Modulating Magnetic Exchange, Spin Dynamics and Intermacrocyclic Interactions *via* an Oxo-bridge in Dihemes Through Stepwise Oxidations

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Experimental Section:

Materials. *Cis*-1,2-bis[chloroiron(III) 5-(2,3,7,8,12,13,17,18- octaethylporphyrinyl)] ethene, P1,[1] *cis*-1,2-bis[μ-oxo iron(III) 5-(2,3,7,8,12,13,17,18-octaethylporphyrinyl)ethene, P2,[2] have been prepared by reported procedure. Reagents and solvents are purchased from commercial sources and purified by standard procedures before use.

P3. A 2.5 mg (0.01 mmol) sample of iodine in 0.5 mL of CH_2Cl_2 and 4.1 mg (0.02 mmol) of $AgClO_4$ in 0.1 mL of acetonitrile were added to 20 mg (0.016 mmol) of P2 in 2 mL of CH_2Cl_2. The mixture was stirred at room temperature for 15 minutes. After filtration of AgI, the product was precipitated by adding n-hexanes. Yield: 15 mg (70%). ***Caution!*** *Perchlorate salts are potentially explosive when heated or shocked. Handle them in milligram quantities with care.* UV-vis (dichloromethane) [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 383 (9.8x 10^4), 582 (1.1x 10^4). ESI-MS: *m/z* 1216.5835 (for $[P2]^+$). EPR data: in dichloromethane (120 K), g = 1.99. IR (KBr): $\nu(ClO_4^-)$, cm^{-1}: 624, 1108, $\nu(C_\alpha–C_{meso})$, cm^{-1}:1554 and ν ($C_\beta–C_\beta$), cm^{-1}: 1629. ^{1}H NMR ($CDCl_3$, 295 K): *meso-H*: 11.9, 12.3; -CH_3: 2.0; CH_2: 9.7, 10.0, 12.1, 14.1, 14.7, 15.7, 20.5, 24.7; C*H*(b): 26.4 ppm.

P4. A 5 mg (0.04 mmol) sample of iodine in 0.5 mL of CH_2Cl_2 and 8.2 mg (0.04 mmol) of $AgClO_4$ in 0.1 mL of acetonitrile were added to 20 mg (0.016 mmol) of P2 in 2 mL of CH_2Cl_2. The mixture was stirred at room temperature for 15 minutes. After filtration of AgI, the product

was precipitated by adding n-hexanes. Yield: 15 mg (70%). ***Caution!*** *Perchlorate salts are potentially explosive when heated or shocked. Handle them in milligram quantities with care.* UV-vis (dichloromethane) [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 376 (8.2x 10^4), 575 (1.2x 10^4). ESI-MS: *m/z* 608.2997(for $[P2]^{2+}$). ^{1}H NMR ($CDCl_3$, 295 K): *meso-H*: 8.3, 8.7; -C*H*$_3$: 1.9; C*H*$_2$:7.4,8.5, 9.5; C*H*$_2$(b): 21.0 ppm.

Instrumentation. Mass spectra were recorded using the electrospray ionization technique in a Waters Micromass QuattroMicro triple quadrupole mass spectrometer instrument. The Bruker Vector 22 FT IR spectrophotometer, using KBr pellets, was used to record all infrared spectra. UV-vis spectra were recorded on a PerkinElmer UV/vis spectrometer. Electron paramagnetic resonance (EPR) spectra were obtained on a Bruker EMX EPR spectrometer. Cyclic voltammetric studies were performed on a BAS Epsilon electrochemical workstation in dichloromethane with 0.1 M tetra(n-butyl)ammonium perchlorate (TBAP) as supporting electrolyte and the reference electrode was Ag/AgCl and the auxiliary electrode was a Pt wire. The concentration of the compounds was in the order of 10^{-3} M. The ferrocene/ferrocenium couple occurs at $E_{1/2}$ = +0.45 (65) V versus Ag/AgCl under the same experimental conditions. ^{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. For a typical spectrum between 2000 and 3000, transients were accumulated with a 50-μs delay time. The residual ^{1}H resonances of the solvents were used as a secondary reference. Variable temperature magnetic susceptibility measurements were carried out in the temperature range of 5-300 K with an applied magnetic field of 0.1 T on polycrystalline samples using a Quantum Design MPMS-XL-5 SQUID magnetometer. The susceptibility data were corrected for the sample holder previously measured using the same conditions and for the diamagnetic contribution of the sample as deduced by using Pascal's constant tables.[3]

X-ray Structure Solution and Refinement.

Crystals were coated with light hydrocarbon oil and mounted in the 100K dinitrogen stream of Bruker SMART APEX CCD diffractometer equipped with CRYO Industries low-temperature apparatus and intensity data were collected using graphite-monochromated Mo Kα radiation (λ= 0.71073 Å). The data integration and reduction were processed with SAINT software.[4] An absorption correction was applied.[5] 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[6] Non-hydrogen atoms were refined anisotropically. In the refinement, hydrogens were treated as riding atoms using SHELXL default parameters.

Crystallographic data and data collection parameters are listed in Table S1a. CCDC 2377591 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Table S1a. Crystal data and structure refinement for P3.

T (K)	100 (2)
Radiation (λ, Å)	Mo K_α (0.71073)
Formula	C_{74} H_{86} Cl Fe_2 N_8 O_5
Crystal size (mm^3)	0.150 x 0.120 x 0.100
Formula weight	1314.65
Crystal system	Monoclinic
Space group	C 2/c
a (Å)	22.192(2)
b (Å)	19.316(2)
c (Å)	20.102(2)
α (°)	90
β (°)	114.152(4)
γ (°)	90
V ($Å^3$)	7862.7(13)
Z	4
d_{calcd}, $g \cdot cm^{-3}$	1.111
μ, mm^{-1}	0.452
F(000)	2780
Reflections collected	46209
Independent reflections	6912
Data/restraints/parameters	6912 / 33 / 463
GOF on F^2	1.182
R_1[a][I>2sigma(I)]	0.1102
wR_2[b][I>2sigma(I)]	0.2586
R_1[a](all data)	0.1177
wR_2[b] (all data)	0.2630

a $R1 = \frac{\sum ||Fo| - |Fc||}{\sum |Fo|}$; b $wR2 = \sqrt{\frac{\sum \left[w(Fo^2 - Fc^2)^2\right]}{\sum \left[w(Fo^2)^2\right]}}$

Table S1b. Selected Bond Lengths (Å) and Bond angles (°) for P3

Fe1-O1	1.948(2)
Fe1-N1	1.988(5)
Fe1-N2	2.017(5)
Fe1-N3	2.007(5)
Fe1-N4	2.019(6)
C37-C38	1.382(17)
Fe-O1-Fe	143.0(3)
O1-Fe1-N1	98.9(3)
O1-Fe1-N2	95.9(2)
O1-Fe1-N3	100.9(2)
O1-Fe1-N4	105.5(2)

Computational Details:

All the single-point calculations and geometry optimizations were performed in the Gaussian 16 suite of programs.[7] The hybrid B3LYP functional along with third-order dispersion correction (D3) was used throughout the calculations. [8] A def2TZVP (def2- triple-ζ-valence-polarized) basis set for the Fe atom and a def2SVP (def2-single- ζ-valence-polarised) basis set for the rest of the atoms were used.[9] Visualization of the molecular orbitals and the corresponding diagrams were made using the Chemcraft software. We have performed broken symmetry DFT calculations in the Gaussian 16 suite of programs to compute the magnetic exchange coupling constants.[10,11] Time-dependent density functional theory (TD-DFT) calculations were performed to compute the UV-visible spectra to investigate the several transitions associated with the molecules. To compute the UV-visible spectra, a set of CAM-B3LYP/LANL2DZ/6-31G** (functional/basis set for Fe metal/basis set for rest of the atoms) tool was used which has been reported to yield the spectrum/transitions with best accuracy.[12] NMR calculations were performed using the gauge independent atomic orbitals (GIAO) method[13] implemented in Orca software[14] where the hybrid B3LYP functional was employed throughout the calculations along with basis sets, IGLO II for H, DKH-def2TZVP for Fe and DKH-def2SVP for rest of the atoms.[15,16] DKH Hamiltonian was employed to account for the

relativistic effects.[17] The third-order dispersion correction with Becke-Johnson damping (D3BJ) was used to capture the non-covalent interactions.[18] We have also performed the CASSCF/NEVPT2 calculations to compute the magnetic anisotropy and ZFS (D and E). To perform CASSCF/NEVPT2 calculations, a basis set of DKH-def2TZVP for Fe, O, N and DKH-def2SVP was used for the rest of the atoms. We incorporated 1 sextet, 24 quartet and 75 doublet roots for the Fe metal centre to compute the ZFS parameters (D and E/D). To compute the hyperfine coupling constant, the basis set of EPR II for H, DKH-def2TZVP for Fe and DKH-def2SVP for the rest of the atoms were used.

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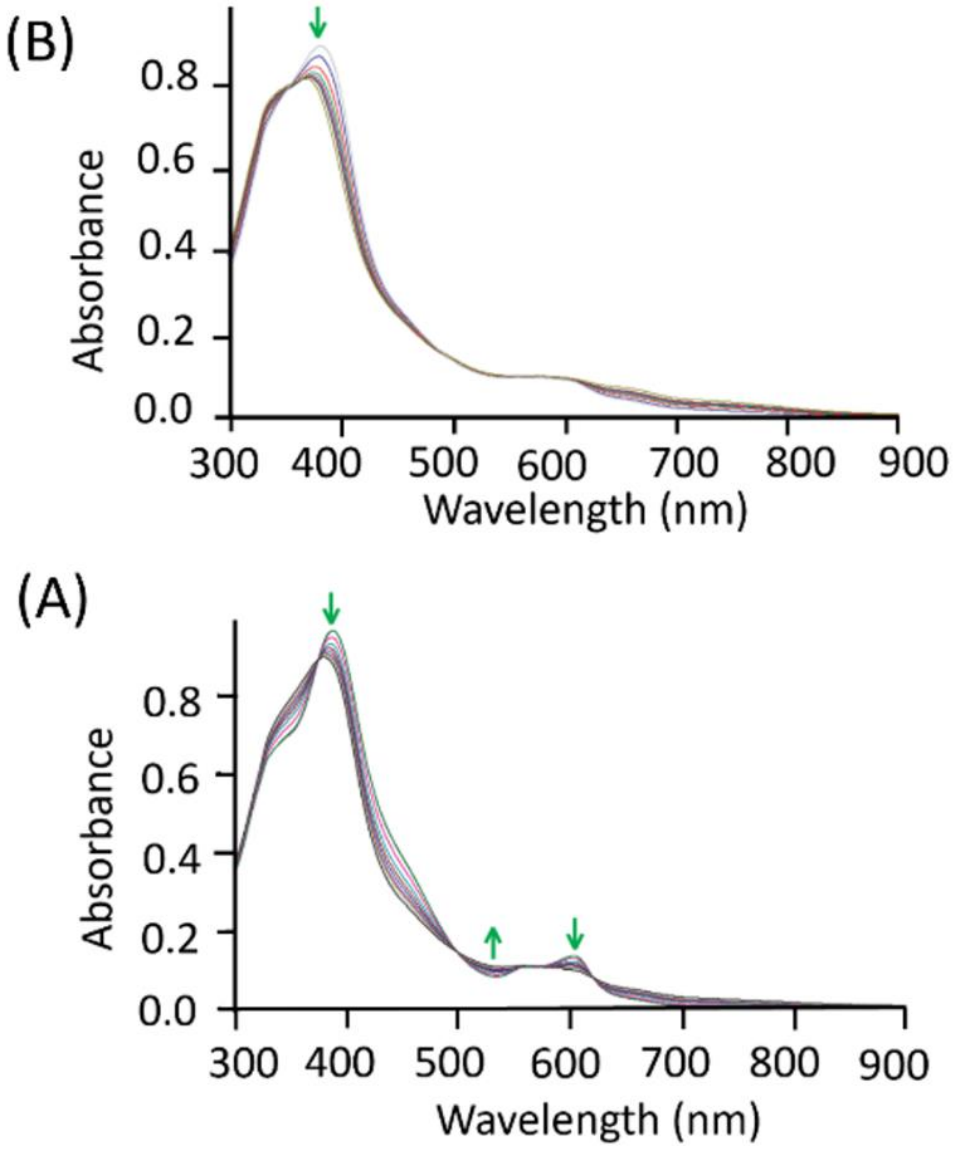


Figure S1. UV-visible spectral changes upon coulometric oxidations under nitrogen of P2 (in dichloromethane at 295 K) at constant potentials of (A) 0.70 and (B) 1.04 V. The arrows indicate the increase or decrease of the band intensity.

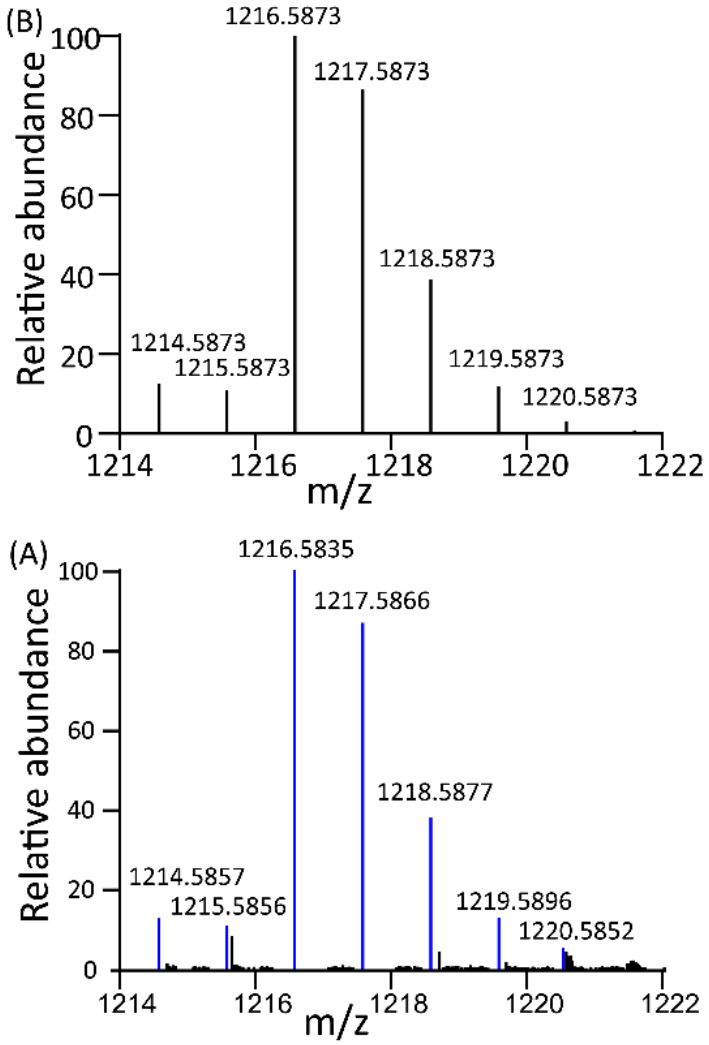


Figure S2. Isotopic distribution pattern of (A) experimental and (B) simulated ESI-MS spectrum (positive ion mode) of $[P2]^+$

