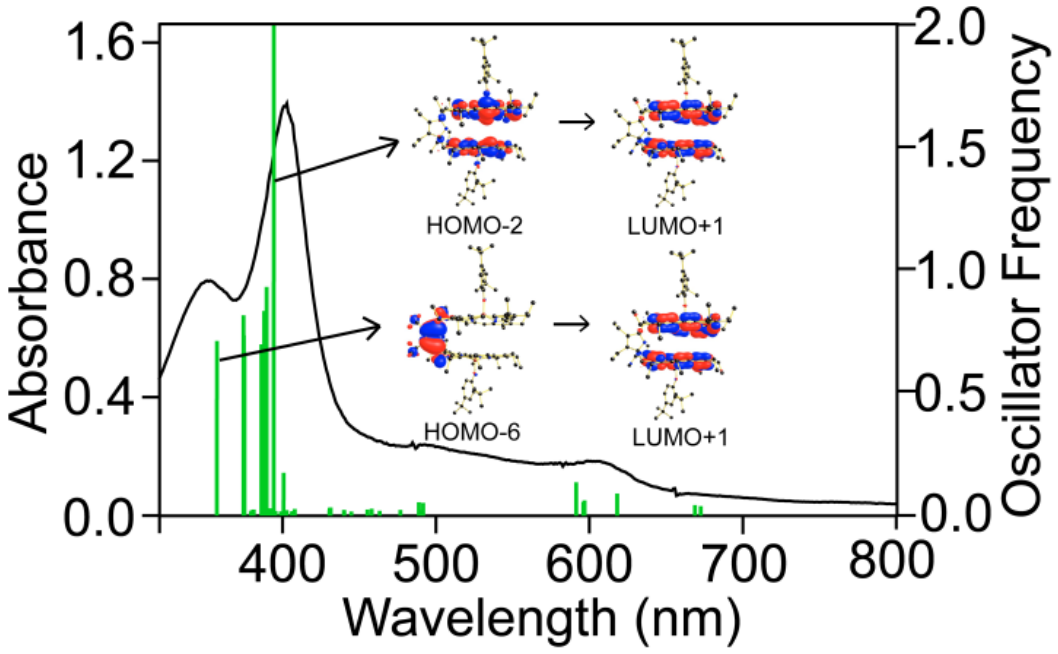


Figure S4. Absorption spectra (curved line, left axis) in CH_2Cl_2 and oscillator strengths (vertical line, right axis) of **2f** obtained from TD-DFT calculations at the ω-B97XD/6-31G**/LANL2DZ level of theory.

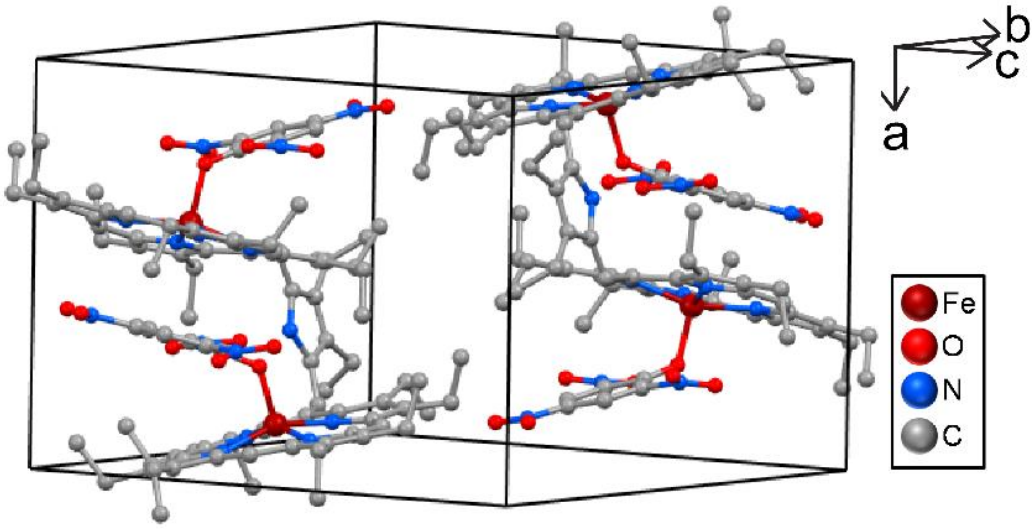


Figure S5. Diagram illustrating the packing of **2a** in the unit cell (H-atoms have been omitted for clarity).

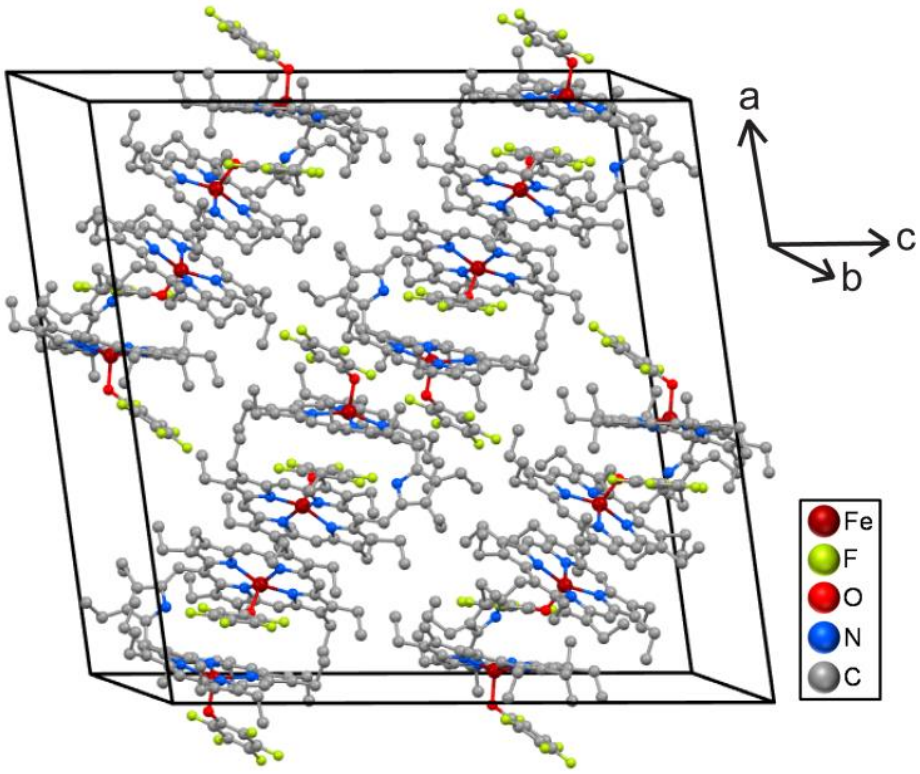


Figure S6. Diagram illustrating the packing of **2b** in the unit cell (H-atoms have been omitted for clarity).

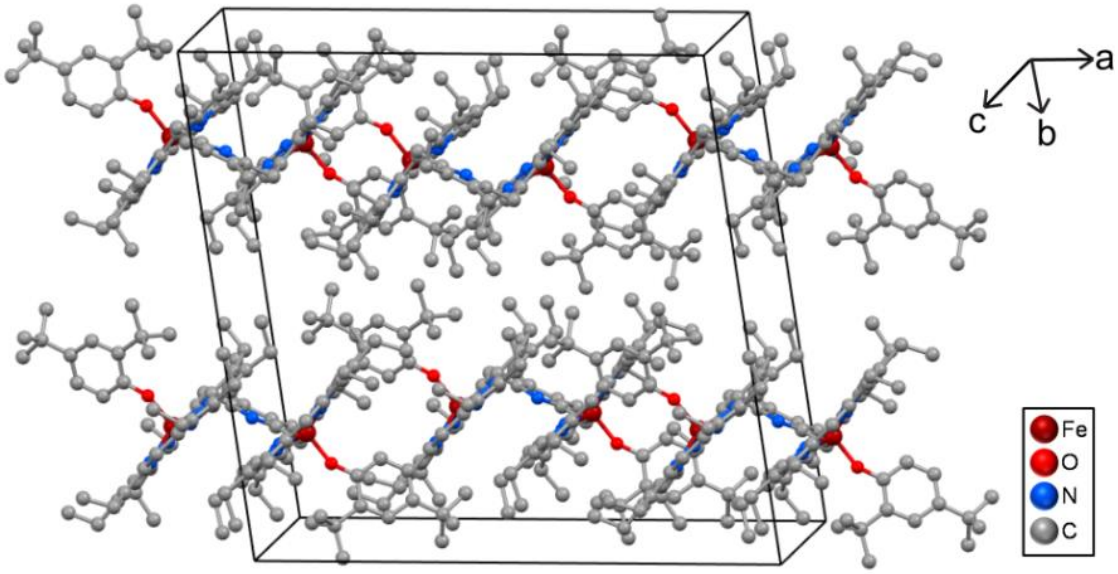


Figure S7. Diagram illustrating the packing of **2f** in the unit cell (H-atoms have been omitted for clarity).

Table S1. Selected bond distances (Å) and angles (°).

Bond distances	**2a**	**2b**	**2f**
Fe1–N1	2.047(3)	2.057(5)	2.0577(13)
Fe1–N2	2.062(3)	2.057(6)	2.0812(14)
Fe1–N3	2.071(3)	2.082(6)	2.0733(13)
Fe1–N4	2.061(3)	2.053(6)	2.0724(14)
Fe2–N5	2.060(3)	2.049(4)	-
Fe2–N6	2.057(4)	2.055(4)	-
Fe2–N7	2.047(3)	2.059(4)	-
Fe2–N8	2.053(3)	2.060(4)	-
Fe1–O1	1.918(3)	1.874(4)	1.8180(11)
Fe2–O2	1.911(3)	1.914(4)	-
Bond angles			
N1–Fe1–N2	88.96(12)	89.2(2)	89.48(5)
N1–Fe1–N3	157.69(13)	157.5(2)	155.81(5)
N1–Fe1–N4	85.91(13)	86.8(2)	85.83(5)
N2–Fe1–N3	86.31(13)	86.5(3)	85.29(5)
N2–Fe1–N4	154.46(13)	158.0(2)	155.50(5)
N3–Fe1–N4	89.01(14)	88.9(3)	89.20(5)
N5–Fe2–N6	89.74(13)	88.68(17)	-
N5–Fe2–N7	160.19(13)	154.4(2)	-
N5–Fe2–N8	84.99(13)	86.47(17)	-
N6–Fe2–N7	85.91(14)	86.66(17)	-
N6–Fe2–N8	153.10(13)	158.3(2)	-
N7–Fe2–N8	90.19(14)	88.60(17)	-

Table S2. Selected structural parameters of **2a**, **2b** and **2f** obtained from DFT calculations.