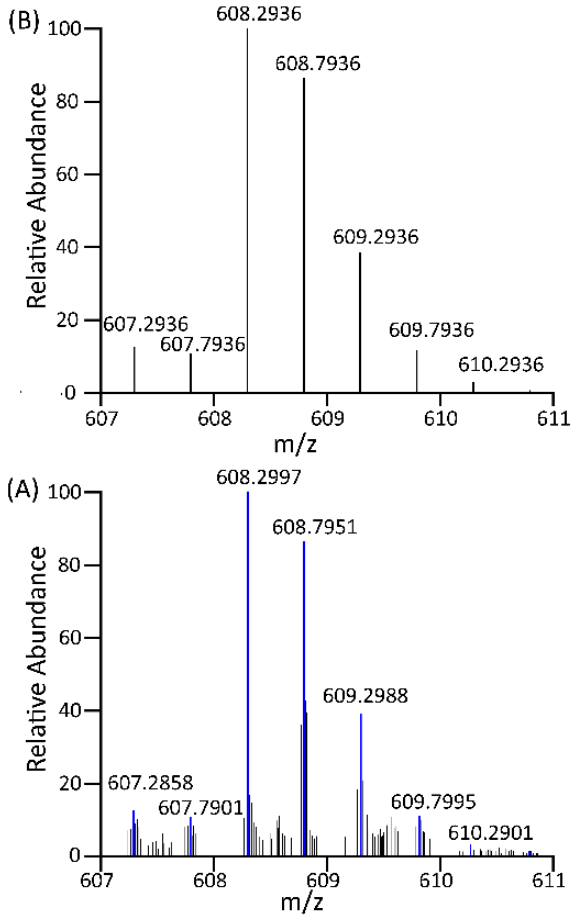


Figure S3. Isotopic distribution pattern of (A) experimental and (B) simulated ESI-MS spectrum (positive ion mode) of $[P2]^{2+}$

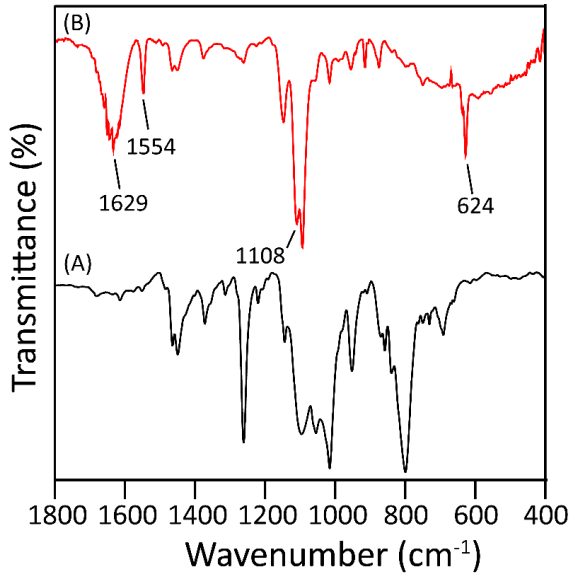


Figure S4. IR spectra (selected portions only) of solid polycrystalline samples of (A) P2, and (B) P3.

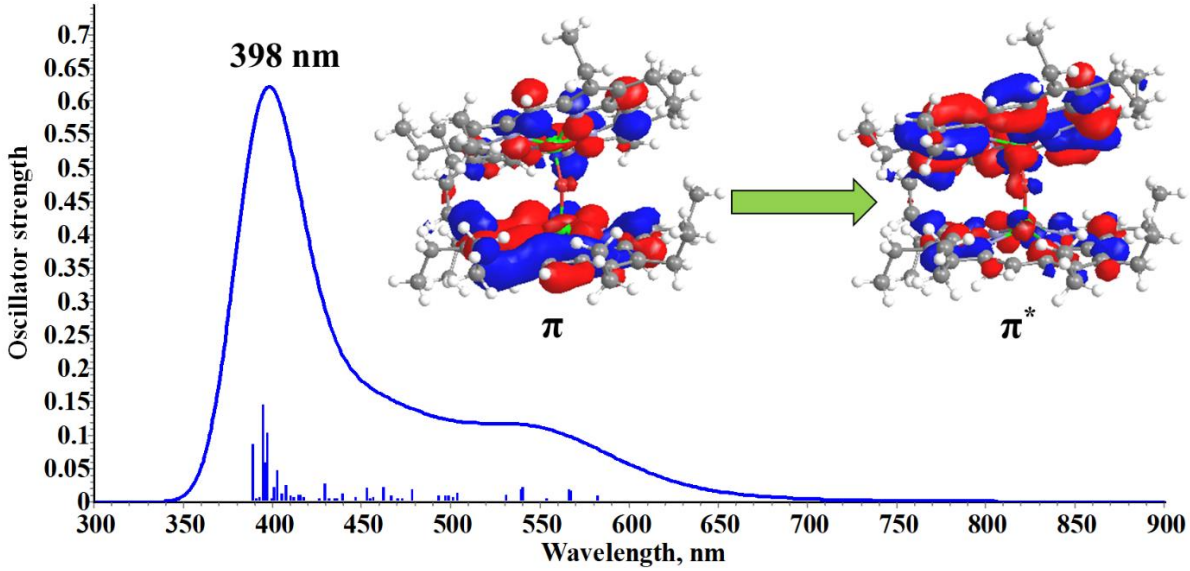


Figure S5. TD-DFT plot of P2 with intense Soret band at around 398nm and Q-band at around 500-600 nm.

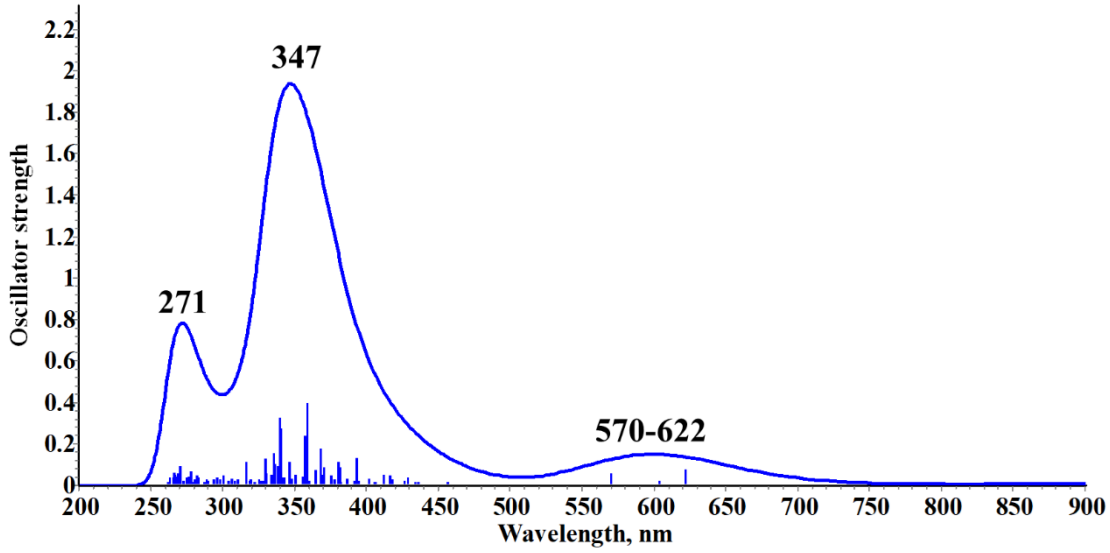


Figure S6. TD-DFT plot of P3 with intense Soret band at around 347nm.