Complex		$Fe–N_p$[a]	Fe–O[b](L)	Fe–O–C[c]	Δ_{24}^{Fe}[d]	Δ_{24}[e]	τ[f]	Fe⋯Fe[g]
2a	Core I	2.089[2.060(3)]	1.957[1.918(3)]	137.3[128.5(2)]	0.43[0.46]	0.04[0.08]	7.52[7.74]	6.78
	Core II	2.083[2.054(3)]	1.963[1.911(3)]	135.5[126.7(3)]	0.43[0.42]	0.13[0.12]	1.10[0.90]	
2b	Core I	2.094[2.062(6)]	1.901[1.874(4)]	122.8[126.6(4)]	0.37[0.39]	0.04[0.02]	1.17[1.56]	6.33
	Core II	2.089[2.055(4)]	1.940[1.914(4)]	119.1[121.9(4)]	0.48[0.47]	0.11[0.16]	0.08[0.10]	
2f		2.088[2.071(13)]	1.895[1.818(11)]	146.8[151.55(11)]	0.51[0.47]	0.14[0.12]	0.06[0.04]	6.21

[a]Average value in Å. [b]Distance (in Å) of axial ligand L. [c]Angle (in °). [d]Displacement (in Å) of iron from the least-squares plane of $C_{20}N_4$ porphyrinato core. [e]Average displacement (in Å) of atoms from the least-squares plane of $C_{20}N_4$ porphyrinato core. [f]tilt-angle (in °). [g]Non-bonding distance (in Å) between two iron(III) centers in a molecule. Parentheses contain the experimental distances from the X-ray structure of the corresponding complexes.

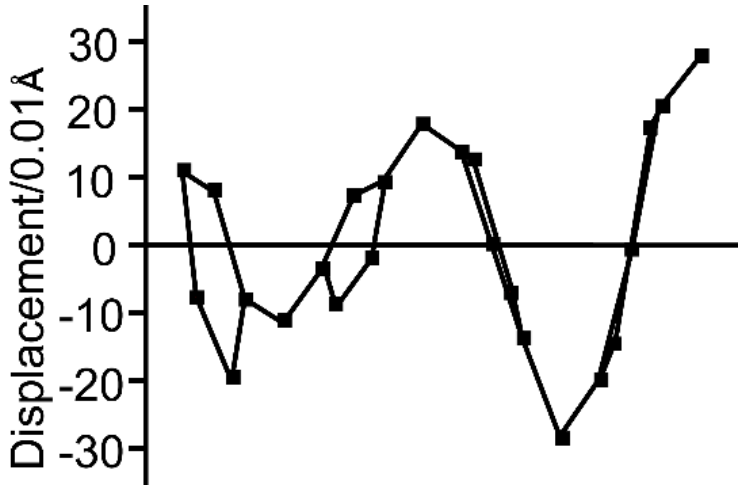


Figure S8. Atom deviations (in units of 0.01 Å) from the least-squares plane of the $C_{20}N_4$ porphyrinato core in **2f**. The horizontal axis represents the atom number in the macrocycle showing the bond connectivity between atoms.

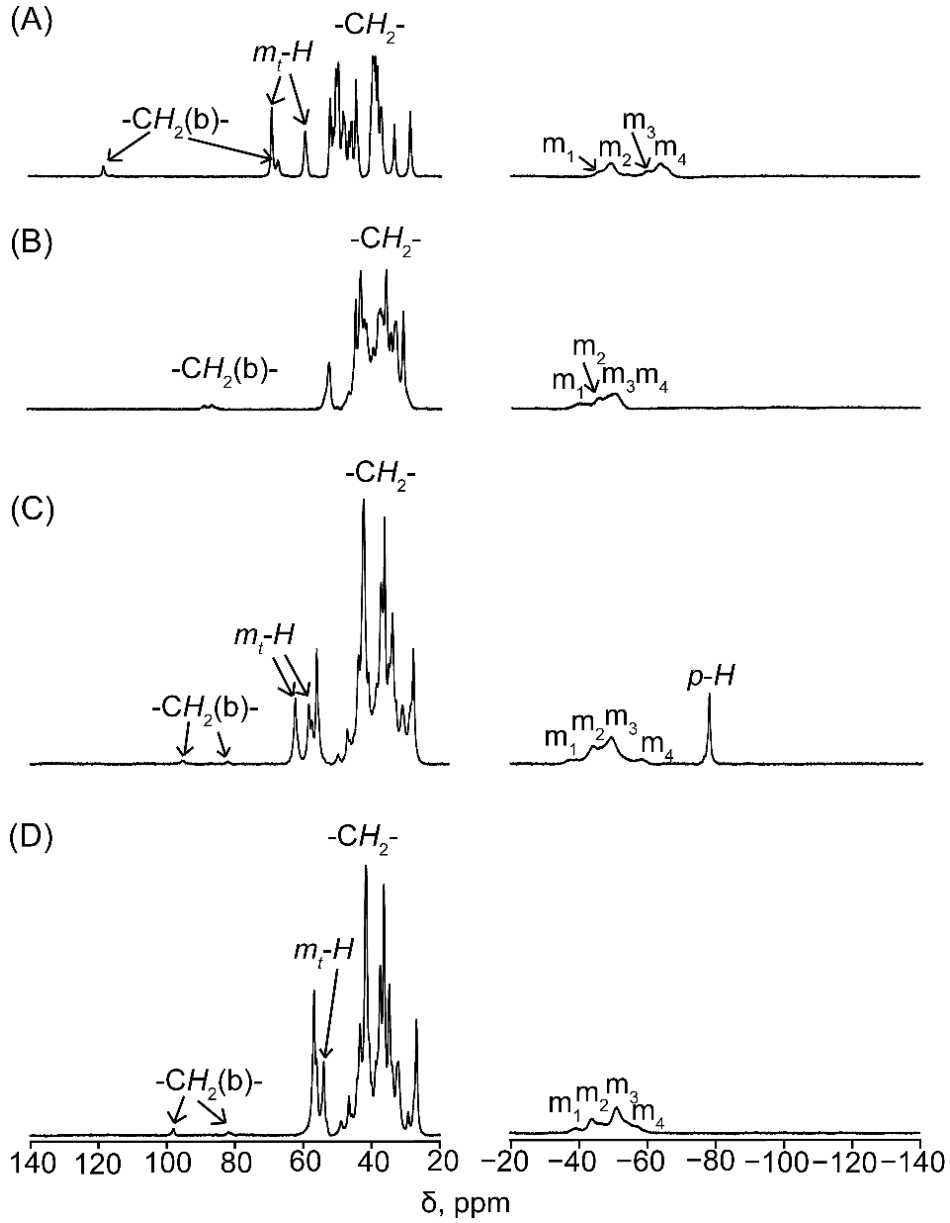


Figure S9. ^{1}H NMR spectra (in $CDCl_3$, at 298 K) of (A) **2a**, (B) **2b**, (C) **2d** and, (D) **2e**.

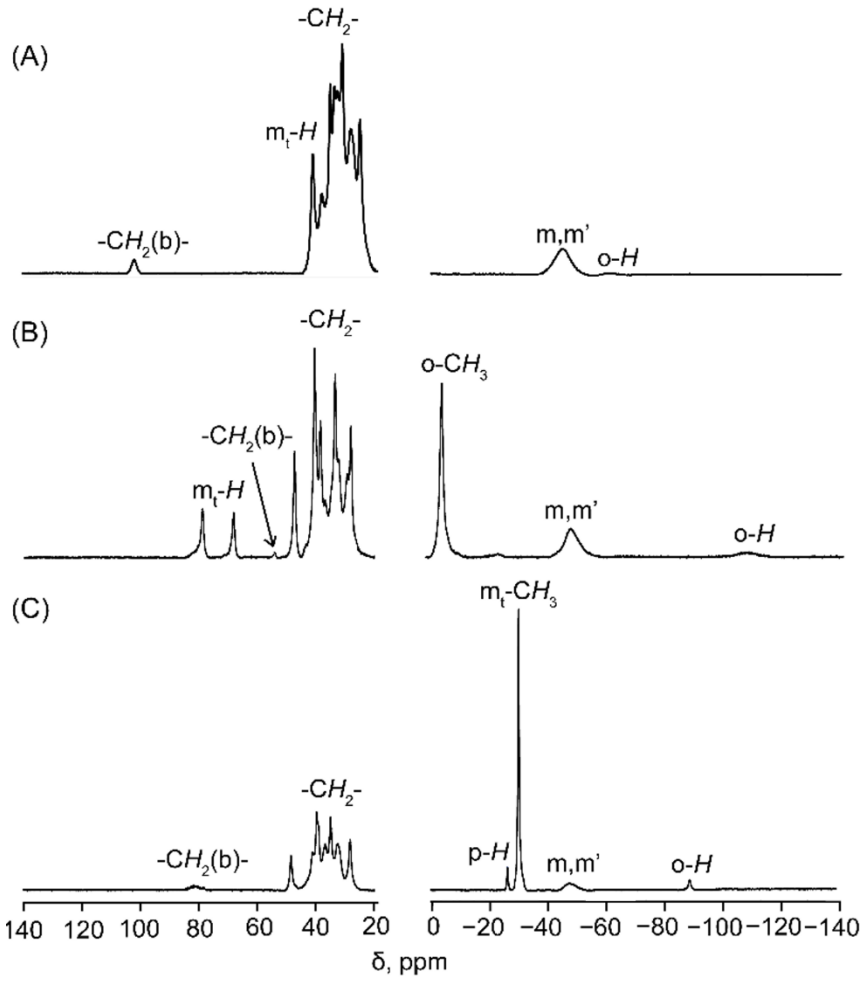


Figure S10. ^{1}H NMR spectra (in $CDCl_3$, at 298 K) of (A) **2f**, (B) **2h**, and (C) **2i**.