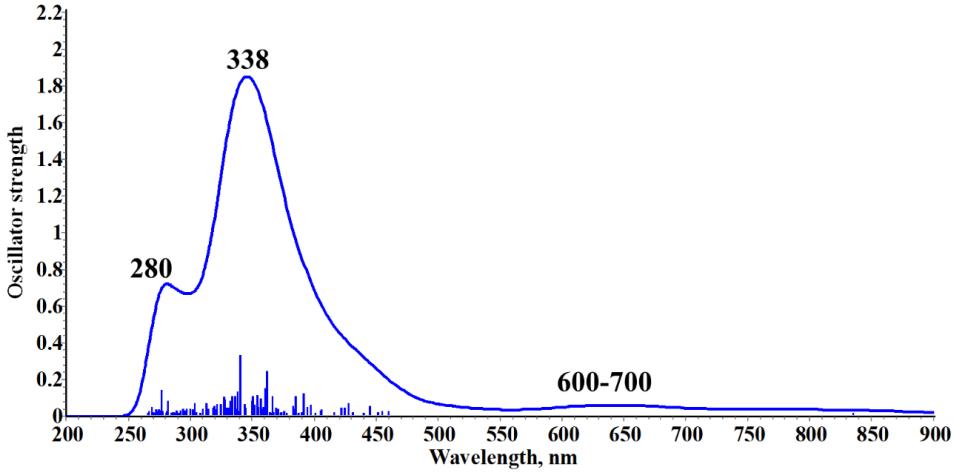
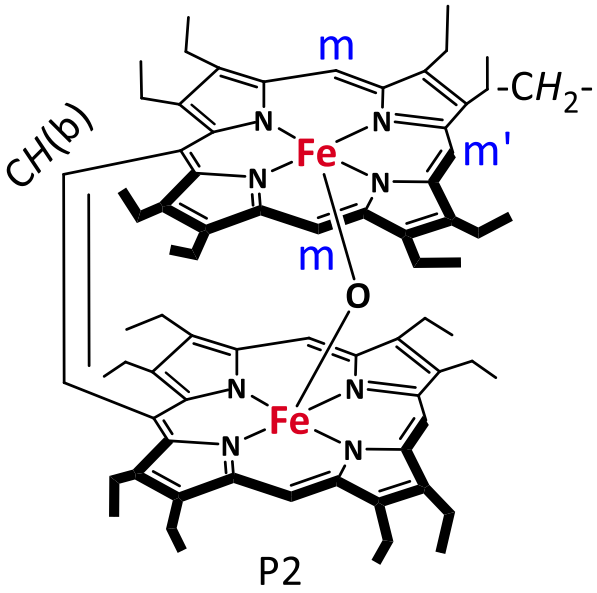


Figure S7. TD-DFT plot of P4 with intense Soret band at around 338nm.

(A)



(B)

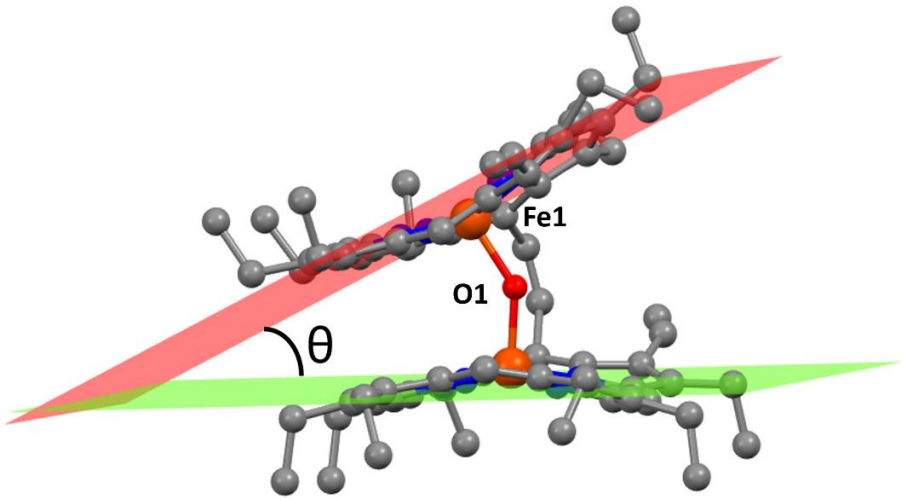


Figure S8. (A) Proton numbering scheme used for ^{1}H NMR (P2 is shown as representative case). (B) Diagram illustrating the angle θ between the two least-squares planes of $C_{20}N_4$ porphyrinato core of P3. (H-atoms have been omitted for clarity).

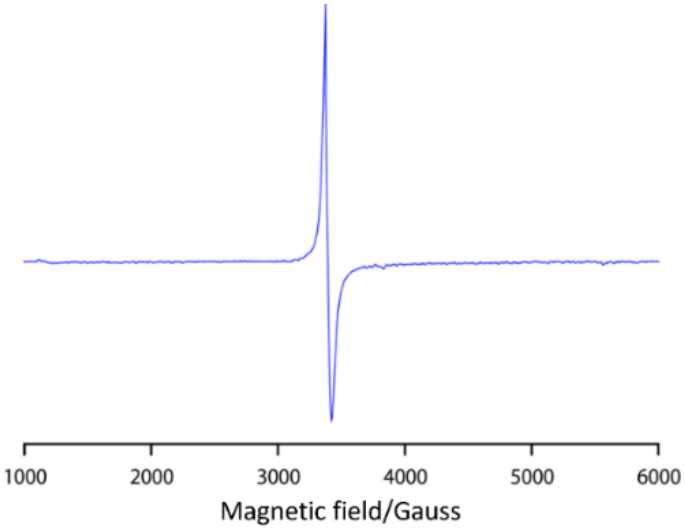


Figure S9: EPR spectra (in dichloromethane at 120 K) of P3.

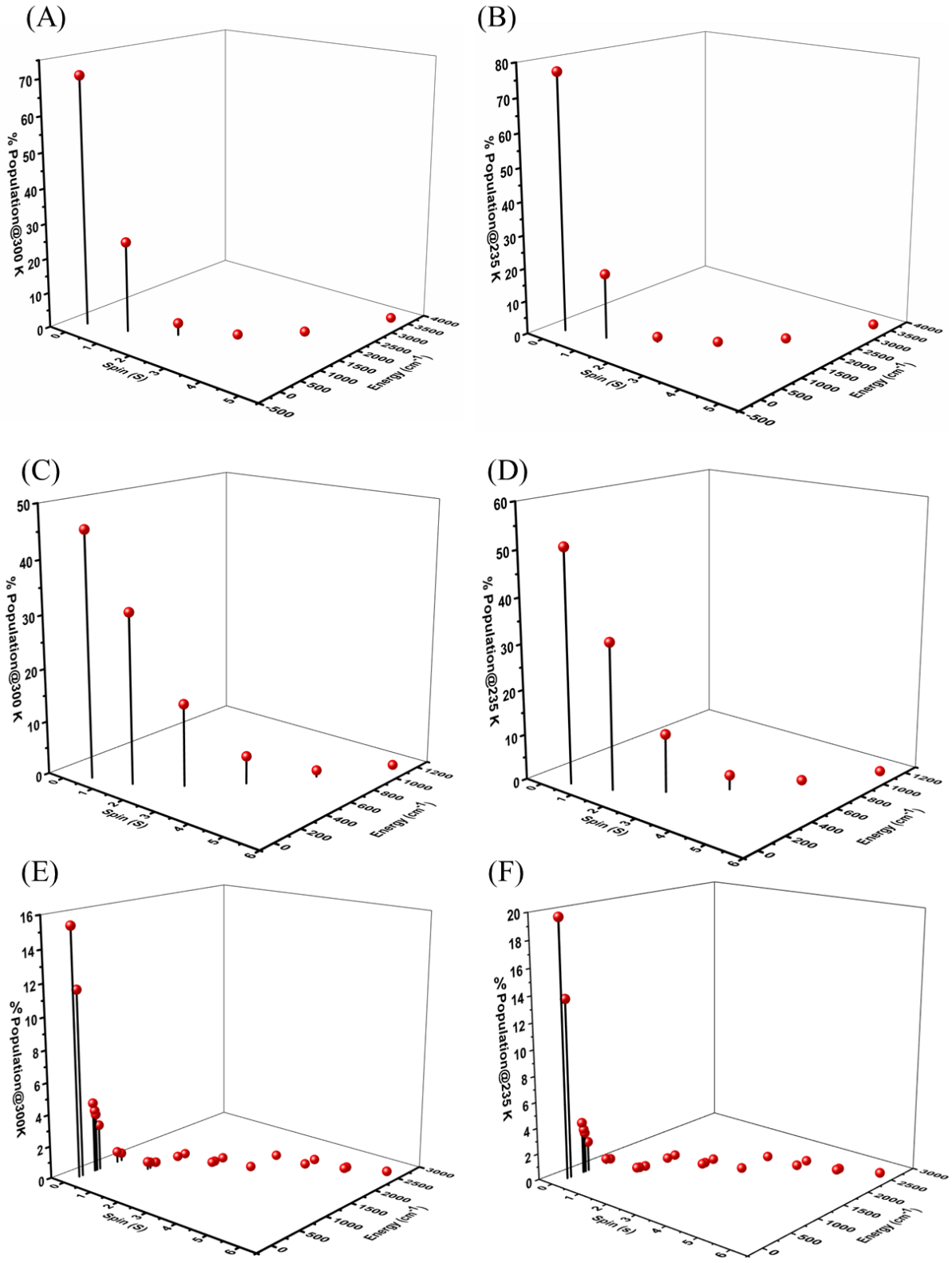


Figure S10. Percentage Boltzmann population of P2 at (A) 300 K (B) 235 K for P3 at (C) 300 K and (D) 235 K and P4 at (E) 235 K and (F) 300 K.

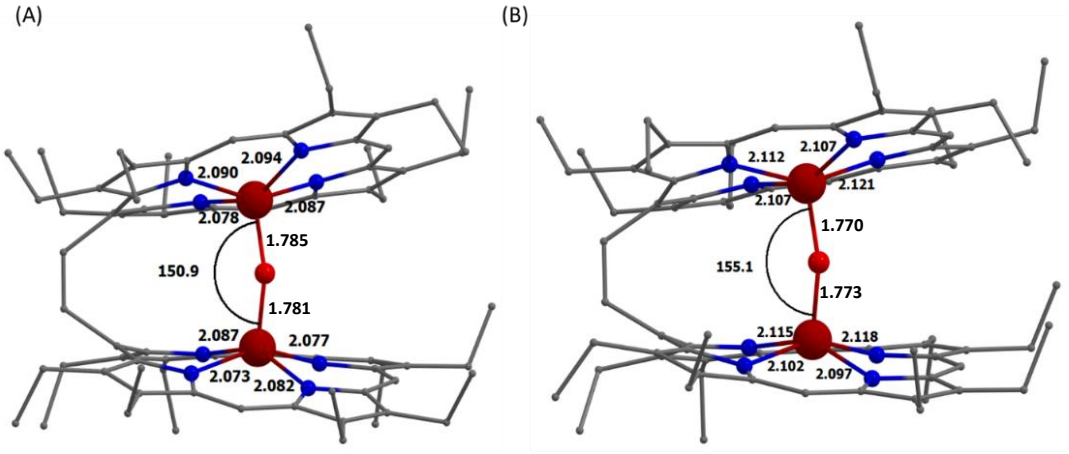


Figure S11. (A) X-ray and (B) DFT optimized structure of P2. Selected bond length (in Å) and bond angles (°) are shown. Hydrogen atoms are omitted for clarity. Colour code: Fe, deep red; O, red; N, blue; C, grey.

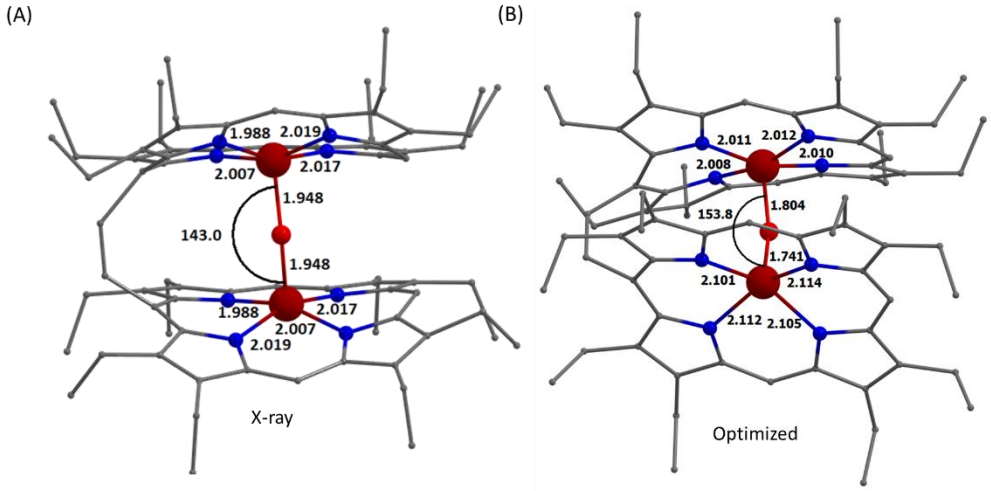


Figure S12. (A) X-ray and (B) DFT optimized structure of P3. Selected bond length (in Å) and bond angles (°) are shown. Hydrogen atoms are omitted for clarity.

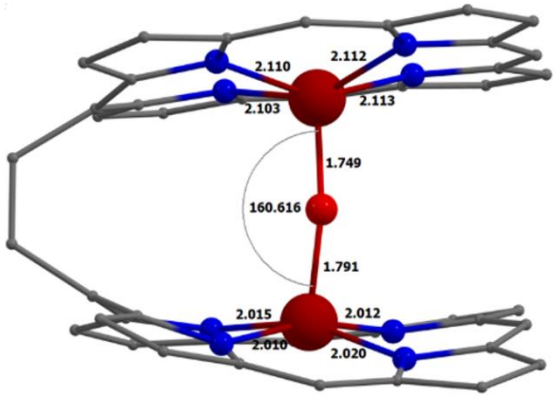


Figure S13. DFT optimized structure of P4. Selected bond length (in Å) and bond angles (°) are shown. Hydrogen atoms are omitted for clarity.