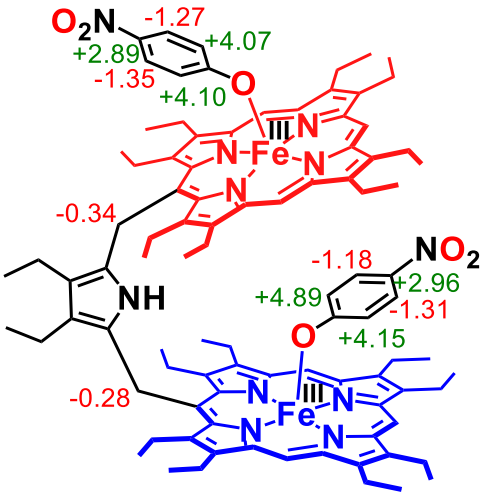


Figure S11. Calculated Mulliken spin densities ($\times 10^{-2}$) for **2c** at the B97D/6-31G**/LANL2DZ level of theory.

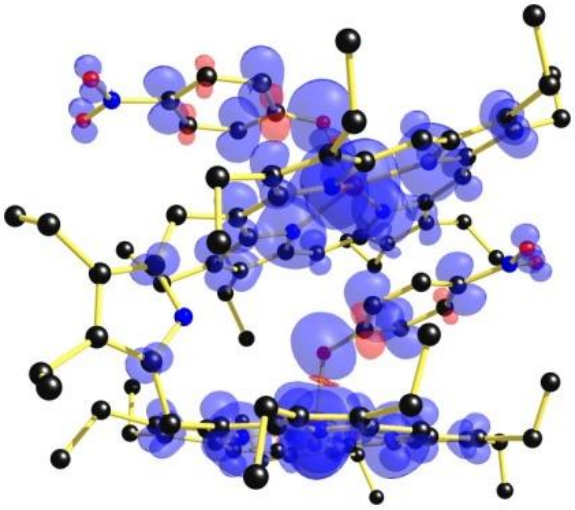


Figure S12. Mulliken spin density plot of **2c** at the B97D/6-31G**/LANL2DZ level of theory (iso-value: 0.001).

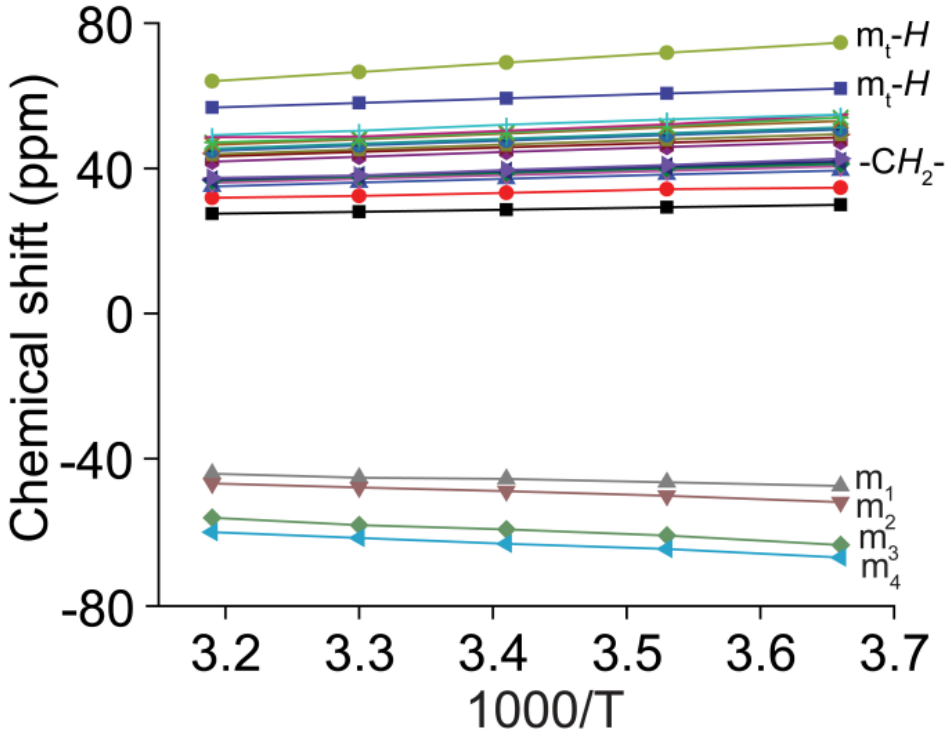
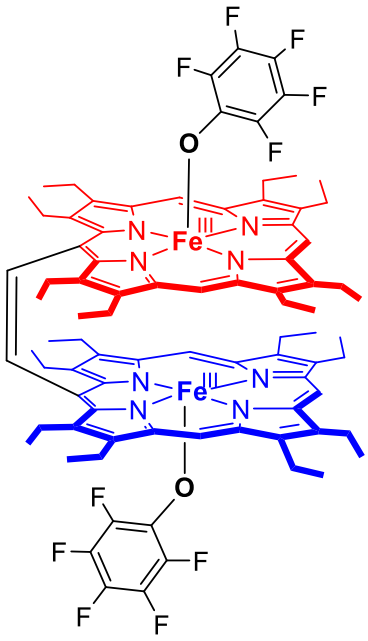


Figure S13. Curie plot (chemical shift *vs*. 1/T) of some proton signals of **2a**.



Scheme S1: Pentafluorophenolato analogue of *cis*-ethene bridged diiron(III) porphyrin dimer.

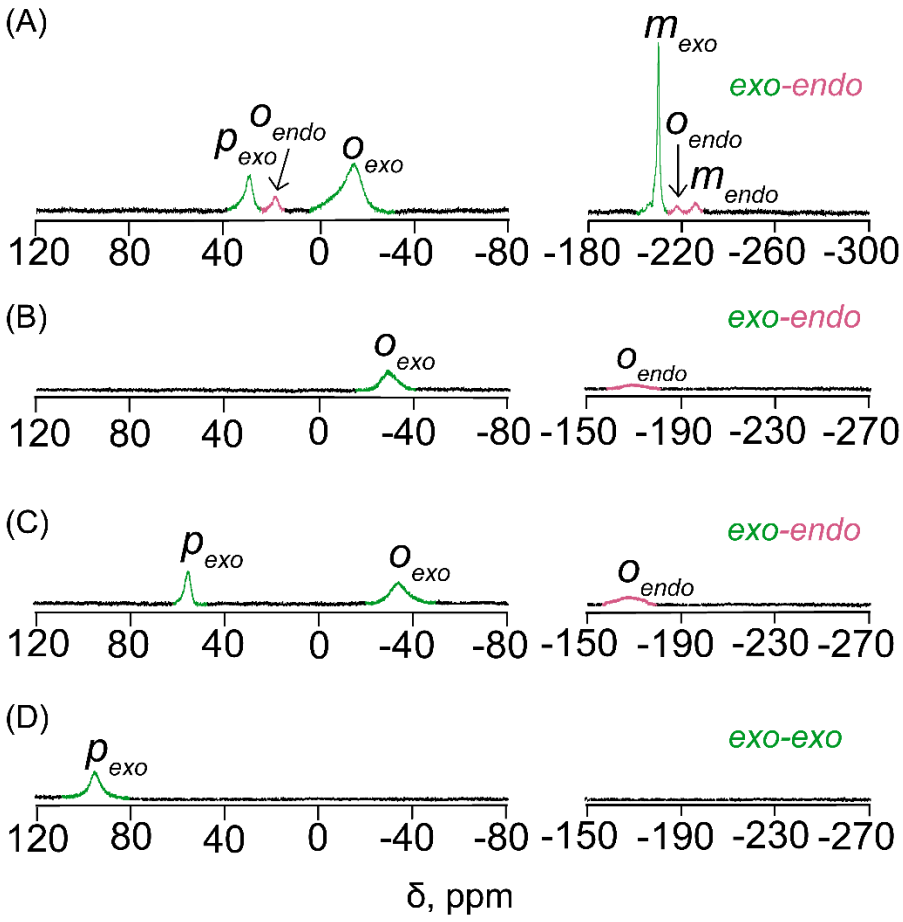


Figure S14. ^{19}F NMR spectra (at 298 K) of (A) **2b** in C_6D_6 and (B) **2d**, (C) **2e** and (D) **2h** in $CDCl_3$.

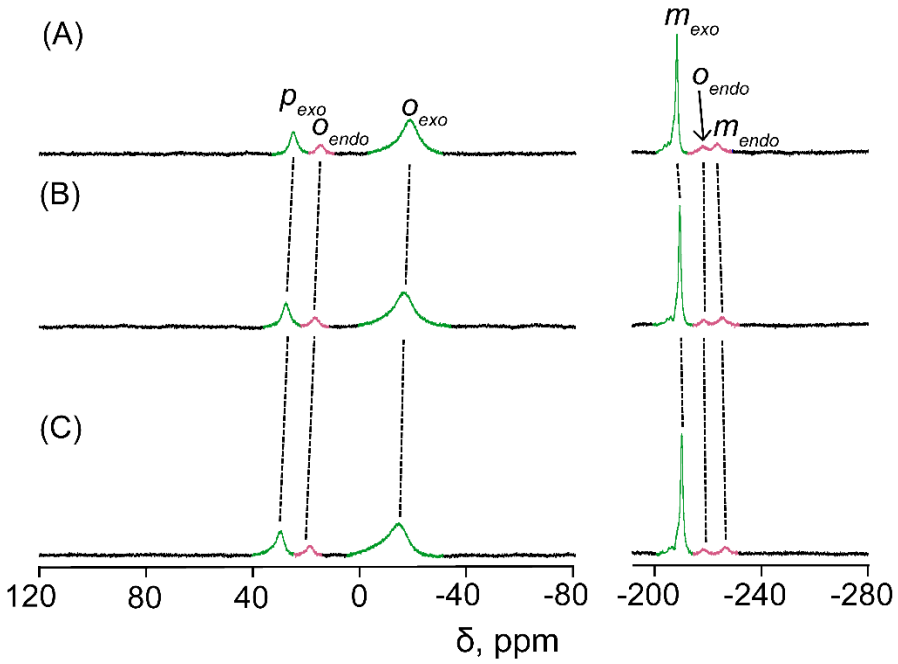


Figure S15. Variable temperature ^{19}F NMR spectra of **2b** (in C_6D_6) at (A) 323 K, (B) 313 K and (C) 298 K.

Table S3. Comparisons of Fe-F Bond Lengths, Fe-O-F Angles, and factors for *exo-endo* dimer (**2b**)

Exo-endo	*o*-F (F_1, F_5)	*m*-F (F_2, F_4)	*p*-F(F_3)
exo-fluorophenol			
r (Fe_{exo}-F), Å	3.80, 3.85	5.85, 5.88	6.66
θ(O-Fe_{exo}-F),[a] deg	46.4, 44.8	48.7, 47.4	47.2
ϕ, deg	171.6, 63.4	159.3, 93.3	126.4
G_{axial}(Fe_{exo}), 10^{21}cm^{-3}	7.77, 8.97 (8.37)[b]	1.53, 1.84 (1.69)[b]	1.30
$G_{rhombic}$(Fe_{exo}), 10^{21}cm^{-3}	7.36, 1.32 (4.34)[c]	2.11, -2.64 (−0.27)[c]	-0.54
r (Fe_{endo}-F), Å	8.0, 8.2	8.9, 9.1	9.4
θ(O-Fe_{endo}-F),[a] deg	29.5, 22.0	42.5, 37.5	44.9
ϕ, deg	87.6,171.6	108.2 ,156.2	132.7
G_{axial}(Fe_{endo}), 10^{21}cm^{-3}	2.50, 2.91 (2.71)	0.89, 1.20 (1.05)	0.61
$G_{rhombic}$(Fe_{endo}), 10^{21}cm^{-3}	−0.47, 0.24 (−0.12)	-0.52, 0.33 (−0.10)	−0.05
G_{axial}(Fe_{endo} + Fe_{exo})	11.44	2.74	1.25
G_{axial}(Fe_{endo} + Fe_{exo})	1.91	−0.37	−0.59

endo-fluorophenol			
r (Fe_{endo}-F), Å	3.75, 3.79	5.89, 5.90	6.66
θ(O-Fe_{endo}-F),[a] deg	45.4, 44.7	46.5, 45.9	44.7
ϕ, deg	29.8, 97.2	0.4, 33.4	67.5
G_{axial}(Fe_{endo}), $10^{21}cm^{-3}$	9.08, 9.47	2.06, 2.20	1.75
$G_{rhombic}$(Fe_{endo}), $10^{21}cm^{-3}$	4.86, -8.80	2.57, 0.99	−1.18
r (Fe_{exo}-F), Å	4.5, 4.0	4.96, 4.46	4.95
θ(O-Fe_{exo}-F),[a] deg	137.6, 148.0	136.9, 144.8	140.1
ϕ,deg	88.4, 46.6	128.7, 23.6	79.5
G_{axial}(Fe_{exo}), $10^{21}cm^{-3}$	18.09, 6.98	4.91, 11.31	6.31
$G_{rhombic}$(Fe_{exo}), $10^{21}cm^{-3}$	−0.24, −4.98	−0.83, 2.54	−3.17
G_{axial}(Fe_{endo} + Fe_{exo})	(27.17, 16.45)	(6.97, 13.51)	8.06
$G_{rhombic}$(Fe_{endo} + Fe_{exo})	(4.62, −13.78)	(9.54, 14.5)	−4.35

[a]Fe-O vector is treated as the z-axis. [b]averaged G_{axial} value and [c]averaged $G_{rhombic}$ value due to assumption of alloweable free rotation.

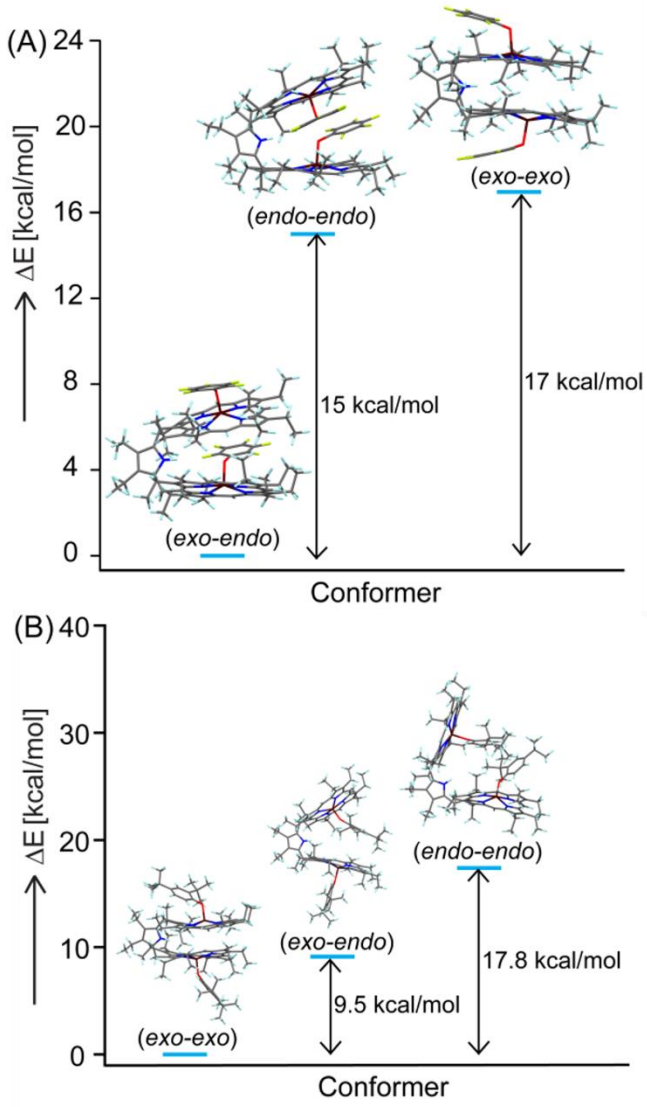


Figure S16. Relative energies of (A) **2b** and (B) **2f** as calculated using unrestricted B97D functional using LANL2DZ basis set for Fe and 6-31G** for all other atoms in chloroform.

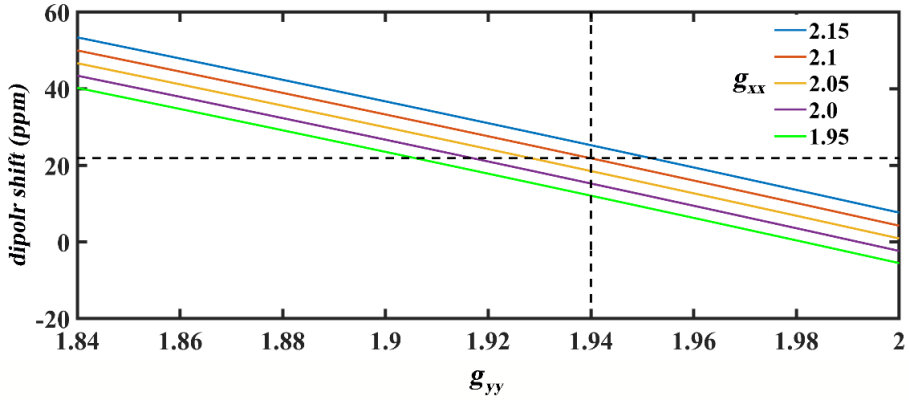


Figure S17. Correlation between metal-centered dipolar shifts and g_{yy} values across a range of g_{xx} values, varying from 1.95 to 2.15 with a 0.05 interval.

2b (*exo-endo*):