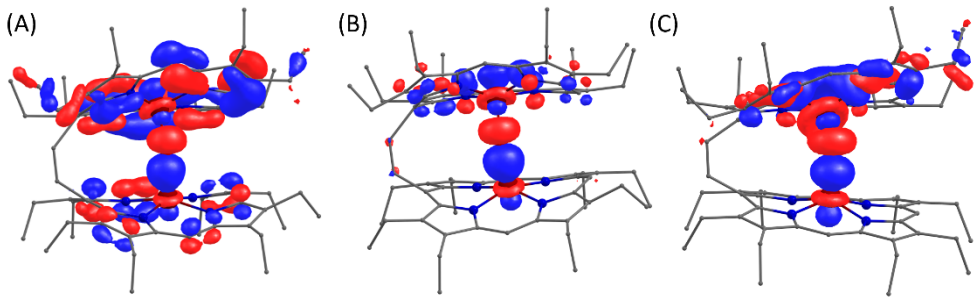


Figure S14. (A) A strong $d_{z^2} - p_z - d_{z^2}$ overlap in P2 (B) A weaker $d_{z^2} - p_z - d_{z^2}$ overlap in P3 (C) A strong $d_{z^2} - p_z - d_{z^2}$ overlap in P4.

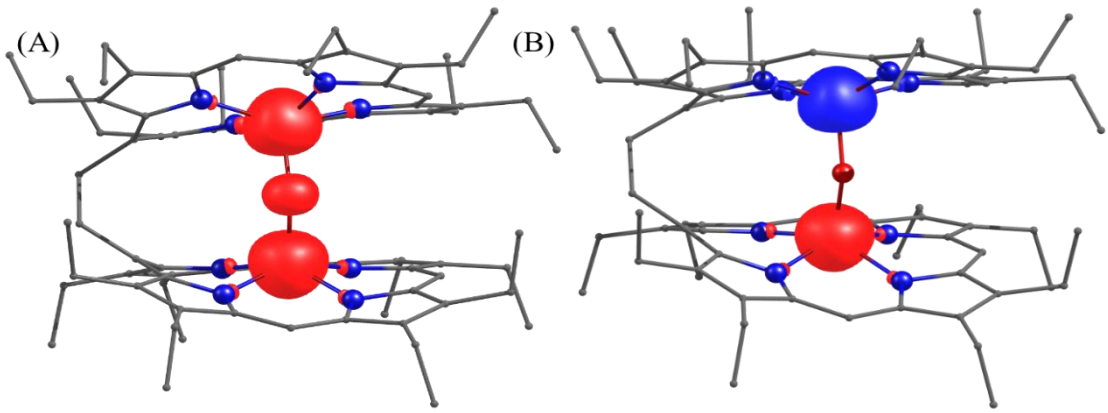


Figure S15. Spin density plot of (A) High-spin state and (B) broken symmetry (BS) state of P2.

Table S2. ^{1}H NMR chemical shift (in ppm) of complex P2

P2	CH=CH (exp)	CH=CH (DFT)	CH_2 (exp)	CH_2 (DFT)	H (m) (exp)	H (m) (DFT)	H (m') (exp)	H (m') (DFT)
	15.1	9.0	4.9	3.6 to 0.10	6.7	11.4	6.5	8.7
		9.0	4.9		6.7	11.4		7.6
			5.6			6.65		
			5.9			8.80		
average	15.1	9.0		3.3	6.7	9.56	6.5	8.16

Table S3. ^{1}H NMR chemical shift (in ppm) of complex P3

P3	CH=CH (exp)	CH=CH (DFT)	CH_2 (exp)	CH_2 (DFT)	H (m) (exp)	H (m) (DFT)	H (m') (exp)	H (m') (DFT)
	26.4	7.13	9 to 25	5.6 to 2.1	11.9	8.3	12.3	7.4
		7.32			11.9	8.4		8.0
						7.4		
						7.2		
average		7.22		3.85		7.82		7.7

Table S4. ^{1}H NMR chemical shift (in ppm) of complex P4

P4	CH=CH (exp)	CH=CH (DFT)	CH_2 (exp)	CH_2 (DFT)	H (m) (exp)	H (m) (DFT)	H (m') (exp)	H (m') (DFT)
	21	8.35	7.4	4.1 to 0.10	8.7	6.5	8.3	6.5
		8.42	7.4		8.7	6.3		7.1
			8.5			8.4		
			9.5			8.3		
Average		8.38		3.4		7.3		6.8

Table S5. DFT computed hyperfine coupling (in MHz) of P3 for the ground state, S_T = ½

P3	CH=CH	CH_2	H (m)	H (m')
	-2.57	0.88 to 0.00	1.96	1.34
	-0.79		2.48	3.18
			1.99	
			2.32	
average	-1.68	0.44	2.18	2.26

Table S6. DFT computed hyperfine coupling (in MHz) of P3 for 1st excited state, S_T = 3/2

P3	CH=CH	CH_2	H (m)	H (m')
	-0.30	0.17 to -0.09	0.64	0.55
	-0.55		0.61	0.66
			0.63	
			0.50	
average	-0.4	0.04	0.5	0.6

Table S7. DFT computed hyperfine coupling (in MHz) of P3 for the 2nd excited state, S_T = 5/2

P3	CH=CH	CH_2	H (m)	H (m')
	-1.53	0.68 to -0.03	1.23	0.81
	-0.64		1.87	2.17
			1.36	
			2.10	
average	-1.00	0.32	1.6	1.4

Table S8. DFT computed hyperfine coupling (in MHz) of P4 for 1st excited state, $S_T = 1$.

P4	CH=CH	CH_2	H (m)	H (m')
	7.3	1.88 to -0.01	1.4	-3.7
	-2.3		1.6	1.5
			-4.2	
			-2.6	
average	2.5	0.9	-3.8	-1.1

Table S9. DFT computed hyperfine coupling (in MHz) of P4 for the 2nd excited state, $S_T = 2$

P4	CH=CH	CH_2	H (m)	H (m')
	1.9	0.81 to -0.05	0.6	-0.9
	-1.5		0.9	0.6
			-1.5	
			-0.2	
average	0.2	0.37	-0.1	-0.15

Table S10. DFT computed ZFS parameters D and E/D and magnetic anisotropy for Fe1/Fe2 metal centres of P3 and P4

	D (cm^{-1})	E/D	g_x	g_y	g_z
P3, Fe1	2.986	0.007	2.000	2.000	2.001
P3, Fe2	2.790	0.009	2.000	2.000	2.001
P4, Fe1	1.088	0.002	2.001	2.001	2.001
P4, Fe2	1.093	0.013	2.001	2.001	2.001

Table S11. Overlap integrals between the d-orbitals of Fe1-Fe2 metal centres in P2.

Overlap integral	d_{xy}	d_{xz}	d_{yz}	$d_{x^2-y^2}$	d_{z^2}
d_{xy}	0.153	0.001	0.007	0.323	0.012
d_{xz}	0.008	0.291	0.283	0.047	0.131
d_{yz}	0.005	0.284	0.301	0.002	0.134
$d_{x^2-y^2}$	0.317	0.004	0.007	0.052	0.013
d_{z^2}	0.002	0.175	0.284	0.042	0.667

Table S12. Overlap integrals between the d-orbitals of Fe1-Fe2 metal centres in P3.

Overlap integral	d_{xy}	d_{xz}	d_{yz}	$d_{x^2-y^2}$	d_{z^2}
d_{xy}	0.522	0.003	0.028	0.009	0.014
d_{xz}	0.001	0.488	0.160	0.013	0.422
d_{yz}	0.001	0.180	0.481	0.004	0.008
$d_{x^2-y^2}$	0.003	0.005	0.003	0.023	0.002
d_{z^2}	0.001	0.213	0.006	0.001	0.015

Table S13. Overlap integrals between the d-orbitals of Fe1-Fe2 metal centres in P4.