26	0.471216000	1.381764000	-2.811090000	6	2.421901000	-2.308801000	-3.874171000	1	-3.117787000	-4.387531000	-5.010821000
26	-1.310026000	-1.146198000	2.242212000	6	3.480487000	-1.749702000	-3.186560000	1	-3.637190000	-3.084484000	-3.906067000
8	-0.235602000	0.603870000	-1.214683000	6	3.085211000	-0.362614000	-2.873551000	1	-1.924691000	-3.531384000	-3.998127000
8	-1.567638000	-0.817572000	4.141657000	6	3.847767000	0.618704000	-2.185106000	6	2.304594000	-3.713399000	-4.402260000
9	-2.961915000	0.400260000	-1.652525000	6	5.474115000	2.899741000	-0.299606000	1	3.307708000	-4.134358000	-4.556235000
9	-4.180431000	-2.050383000	-1.694494000	1	5.384952000	3.490393000	0.624433000	1	1.821200000	-3.694376000	-5.392260000
9	-2.703719000	-4.323918000	-1.288356000	1	5.767088000	1.898959000	0.033712000	6	1.497805000	-4.632298000	-3.456798000
9	-0.006650000	-4.144405000	-0.797736000	6	6.589499000	3.542624000	-1.157618000	1	1.448653000	-5.656877000	-3.855565000
9	1.226058000	-1.704951000	-0.765946000	1	7.550990000	3.514919000	-0.623708000	1	0.473599000	-4.257268000	-3.330586000
9	-3.735198000	0.931228000	4.199143000	1	6.343207000	4.590938000	-1.377673000	1	1.959717000	-4.661561000	-2.461388000
9	-3.430516000	3.488337000	5.096752000	1	6.715131000	3.024778000	-2.120822000	6	4.716153000	-2.572579000	-2.882885000
9	-0.969753000	4.366220000	5.966128000	6	3.594409000	5.371050000	-0.315817000	1	5.182647000	-2.292388000	-1.933248000
9	1.162650000	2.648525000	5.993062000	1	2.718427000	5.725559000	0.249000000	1	4.387628000	-3.612672000	-2.741638000
9	0.882421000	0.082587000	5.080297000	1	4.420589000	5.295086000	0.405192000	6	5.749720000	-2.552764000	-4.035066000
7	2.141813000	2.414366000	-2.106160000	6	3.952721000	6.423647000	-1.393631000	1	6.624487000	-3.170291000	-3.780387000
7	-0.572824000	3.195957000	-2.981473000	1	4.163452000	7.398438000	-0.928566000	1	6.100511000	-1.533058000	-4.255430000
7	-0.932414000	0.615312000	-4.169568000	1	3.121872000	6.546871000	-2.103462000	1	5.299147000	-2.949170000	-4.957313000
7	1.796815000	-0.145063000	-3.348108000	1	4.838101000	6.110132000	-1.965337000	6	5.270137000	0.238989000	-1.806704000
7	0.162122000	-2.629626000	2.183562000	6	-1.264842000	6.715592000	-1.838884000	1	5.698293000	-0.415435000	-2.569798000
7	-2.747964000	-2.609498000	1.829241000	1	-2.003327000	7.358897000	-2.340788000	1	5.907313000	1.126436000	-1.847111000
7	-2.671734000	0.231424000	1.464684000	1	-0.277295000	7.177240000	-2.002107000	6	5.360470000	-0.412935000	-0.452217000
7	0.239191000	0.209426000	1.881553000	6	-1.562802000	6.681613000	-0.319716000	6	6.460210000	-0.951168000	0.211448000
7	4.273103000	-0.526779000	0.387168000	1	-1.491471000	7.689401000	0.116500000	6	6.009592000	-1.387883000	1.501680000
1	3.328812000	-0.238133000	0.159056000	1	-0.850191000	6.025165000	0.201617000	6	4.644946000	-1.112438000	1.579617000
6	3.390357000	1.902313000	-1.773475000	1	-2.573473000	6.292703000	-0.134332000	6	7.868547000	-0.964217000	-0.324157000
6	4.121421000	2.911484000	-0.980432000	6	-3.640209000	5.302628000	-3.563689000	1	8.466294000	-1.709316000	0.220996000
6	3.300561000	4.023229000	-0.916013000	1	-3.885051000	4.993981000	-4.592733000	1	7.863804000	-1.276840000	-1.382607000
6	2.080299000	3.696602000	-1.607813000	1	-3.589168000	6.402177000	-3.565925000	6	8.555635000	0.416888000	-0.212279000
6	1.003200000	4.586238000	-1.721924000	6	-4.772314000	4.845921000	-2.613129000	1	9.588152000	0.382313000	-0.594413000
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6	-0.220543000	4.368000000	-2.352033000	1	-4.588691000	5.214202000	-1.594915000	1	8.001696000	1.172416000	-0.787180000
6	-1.290644000	5.346312000	-2.456333000	1	-4.819665000	3.748089000	-2.568149000	6	6.854644000	-2.039367000	2.566252000
6	-2.300206000	4.742179000	-3.178261000	6	-4.446410000	0.311307000	-5.477903000	1	6.303035000	-2.048007000	3.519697000
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6	-3.000832000	0.129466000	-5.116227000	1	-5.066239000	0.972308000	-3.490527000	1	6.409772000	-4.137856000	2.100754000
6	-2.235982000	-1.016778000	-5.198581000	1	-5.234780000	-0.767539000	-3.743713000	6	1.539893000	-2.475460000	2.161362000
6	-0.947559000	-0.688390000	-4.616819000	6	-2.625792000	-2.372063000	-5.718925000	6	2.168780000	-3.800335000	2.056240000
6	0.132231000	-1.562107000	-4.523714000	1	-1.842525000	-2.744260000	-6.400280000	6	1.144690000	-4.726731000	2.132427000
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6	1.384891000	-1.314002000	-3.949783000	6	-2.842082000	-3.409034000	-4.589729000	6	-1.349839000	-4.592063000	2.173887000

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6	-3.842632000	-4.660348000	1.798705000	6	-4.027015000	-6.151141000	1.831223000	1	2.390409000	4.098696000	1.799957000
6	-4.780328000	-3.689723000	1.509617000	1	-5.080256000	-6.383660000	2.049211000	6	0.688561000	4.498782000	3.080838000
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6	-4.021443000	0.049973000	1.246161000	1	-2.567428000	-6.598431000	0.259874000	6	3.630727000	1.814717000	2.589981000
6	-4.659521000	1.317390000	0.946237000	1	-4.233218000	-6.442831000	-0.328445000	1	3.847884000	2.740381000	2.039922000
6	-3.666456000	2.272250000	0.969249000	6	-6.246257000	-3.862703000	1.231430000	1	4.405722000	1.112828000	2.275283000
6	-2.437214000	1.575209000	1.290442000	1	-6.530971000	-3.236161000	0.370257000	6	3.751445000	2.104908000	4.104781000
6	-1.191631000	2.178980000	1.419105000	1	-6.442077000	-4.906243000	0.942921000	1	4.791188000	2.350684000	4.370072000
1	-1.156270000	3.253240000	1.258815000	6	-7.122686000	-3.489855000	2.451583000	1	3.427648000	1.241367000	4.703296000
6	0.023883000	1.559020000	1.719903000	1	-8.191699000	-3.609386000	2.218418000	1	3.106737000	2.948038000	4.383977000
6	1.244957000	2.293128000	1.921708000	1	-6.943891000	-2.446953000	2.751590000	6	3.670785000	-1.262222000	2.720235000
6	2.234566000	1.371582000	2.214669000	1	-6.876700000	-4.133499000	3.309175000	1	3.832777000	-0.472115000	3.465499000
6	1.590487000	0.044535000	2.164600000	6	-6.102938000	1.485264000	0.570255000	1	3.874015000	-2.186359000	3.269961000
6	2.200230000	-1.226180000	2.315905000	1	-6.427041000	2.514507000	0.786161000	6	-0.832228000	-0.574871000	-1.195109000
6	3.564872000	-4.181746000	1.627350000	1	-6.731158000	0.819445000	1.182952000	6	-2.224792000	-0.707056000	-1.433291000
1	3.724043000	-5.244795000	1.861640000	6	-6.324605000	1.173293000	-0.929177000	6	-2.850454000	-1.951804000	-1.454309000
1	4.354173000	-3.632217000	2.144547000	1	-7.392817000	1.214096000	-1.191726000	6	-2.101562000	-3.117088000	-1.246778000
6	3.750267000	-3.973627000	0.105232000	1	-5.931617000	0.178211000	-1.177355000	6	-0.727729000	-3.021434000	-0.999919000
1	4.771398000	-4.248890000	-0.196388000	1	-5.784880000	1.905021000	-1.546602000	6	-0.105453000	-1.770497000	-0.976401000
1	3.581856000	-2.926901000	-0.169736000	6	-3.787051000	3.750278000	0.742250000	6	-1.436014000	0.417118000	4.606118000
1	3.033779000	-4.590679000	-0.455321000	1	-4.761351000	3.963406000	0.280163000	6	-2.521388000	1.331471000	4.630912000
6	1.234210000	-6.227057000	2.053068000	1	-3.020232000	4.076578000	0.021756000	6	-2.376123000	2.642871000	5.096873000
1	0.486455000	-6.670771000	2.729837000	6	-3.651689000	4.566286000	2.048975000	6	-1.130173000	3.090261000	5.555099000
1	2.215652000	-6.559668000	2.421696000	1	-3.773804000	5.641864000	1.850422000	6	-0.040199000	2.208831000	5.557800000
6	1.010288000	-6.779124000	0.624974000	1	-2.667159000	4.411254000	2.511523000	6	-0.190381000	0.903853000	5.083190000
1	1.068877000	-7.878215000	0.622422000	1	-4.409541000	4.252452000	2.779323000				

2b (*exo-exo*):

26	3.443314000	0.836621000	0.636224000	6	1.182916000	-1.019701000	1.700447000	6	1.824950000	4.780165000	1.549443000
26	-3.159941000	1.430418000	-0.882191000	6	4.674201000	-0.835372000	2.547026000	6	3.045175000	5.165670000	1.029223000
8	4.580217000	0.435601000	2.176978000	6	0.011416000	-0.951217000	2.595322000	6	3.699365000	3.950751000	0.573763000
7	1.578826000	0.270858000	1.377416000	6	5.584479000	-1.727372000	1.920916000	6	4.876825000	3.907124000	-0.178852000
7	2.924656000	2.848778000	0.868048000	6	-0.230648000	0.391798000	2.810071000	1	5.403539000	4.847200000	-0.333088000
7	4.791013000	1.530294000	-0.807573000	6	5.584020000	-3.098243000	2.189700000	6	5.358287000	2.786253000	-0.863504000
7	3.463902000	-1.046142000	-0.265133000	6	0.729716000	1.132952000	2.036378000	6	6.463712000	2.800367000	-1.806996000
7	-3.859678000	-0.260462000	0.128743000	6	4.691241000	-3.626656000	3.133385000	6	6.539123000	1.529984000	-2.341375000
7	-4.121596000	2.647904000	0.540129000	6	0.784892000	2.531584000	2.018426000	6	5.497196000	0.750420000	-1.696189000
7	-1.857186000	3.056306000	-1.150604000	1	-0.017840000	3.051117000	2.535485000	6	5.270096000	-0.606813000	-1.906686000
7	-1.696807000	0.164425000	-1.681842000	6	3.824365000	-2.765912000	3.816922000	1	5.909247000	-1.093377000	-2.640185000
7	-0.490354000	-3.385748000	0.146270000	6	3.814416000	-1.397341000	3.526510000	6	4.362903000	-1.433293000	-1.234452000
1	-0.377838000	-2.389153000	0.006532000	6	1.785157000	3.332013000	1.471647000	6	4.296408000	-2.854549000	-1.430879000