Overlap integral	d_{xy}	d_{xz}	d_{yz}	$d_{x^2-y^2}$	d_{z^2}
d_{xy}	0.002	0.021	0.004	0.054	0.025
d_{xz}	0.095	0.196	0.131	0.110	0.019
d_{yz}	0.002	0.148	0.731	0.003	0.005
$d_{x^2-y^2}$	0.002	0.002	0.009	0.213	0.006
d_{z^2}	0.015	0.107	0.003	0.007	0.647

To compute the magnetic exchanges, J_O and $J_{CH=CH}$, we have used two models (see Figures S16A and B). In the computation of $J_{CH=CH}$, -O^{2-}-bridging atom was used as point charge (net Mulliken charge on oxygen bridged atom, $\Delta\delta_O$ = -0.67) while in the case of J_O computation, -CH=CH- atoms were used as point charges ($\Delta\delta_C$ = 0.22, $\Delta\delta_H$ = -0.07).

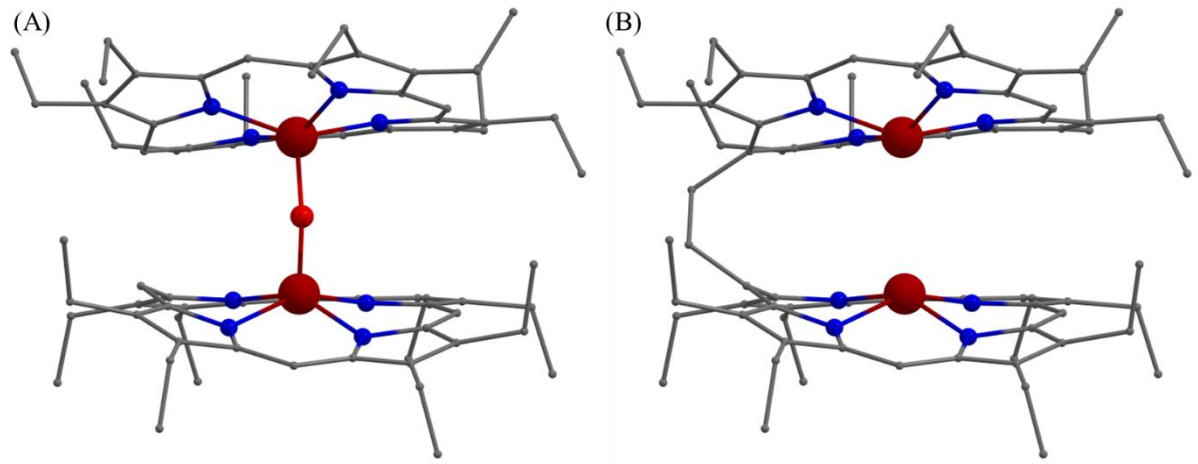


Figure S16. (A) the model used to compute J_O where the CH=CH group was used as the point charge (B) model used to compute the $J_{CH=CH}$ where the O^{2-} bridging ion was used as the point charge.

The cooperative enhancement by porphyrins in antiferromagnetic coupling (J_{coop}) could be defined as

$$J_{coop} = J_{Fe\text{-}Fe} - (J_O + J_{CH=CH}).$$

The coordinates of X-ray structures (P2 and P3)/optimised (P4) along with corresponding excited state energies and oscillator strength.

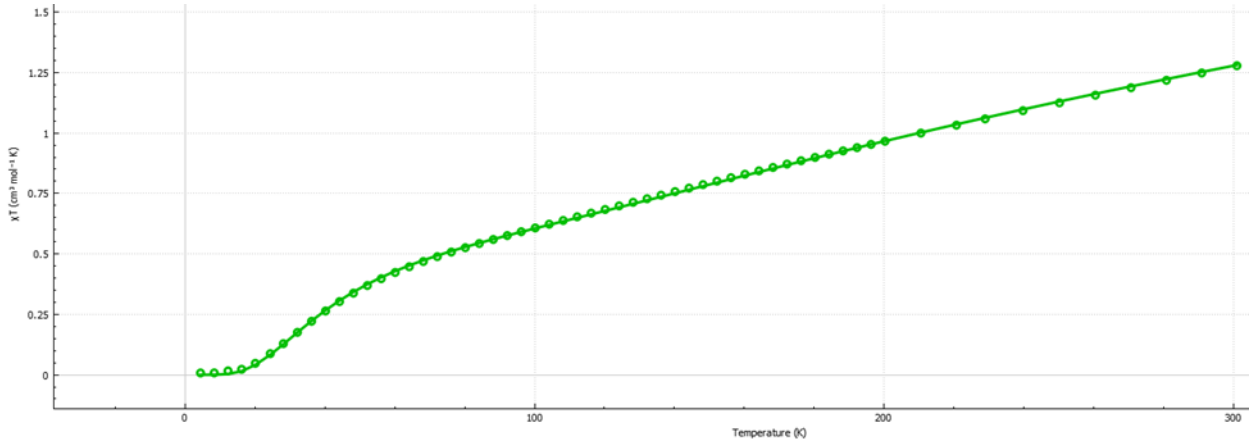


Figure S17(A). χT vs T fitting for complex **P4** using PHI without taking DFT computed J's as initial parameters in the PHI input which gives a good fit but unreliable J's (see Table S14).

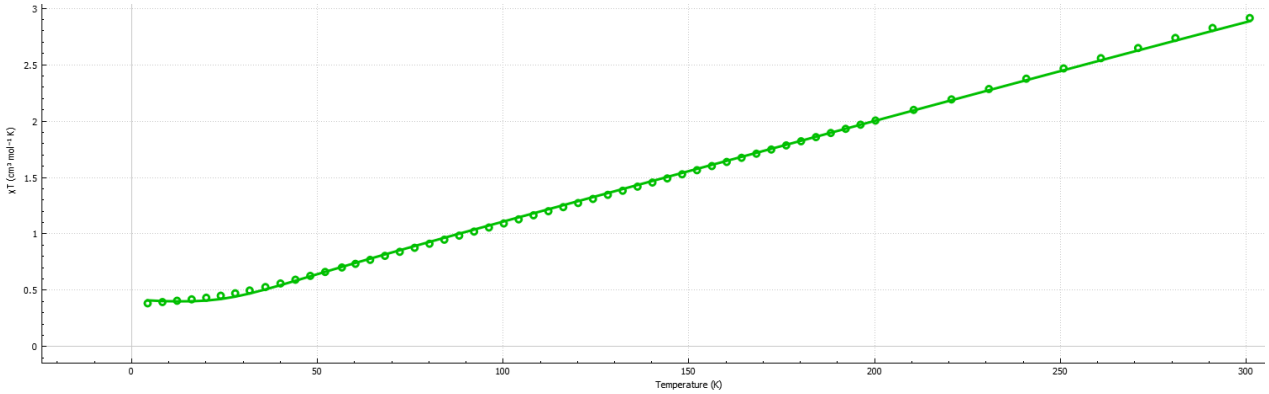


Figure S17 (B). χT vs T fitting for complex **P3** using PHI without taking DFT computed J's as initial parameters in the PHI input.

Table S14. The J's obtained from DFT calculations, from PHI fit with and without taking initial parameters from the DFT computed J's.

Exchange type	**Spin centres**	P4		
		J_{DFT} (cm^{-1})	J_{sim} (cm^{-1}) with guidance from DFT computed J values	**J_{sim} (cm^{-1}) without guidance from DFT computed J values**
$J_{Fe\text{-}Fe}$	$\boldsymbol{Fe1 - Fe2}$	−106.1	−116.1	**-179.2**
$J_{Fe\text{-}r}$	$\boldsymbol{Fe1 - Fe1_{rad}/Fe1 - Fe1_{rad}}$	−26.5	−27.2	**24.6**
$J_{Fe\text{-}r}$	$\boldsymbol{Fe1 - Fe2_{rad}/Fe2 - Fe1_{rad}}$	-	-	**75.4**
$J_{r\text{-}r}$	$\boldsymbol{Fe1_{rad} - Fe2_{rad}}$	−3.1	−2.4	**-3.4**

Table S15. The xyz coordinate of the X-ray/optimised structures along with corresponding TD-DFT excited state energies with oscillator strength.