6	3.376645000	-3.359114000	-0.525946000	1	9.229803000	0.923268000	-1.934381000	1	0.484136000	2.126348000	-3.419483000
6	2.836957000	-2.197298000	0.197020000	6	5.163387000	-3.625798000	-2.387804000	6	-0.724488000	0.622759000	-2.543566000
6	1.843497000	-2.180973000	1.213464000	1	5.277808000	-3.057653000	-3.324347000	6	-0.118075000	-0.475569000	-3.245516000
6	-0.867482000	-2.004747000	3.238893000	1	4.673844000	-4.572436000	-2.655240000	6	-0.705776000	-1.635286000	-2.781663000
1	-1.891926000	-1.602150000	3.266808000	6	6.558780000	-3.916880000	-1.784321000	6	-1.735465000	-1.217177000	-1.809732000
1	-0.934273000	-2.918811000	2.642373000	1	7.200726000	-4.434479000	-2.513159000	6	-2.643059000	-2.043694000	-1.094262000
6	-0.435488000	-2.336139000	4.687990000	1	6.462554000	-4.542693000	-0.887606000	6	-4.542506000	-3.924566000	0.965136000
1	-1.071545000	-3.130448000	5.107744000	1	7.048537000	-2.980500000	-1.480483000	1	-3.585486000	-4.438683000	0.828964000
1	-0.524129000	-1.444960000	5.326768000	6	3.072329000	-4.844490000	-0.515423000	1	-4.805002000	-4.075066000	2.023593000
1	0.611225000	-2.662872000	4.733089000	1	2.698653000	-5.214304000	0.440665000	6	-5.656005000	-4.574464000	0.106410000
6	-1.256758000	1.015945000	3.716046000	1	4.023685000	-5.370629000	-0.690373000	1	-5.762706000	-5.641024000	0.355916000
1	-1.640683000	0.257948000	4.412236000	6	2.068015000	-5.249362000	-1.618787000	1	-5.454707000	-4.491761000	-0.970250000
1	-0.763009000	1.785393000	4.332475000	1	1.947568000	-6.343108000	-1.639068000	1	-6.617062000	-4.071041000	0.287199000
6	-2.429435000	1.640678000	2.939651000	1	2.417574000	-4.915196000	-2.606973000	6	-6.254259000	-1.904497000	2.503536000
1	-3.179344000	2.068645000	3.620680000	1	1.087799000	-4.803802000	-1.423882000	1	-6.626478000	-2.927220000	2.351877000
1	-2.915704000	0.880172000	2.320777000	6	1.397836000	-3.518688000	1.785267000	1	-7.129216000	-1.240941000	2.423436000
1	-2.087494000	2.433601000	2.262930000	1	2.254518000	-4.196489000	1.853088000	6	-5.635639000	-1.780356000	3.917160000
6	0.740854000	5.641046000	2.133984000	1	1.098368000	-3.376862000	2.827993000	1	-6.374754000	-2.023335000	4.695450000
1	-0.238446000	5.275144000	1.785972000	6	0.292434000	-4.146995000	0.983694000	1	-5.269715000	-0.756823000	4.086885000
1	0.849891000	6.667824000	1.754427000	6	-0.190073000	-5.451975000	0.933876000	1	-4.779767000	-2.464449000	4.020639000
6	0.764716000	5.659631000	3.681637000	6	0.342863000	-6.607712000	1.735532000	6	-6.786043000	3.287029000	3.124570000
1	-0.048726000	6.287528000	4.075907000	1	0.150681000	-7.551953000	1.201635000	1	-7.578076000	2.607105000	2.772392000
1	1.723121000	6.057733000	4.046375000	1	1.438235000	-6.518432000	1.834623000	1	-7.249142000	4.277395000	3.247785000
1	0.646902000	4.643182000	4.084586000	6	-0.283893000	-6.678227000	3.148231000	6	-6.254861000	2.791502000	4.492029000
6	3.587421000	6.559888000	0.877099000	1	0.113420000	-7.530356000	3.722019000	1	-7.068962000	2.724957000	5.229485000
1	4.664538000	6.563178000	1.109225000	1	-1.377265000	-6.784236000	3.077017000	1	-5.488513000	3.480561000	4.877105000
1	3.102770000	7.215798000	1.615820000	1	-0.072202000	-5.754197000	3.707827000	1	-5.793879000	1.798267000	4.388883000
6	3.372790000	7.141431000	-0.541100000	6	-3.579312000	-1.601763000	-0.120590000	6	-5.074366000	5.888395000	2.205913000
1	3.784040000	8.159788000	-0.609531000	6	-4.434525000	-2.432094000	0.739024000	1	-4.078661000	6.304278000	2.432188000
1	2.300352000	7.181014000	-0.780190000	6	-5.250187000	-1.561204000	1.437924000	1	-5.648756000	5.912110000	3.144037000
1	3.862057000	6.513187000	-1.298398000	6	-4.886779000	-0.227108000	1.051544000	6	-5.770110000	6.779885000	1.148667000
6	7.355085000	3.979140000	-2.074760000	6	-5.505633000	0.914369000	1.573144000	1	-5.852017000	7.818206000	1.504176000
1	6.747519000	4.894638000	-2.164576000	1	-6.322565000	0.741056000	2.270381000	1	-6.780650000	6.401604000	0.934619000
1	7.865546000	3.840303000	-3.039853000	6	-5.147426000	2.242382000	1.363395000	1	-5.202213000	6.776053000	0.206592000
6	8.408664000	4.175748000	-0.957623000	6	-5.693031000	3.370160000	2.096892000	6	-0.833721000	6.680934000	-1.055280000
1	9.045180000	5.048182000	-1.169318000	6	-4.934334000	4.466102000	1.742422000	1	-0.943462000	6.898558000	0.018759000
1	9.049448000	3.285549000	-0.874611000	6	-3.956746000	3.995330000	0.776568000	6	-1.876614000	7.498119000	-1.855458000
1	7.916090000	4.328610000	0.013968000	6	-2.951404000	4.786012000	0.213915000	1	-1.760698000	8.575599000	-1.663315000
6	7.538613000	0.987653000	-3.322288000	1	-2.926426000	5.835912000	0.499991000	1	-2.898125000	7.200715000	-1.576034000
1	7.949358000	1.813336000	-3.923127000	6	-1.974610000	4.349359000	-0.684000000	1	-1.756405000	7.319197000	-2.934097000
1	7.039030000	0.300203000	-4.023763000	6	-0.968449000	5.203531000	-1.291166000	6	0.890496000	4.788032000	-3.061980000
6	8.695951000	0.242026000	-2.613137000	6	-0.255597000	4.409010000	-2.166351000	1	0.706318000	4.396440000	-4.076149000
1	9.413220000	-0.156524000	-3.346502000	6	-0.807057000	3.072845000	-2.043280000	1	0.933073000	5.884046000	-3.149508000
1	8.306219000	-0.593868000	-2.013574000	6	-0.324858000	1.952280000	-2.713848000	6	2.248061000	4.260541000	-2.542391000

1	3.069958000	4.578362000	-3.201920000	1	-2.064534000	-3.472392000	-4.462013000	6	-4.414300000	-0.747509000	-3.554049000
1	2.253804000	3.164012000	-2.483015000	6	-2.520850000	-3.543089000	-1.332238000	6	-4.953625000	-2.032028000	-3.695627000
1	2.438814000	4.646111000	-1.536093000	1	-3.476442000	-4.041362000	-1.165705000	6	-6.071427000	-2.417040000	-2.945707000
6	0.991638000	-0.361242000	-4.255368000	1	-2.316071000	-3.725878000	-2.391124000	6	-6.663343000	-1.495925000	-2.069742000
1	0.893587000	-1.167380000	-4.996966000	6	-1.476258000	-4.154607000	-0.432202000	6	-6.143032000	-0.203958000	-1.965909000
1	0.894324000	0.583282000	-4.811545000	6	-1.313767000	-5.456846000	0.042810000	9	-6.564240000	-3.671309000	-3.053519000
6	2.385827000	-0.442588000	-3.596271000	6	-2.135733000	-6.644463000	-0.378031000	9	-7.729201000	-1.867516000	-1.327807000
1	3.184519000	-0.345194000	-4.347274000	1	-2.143263000	-7.394313000	0.428835000	9	-4.389661000	-2.922579000	-4.543860000
1	2.509570000	-1.405422000	-3.083825000	1	-3.183063000	-6.334355000	-0.532229000	9	-3.313042000	-0.424392000	-4.264180000
1	2.518944000	0.346024000	-2.843298000	6	-1.604562000	-7.293454000	-1.677666000	9	-6.740348000	0.670510000	-1.128570000
6	-0.249462000	-2.975919000	-3.318459000	1	-2.218649000	-8.157892000	-1.976025000	9	4.650179000	-4.956512000	3.364250000
1	-0.318982000	-3.774002000	-2.576011000	1	-0.567010000	-7.633598000	-1.539321000	9	6.430309000	-3.925840000	1.539927000
1	0.823346000	-2.888774000	-3.543715000	1	-1.609986000	-6.561882000	-2.500281000	9	6.432082000	-1.249316000	0.984590000
6	-0.982926000	-3.379200000	-4.618904000	1	0.178883000	7.002445000	-1.340373000	9	2.915894000	-0.607408000	4.150611000
1	-0.597846000	-4.339287000	-4.995331000	8	-4.387911000	1.368498000	-2.404985000	9	2.953329000	-3.283677000	4.714180000
1	-0.832070000	-2.613262000	-5.393901000	6	-4.967028000	0.197458000	-2.652708000				

2b (*endo-endo*):

26	-0.584024000	2.092721000	-1.828381000	6	-3.577459000	1.239063000	-1.678418000	6	-5.979797000	0.900169000	-0.438374000
8	-0.384693000	1.527911000	0.005984000	6	-4.678405000	-1.959398000	-1.269253000	1	-6.160510000	1.227725000	0.596404000
7	-0.410087000	4.181657000	-1.605871000	6	3.324398000	1.531004000	-3.670672000	1	-5.781153000	-0.172859000	-0.371679000
7	-0.952628000	0.316447000	-2.852276000	6	2.015614000	4.424689000	-1.944391000	6	-7.076341000	-2.781013000	-1.711264000
7	-2.673777000	2.292243000	-1.718803000	1	2.862001000	5.101689000	-1.842775000	1	-7.332976000	-1.767610000	-2.062205000
7	-3.681798000	-2.242617000	-0.358398000	6	-2.341888000	1.543428000	1.384293000	1	-7.894323000	-3.102422000	-1.047583000
1	-2.771555000	-1.798350000	-0.339452000	6	0.019162000	-0.413908000	-3.499150000	6	4.860297000	4.606787000	-4.217399000
7	1.317491000	2.193308000	-2.699375000	6	-2.883038000	3.543864000	2.644019000	1	4.009909000	5.302572000	-4.157158000
6	-1.383288000	5.003184000	-1.083697000	6	-0.486276000	-1.714883000	-3.852186000	1	4.811328000	4.098036000	-5.191657000
6	-4.586776000	2.996438000	-0.620357000	6	1.330499000	-0.008164000	-3.770083000	1	5.792566000	5.190271000	-4.173826000
6	-0.746329000	3.344129000	1.522817000	1	1.953512000	-0.721779000	-4.303377000	6	4.800597000	3.575410000	-3.066460000
6	-0.820608000	6.283170000	-0.693376000	6	-4.522887000	-0.975663000	-2.396795000	1	5.662346000	2.895580000	-3.129747000
6	-4.778757000	1.666927000	-0.942613000	1	-5.447008000	-0.394008000	-2.482717000	1	4.886110000	4.094147000	-2.099820000
6	-1.114553000	2.101457000	0.946861000	1	-4.450589000	-1.504333000	-3.354083000	6	4.003696000	0.697890000	-5.962464000
6	0.766304000	4.903363000	-1.545643000	6	-1.602898000	7.416098000	-0.093460000	1	4.719455000	0.059703000	-6.502792000
6	0.526414000	6.220602000	-0.984716000	1	-0.908865000	8.131476000	0.372464000	1	4.084415000	1.722803000	-6.354530000
6	-1.626767000	4.074188000	2.326637000	1	-2.243242000	7.027999000	0.715223000	1	2.986419000	0.336283000	-6.172997000
6	3.536897000	2.765218000	-3.090567000	6	4.288172000	0.677020000	-4.441907000	6	-6.997413000	-3.732775000	-2.928386000
6	1.940504000	1.188125000	-3.404637000	1	4.234344000	-0.356784000	-4.067967000	1	-6.762213000	-4.756499000	-2.599021000
6	2.267506000	3.175556000	-2.519130000	1	5.312342000	1.027623000	-4.254004000	1	-6.200258000	-3.411217000	-3.615733000
6	-5.785602000	-2.738810000	-0.939933000	6	-1.785821000	-1.793699000	-3.390673000	1	-7.947785000	-3.754913000	-3.484946000
6	-2.093427000	-0.478657000	-2.795450000	6	1.571595000	7.284958000	-0.810824000	6	-6.196399000	4.946151000	-0.784091000
6	-3.280473000	3.367251000	-1.101104000	1	2.498949000	6.834752000	-0.421123000	1	-6.798880000	4.437788000	-1.551360000
6	-3.335647000	-0.031392000	-2.270263000	1	1.231899000	8.013529000	-0.059400000	1	-5.448217000	5.564348000	-1.301521000
6	-3.228570000	2.269187000	2.178191000	6	-5.509551000	3.910487000	0.137753000	1	-6.855519000	5.609005000	-0.203459000
6	-2.704624000	4.618147000	-0.860168000	1	-4.946822000	4.438779000	0.923710000	6	-2.476411000	8.150611000	-1.137894000
1	-3.343000000	5.352989000	-0.374499000	1	-6.277511000	3.316878000	0.652052000	1	-3.186539000	7.453982000	-1.607271000

1	-1.846755000	8.576388000	-1.933446000
1	-3.046193000	8.966540000	-0.668054000
6	1.879147000	8.020044000	-2.138232000
1	0.972427000	8.509243000	-2.524303000
1	2.229470000	7.308796000	-2.900944000
1	2.655478000	8.786347000	-1.991880000
6	-7.261935000	1.158477000	-1.262319000
1	-7.523718000	2.226740000	-1.243578000
1	-8.106767000	0.584858000	-0.851869000
1	-7.131653000	0.869291000	-2.316494000
6	-2.575785000	-3.079397000	-3.529239000
1	-3.326478000	-3.197381000	-2.743125000
1	-1.868217000	-3.909888000	-3.382661000
6	-3.230205000	-3.243044000	-4.921583000
1	-3.942186000	-2.431396000	-5.135447000
1	-3.771703000	-4.199421000	-4.982635000
1	-2.464738000	-3.223057000	-5.711454000
6	0.330976000	-2.789343000	-4.516230000
1	0.898324000	-2.353990000	-5.354925000
1	-0.333766000	-3.549518000	-4.950020000
6	1.303228000	-3.458825000	-3.518962000
1	1.903741000	-4.237986000	-4.014348000
1	0.736837000	-3.917125000	-2.701053000
1	1.980149000	-2.719644000	-3.071161000
7	3.331450000	-3.099935000	0.777721000
7	-0.078547000	-2.049443000	2.793329000
7	0.471842000	-3.846595000	0.660286000
7	2.775001000	-1.316349000	2.917047000
6	3.419221000	-4.070339000	-0.195221000
6	-0.044428000	-5.532140000	-0.834981000
6	4.751221000	-4.091959000	-0.775259000
6	-1.244457000	-5.087534000	-0.308669000
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6	4.445981000	0.157698000	3.585856000
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1	5.645130000	1.864924000	4.036715000
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9	1.489479000	1.321522000	2.015986000	9	3.410612000	-1.090917000	-1.630853000	9	0.446222000	3.886929000	1.207054000
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2f (*exo-exo*):

26	2.640421000	-0.927296000	0.302418000	1	4.780938000	2.538675000	2.252450000	1	9.836185000	-0.789511000	-1.042717000
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7	2.247724000	-2.929399000	-0.221143000	6	3.785615000	-3.060182000	-2.160446000	1	4.078114000	0.409244000	5.279042000
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6	-6.603539000	-0.019357000	-0.791886000
1	-7.255361000	-0.205155000	0.060669000
6	-5.670978000	1.018074000	-0.708011000
1	-5.585224000	1.611671000	0.200604000
6	-6.678594000	-0.819162000	-1.945560000
6	-4.392773000	2.407560000	-4.632280000
1	-5.463105000	2.513384000	-4.869371000
1	-3.809600000	2.690958000	-5.523596000
1	-4.140677000	3.092075000	-3.812598000
6	-4.063400000	0.942235000	-4.240031000
6	-4.388860000	0.043914000	-5.454756000
1	-4.139973000	-1.009345000	-5.253566000
1	-3.788669000	0.378769000	-6.313857000
1	-5.451909000	0.104264000	-5.734664000
6	-7.648888000	-2.002829000	-2.095805000
6	-8.474733000	-2.253170000	-0.816242000
1	-7.820651000	-2.485527000	0.037607000

1	-9.146858000	-3.109629000	-0.975165000	1	-2.287204000	-0.199501000	-3.657305000	6	-6.854564000	-3.296924000	-2.407723000
1	-9.088434000	-1.378190000	-0.554607000	6	-8.630897000	-1.720636000	-3.262567000	1	-6.255820000	-3.191612000	-3.323214000
6	-2.545699000	0.820293000	-3.968637000	1	-9.220678000	-0.813937000	-3.059051000	1	-7.548025000	-4.141994000	-2.544011000
1	-2.226917000	1.512002000	-3.185838000	1	-9.323043000	-2.568679000	-3.388749000	1	-6.173767000	-3.540347000	-1.580201000
1	-1.988798000	1.053028000	-4.891134000	1	-8.089793000	-1.573530000	-4.208591000				

2f (*exo-endo*):

26	3.567448000	-0.778724000	-0.201496000	6	2.510765000	-4.344305000	-4.519996000	6	-6.437203000	-2.238769000	1.985122000
8	5.269784000	-0.362382000	-0.829305000	6	4.741584000	-2.735068000	5.042404000	6	-0.618138000	6.202140000	0.465628000
7	3.176776000	-2.543202000	-1.284709000	6	3.172887000	2.948436000	1.968994000	6	-2.919885000	2.212537000	1.868806000
7	3.132313000	0.780247000	1.136418000	6	3.876454000	-6.127507000	-2.185747000	6	-5.667864000	2.216227000	-1.496438000
7	2.343037000	0.278732000	-1.545349000	6	0.638719000	0.592423000	-4.871566000	6	-3.137484000	3.182052000	0.857412000
7	-0.223915000	4.026321000	0.165522000	6	0.587887000	3.218487000	-3.214456000	6	-6.781844000	1.491167000	-1.924341000
7	3.870570000	-2.062573000	1.442718000	6	1.678736000	7.148431000	-0.375901000	6	-4.008009000	3.010556000	-0.254649000
6	2.705282000	-2.593973000	-2.570415000	6	8.265779000	0.469960000	-4.006450000	6	-1.175889000	4.935482000	0.579975000
6	1.250933000	0.799549000	-3.511875000	6	6.413364000	-5.602944000	2.725392000	6	-5.162141000	-2.823843000	3.765605000
6	7.466909000	0.267849000	-1.580672000	6	10.613455000	1.204737000	0.469614000	6	-7.469636000	-2.248937000	1.052668000
6	2.881264000	-3.927173000	-3.124321000	6	10.874545000	1.298409000	1.985198000	6	-3.093534000	0.324610000	3.027512000
6	1.282708000	1.951698000	-2.760766000	6	5.935319000	1.116327000	-3.408308000	6	-2.083320000	1.111468000	3.688398000
6	6.520529000	0.004404000	-0.542113000	6	4.942397000	-5.286778000	3.061866000	6	-3.561098000	-0.886697000	3.543441000
6	3.620398000	-3.806398000	-0.985113000	6	6.166299000	-2.249538000	5.375915000	6	-2.557700000	4.580853000	1.080713000
6	3.460500000	-4.683996000	-2.133909000	6	1.518753000	7.704680000	-1.804067000	6	-9.439103000	0.165527000	-2.908748000
6	8.752875000	0.646575000	-1.184583000	6	1.658612000	0.592341000	-6.029150000	6	-4.571722000	-3.462746000	4.991663000
6	4.536596000	-3.878372000	2.727265000	6	3.571141000	-3.975826000	-5.576374000	6	-1.985689000	2.301437000	3.008065000
6	4.042913000	-1.668993000	2.746022000	6	11.600464000	0.170754000	-0.123987000	6	-9.898849000	-2.332244000	-0.902059000
6	4.164085000	-3.404997000	1.404235000	6	5.385622000	-6.325513000	-2.429326000	6	-5.757762000	3.942364000	-3.453735000
6	0.711862000	6.041596000	-0.042539000	6	1.380991000	4.066694000	-4.228896000	6	-3.348843000	5.101063000	-1.853875000
6	2.874444000	2.100795000	0.800020000	6	3.186835000	4.447793000	2.162177000	6	-1.265155000	7.504164000	0.862397000
6	1.921232000	-0.224450000	-2.750306000	6	10.896272000	2.593544000	-0.152334000	6	-8.465583000	-3.969070000	4.121574000
6	2.338489000	2.500402000	-0.452267000	6	4.543391000	5.091004000	1.805086000	6	-7.201111000	-4.359505000	3.330825000
6	8.215077000	0.511293000	1.143186000	6	3.945896000	2.466273000	4.390631000	6	-5.014418000	-2.799556000	6.311161000
6	2.110852000	-1.523985000	-3.225875000	6	2.785729000	2.408711000	5.402868000	6	-0.942801000	7.942515000	2.304322000
6	2.001375000	1.619123000	-1.515203000	7	-6.838311000	-0.252950000	-0.220346000	6	-7.067010000	4.741800000	-3.288275000
6	0.930988000	4.681276000	-0.212666000	7	-3.565087000	0.984771000	1.920110000	6	-10.417687000	1.299417000	-2.544361000
6	4.452572000	-2.795076000	3.568189000	7	-4.913345000	1.970197000	-0.374341000	6	-11.004387000	-2.004450000	0.121005000
6	4.083710000	-4.204712000	0.266900000	7	-5.435796000	-1.297714000	2.036744000	6	-4.030403000	6.469305000	-1.653048000
6	6.920691000	0.131651000	0.800910000	6	-7.360450000	0.383947000	-1.317583000	6	-1.069748000	3.404670000	3.492988000
6	3.522521000	0.760892000	2.452459000	6	-5.196429000	3.401011000	-2.166039000	6	-1.698069000	4.276828000	4.599382000
6	9.167548000	0.780659000	0.154174000	6	-8.575657000	-0.277955000	-1.761015000	6	-1.299488000	0.662271000	4.892734000
6	3.548785000	2.099663000	2.983911000	6	-4.164186000	3.908017000	-1.410574000	6	-0.174146000	-0.333731000	4.547640000
6	6.647728000	-1.316181000	-3.374066000	6	-7.669077000	-1.314535000	0.038625000	26	-4.890453000	0.084448000	0.545461000
6	3.888870000	-0.363945000	3.196405000	6	-8.770733000	-1.338599000	-0.909241000	8	-3.863905000	-0.932812000	-0.639376000
6	7.086538000	0.137497000	-3.069408000	6	-6.277545000	-3.204686000	3.059443000	6	-3.186112000	-2.838156000	-1.966879000
6	2.177039000	3.993352000	-0.718879000	6	-4.656234000	-1.626730000	3.116367000	6	-3.217149000	-2.102065000	-0.742103000

6	-2.536341000	-4.076710000	-1.944436000
6	-1.888473000	-3.843467000	0.344686000
6	-2.536194000	-2.612508000	0.378089000
6	-1.891730000	-4.621137000	-0.818559000
6	-1.268096000	-6.026617000	-0.892949000
6	-0.479275000	-6.379886000	0.382901000
6	-2.399944000	-7.068874000	-1.068579000
6	-0.298699000	-6.127480000	-2.093462000
6	-3.845499000	-2.307914000	-3.256035000
6	-5.377012000	-2.222873000	-3.061335000
6	-3.279433000	-0.909073000	-3.602936000
6	-3.581302000	-3.221607000	-4.470825000

2f (*endo-endo*)

26	-4.777999000	-0.026900000	0.593296000
8	-3.428299000	-1.215800000	0.114196000
7	-6.454399000	-0.811800000	-0.420204000
7	-3.815099000	1.327600000	1.886496000
7	-4.717699000	1.549600000	-0.797104000
7	-0.369199000	4.290000000	-0.348204000
7	-5.575199000	-1.015500000	2.290196000
6	-6.774799000	-0.539200000	-1.725704000
6	-4.848299000	2.533500000	-2.884104000
6	-2.142899000	-3.186200000	-0.415204000
6	-7.782099000	-1.467800000	-2.208804000
6	-4.022299000	3.326900000	-2.122904000
6	-3.029099000	-2.126000000	-0.780304000
6	-7.229399000	-1.885300000	-0.050604000
6	-8.067099000	-2.308900000	-1.160004000
6	-1.795899000	-4.096400000	-1.417704000
6	-6.522899000	-2.658100000	3.629596000
6	-5.046499000	-0.944400000	3.552896000
6	-6.471799000	-2.055300000	2.307096000
6	-1.074799000	6.409400000	-0.403704000
6	-3.177099000	2.524300000	1.601596000
6	-5.290199000	1.451100000	-2.042904000
6	-3.274999000	3.204500000	0.358896000
6	-3.108399000	-2.972800000	-3.071604000
6	-6.209799000	0.489900000	-2.468604000
6	-3.954599000	2.707700000	-0.786904000
6	-1.460999000	5.107800000	-0.115004000
6	-5.630499000	-1.963400000	4.409496000
6	-7.225099000	-2.471000000	1.212296000
6	-3.480699000	-2.038200000	-2.109404000
6	-3.543999000	1.025100000	3.198696000
6	-2.256699000	-4.034200000	-2.746404000
6	-2.661199000	2.011400000	3.767296000
6	-0.632599000	-4.519700000	1.163696000
6	-4.087499000	-0.020800000	3.947196000
6	-1.612199000	-3.338000000	1.022596000
6	-2.837299000	4.671200000	0.339996000
6	-8.392799000	-1.453300000	-3.582404000
6	-5.315299000	-2.158700000	5.866196000
6	-2.434199000	2.959400000	2.798696000
6	-9.065399000	-3.432200000	-1.113404000
6	-5.250099000	2.721900000	-4.322904000
6	-3.317299000	4.532400000	-2.700304000
6	-1.918500000	7.649800000	-0.256304000
6	-2.795699000	-3.598400000	1.984896000
6	-8.860199000	-3.357700000	4.367896000
6	-1.824199000	-5.109900000	-3.759204000
6	-2.424299000	-4.867900000	-5.157504000
6	-0.853299000	-2.058600000	1.451796000
6	-7.421199000	-3.795300000	4.029696000
6	-6.072399000	-1.192000000	6.798396000
6	-1.720200000	8.384000000	1.084096000
6	-6.658399000	3.321700000	-4.515704000
6	-9.553299000	-0.449900000	-3.734504000
6	-0.282299000	-5.114800000	-3.893004000
6	-10.415599000	-3.035500000	-0.483804000
6	-4.192199000	5.795600000	-2.828104000
6	-1.545299000	4.155500000	3.065896000
6	-2.294799000	-6.501200000	-3.269904000
6	-2.246599000	5.300100000	3.826496000
6	-2.098099000	1.961400000	5.162996000
6	-0.926899000	0.972200000	5.316196000
7	6.579801000	-0.003100000	0.041896000
7	3.037901000	0.891300000	-1.842604000
7	4.521101000	2.072800000	0.259696000
7	5.074501000	-1.237800000	-2.045004000
6	7.148501000	0.729600000	1.052496000
6	4.774301000	3.554200000	2.016796000
6	8.456701000	0.196900000	1.392996000
6	3.652501000	3.943700000	1.320896000
6	7.477101000	-0.993200000	-0.268604000
6	8.664201000	-0.878900000	0.562896000
6	5.948401000	-3.143500000	-3.039904000
6	4.199701000	-1.705100000	-2.996104000
6	6.149301000	-2.096200000	-2.053304000
6	0.287501000	6.368300000	-0.838604000
6	2.387801000	2.116700000	-1.857404000
6	5.321801000	2.414300000	1.325996000
6	2.609101000	3.137800000	-0.903304000
6	6.533701000	1.812800000	1.670296000
6	3.523201000	3.027100000	0.182696000
6	0.702501000	5.044400000	-0.792104000
6	4.726501000	-2.904600000	-3.623604000
6	7.265401000	-1.979600000	-1.230004000
6	2.534001000	0.155200000	-2.884304000
6	1.501801000	0.894400000	-3.570504000
6	3.012701000	-1.073600000	-3.346404000
6	2.070901000	4.542400000	-1.203004000
6	9.384001000	0.765900000	2.430196000
6	4.053901000	-3.675000000	-4.725804000
6	1.432601000	2.132700000	-2.979804000
6	9.872801000	-1.768500000	0.475096000
6	5.343601000	4.159700000	3.271496000
6	2.704701000	5.016700000	1.803596000
6	1.090600000	7.543800000	-1.334304000
6	8.063601000	-3.796100000	-4.303004000
6	6.930801000	-4.237100000	-3.354704000
6	4.287401000	-3.081200000	-6.129304000
6	0.881300000	7.849700000	-2.830404000
6	6.533301000	5.111700000	3.030096000
6	10.209301000	1.967800000	1.929496000
6	10.839601000	-1.387400000	-0.663504000
6	3.217201000	6.463700000	1.675696000
6	0.539801000	3.221500000	-3.532104000
6	1.184901000	4.001700000	-4.696304000
6	0.687701000	0.378600000	-4.726904000
6	-0.493799000	-0.507000000	-4.287204000
26	4.550301000	0.141500000	-0.552704000
8	3.719801000	-0.884800000	0.776096000
6	3.455401000	-2.420400000	2.625296000
6	3.611801000	-2.140200000	1.235296000
6	3.390401000	-3.770300000	3.005096000
6	3.568901000	-4.536200000	0.749596000
6	3.637001000	-3.217400000	0.324296000
6	3.457901000	-4.850600000	2.113196000
6	4.787801000	-0.595300000	3.721996000
6	3.413101000	-1.301800000	3.685596000
6	3.123301000	-1.836500000	5.103996000

6	3.449701000	-6.320100000	2.574396000	6	2.305601000	-0.275000000	3.350696000	6	2.317901000	-7.098200000	1.86239600
6	4.809501000	-6.966700000	2.212496000	6	3.240201000	-6.462500000	4.094296000				