P2	X-ray xyz coordinates			Excites state energies	Oscillator strength
Fe	-0.35668	-0.27552	-1.64695	806.21	0
Fe	0.133528	-0.05477	1.763518	792.42	0.0001
O	-0.17556	-0.60612	0.098134	788.44	0
N	0.309318	1.677054	-1.89856	777.48	0.0001
N	-2.29512	0.469153	-1.85744	775.47	0.0002
N	-1.1127	-2.017	-2.53121	764.28	0.0001
N	1.512595	-0.83241	-2.39658	744.93	0.0001
N	0.825676	1.908984	1.615816	737.28	0
N	-1.68938	0.758964	2.335999	681.4	0.001
N	-0.38005	-1.67766	2.961901	671.14	0.0013
N	2.117937	-0.54062	2.115519	659.29	0.0003
C	1.619879	2.101175	-1.97514	651.62	0.0004
C	1.664073	3.552987	-2.00916	637.15	0
C	0.397322	3.99076	-1.87256	628.66	0
C	-0.44438	2.817933	-1.76395	628.34	0
C	-1.80847	2.835543	-1.53502	622.44	0.0007
C	-2.69172	1.766523	-1.6041	619.46	0.0015
C	-4.13805	1.842245	-1.53612	619.06	0.0006
C	-4.61719	0.601177	-1.79061	598.76	0.0006
C	-3.46974	-0.25967	-1.96964	597.9	0.0036
C	-3.50982	-1.6127	-2.26811	582.91	0.0002
H	-4.36702	-2.02235	-2.28115	582.45	0.0086
C	-2.42673	-2.42851	-2.54896	567.71	0.0168
C	-2.50733	-3.81649	-2.95021	566.5	0.0184
C	-1.23914	-4.24533	-3.18134	553.91	0.0052
C	-0.37223	-3.11139	-2.91767	552.96	0.0009
C	1.009608	-3.14537	-2.99083	546.17	0.0008
H	1.3985	-3.9729	-3.24977	543.98	0.001
C	1.885352	-2.11173	-2.73077	539.92	0.0214

C	3.319473	-2.217	-2.80921	539.35	0.0189
C	3.820199	-0.99323	-2.49104	530.68	0.0105
C	2.676901	-0.12187	-2.24094	527.28	0.0032
C	2.715892	1.24749	-1.96723	523.34	0.001
C	2.852702	4.41397	-2.33324	519.65	0.0004
H	3.65204	4.051333	-1.87576	503.49	0.0135
H	2.695092	5.329524	-1.98916	501.22	0.0059
C	3.119964	4.484823	-3.82563	498.9	0.0089
H	3.911609	5.039002	-3.98925	496.94	0.0081
H	2.344833	4.879142	-4.27706	493.12	0.0076
H	3.275064	3.579371	-4.17368	485.43	0.0016
C	-0.09022	5.41185	-1.93047	478.77	0.0001
H	-0.81072	5.531131	-1.26286	478.43	0.0174
H	0.653145	6.016905	-1.68319	477.41	0.0027
C	-0.61073	5.805374	-3.27756	475.56	0.0004
H	-0.92599	6.732802	-3.24886	472.59	0.0022
H	-1.35403	5.214765	-3.52542	472.41	0.0054
H	0.104503	5.723157	-3.94131	470.84	0.0011
C	-4.92531	3.106984	-1.3269	470.52	0.0011
H	-4.48038	3.654967	-0.63035	469.91	0.0053
H	-5.83019	2.874112	-0.99725	466.46	0.0075
C	-5.05881	3.931347	-2.59511	461.87	0.0222
H	-5.56097	4.751325	-2.3993	460.86	0.0001
H	-5.53137	3.411002	-3.27408	460.77	0.0004
H	-4.16722	4.167747	-2.92441	457.22	0.0023
C	-6.05212	0.17211	-1.95613	456.37	0.0063
H	-6.6278	0.75384	-1.39708	454.35	0.0046
H	-6.15014	-0.75555	-1.62231	452.59	0.0197
C	-6.53633	0.232294	-3.39001	446.36	0.0065
H	-7.47647	-0.03785	-3.42703	444.83	0.0024
H	-5.99955	-0.37443	-3.94101	443.06	0.0024
H	-6.44608	1.148169	-3.72741	441.31	0.0036
C	-3.75364	-4.6497	-3.01289	438.85	0.0114

H	-3.65926	-5.31806	-3.73712	437.89	0.0014
H	-4.52182	-4.06629	-3.2386	436.36	0.0051
C	-4.04612	-5.36924	-1.71318	435.84	0.0014
H	-4.85527	-5.91346	-1.81486	434.98	0.0045
H	-4.18088	-4.7119	-1.0009	432.72	0.0002
H	-3.28903	-5.94933	-1.48295	431.72	0.0055
C	-0.7669	-5.57332	-3.68543	429.88	0.0038
H	-1.45134	-6.25988	-3.48111	429.53	0.0003
H	0.065075	-5.826	-3.2119	428.93	0.0262
C	-0.50472	-5.56033	-5.17441	427.25	0.0007
H	-0.20277	-6.44665	-5.4607	426.8	0.0014
H	0.188756	-4.89715	-5.37839	426.07	0.0047
H	-1.3281	-5.32404	-5.65028	424.73	0.0015
C	4.059387	-3.48476	-3.12253	423.66	0.004
H	4.964855	-3.25727	-3.45358	423	0.0011
H	3.586152	-3.9642	-3.84487	421.31	0
C	4.186685	-4.39475	-1.92529	417.52	0.0062
H	4.674215	-5.20485	-2.18183	415.58	0.0103
H	3.293169	-4.6393	-1.60527	414.93	0.0005
H	4.674217	-3.93096	-1.21388	414.28	0.0091
C	5.293882	-0.63386	-2.47883	412.37	0.0011
H	5.486898	-0.0343	-1.71306	412.11	0.0067
H	5.840209	-1.45281	-2.37781	410.56	0.0021
C	5.621769	0.024682	-3.7078	409.83	0.0085
H	6.549134	0.336202	-3.67475	407.5	0.0243
H	5.024102	0.79044	-3.83875	404.84	0.011
H	5.514717	-0.60435	-4.45296	402.8	0.0464
C	3.977449	1.829787	-1.28132	400.63	0.0214
H	4.666321	2.155809	-1.84981	399.55	0.0047
C	4.180193	1.91168	0.021837	398.31	0.0008
H	4.997881	2.293823	0.319525	397.23	0.0746
C	2.114793	2.300036	1.326368	396.79	0.1026
C	2.193869	3.753694	1.296666	395.45	0.0581

C	0.938299	4.214764	1.489096	394.66	0.146
C	0.082239	3.064612	1.651976	393.37	0.0023
C	-1.29314	3.11295	1.821338	392.9	0.0066
C	-2.1234	2.050834	2.143206	390.71	0.0056
C	-3.54128	2.14355	2.410366	389.17	0.0858
C	-3.97459	0.892934	2.725316	387.03	0.0023
C	-2.81764	0.038193	2.698745	384.46	0.02
C	-2.79044	-1.28923	3.110721	383.4	0.0036
H	-3.62877	-1.69909	3.287261	378.6	0.0125
C	-1.6675	-2.07046	3.289417	378.03	0.0049
C	-1.64392	-3.39094	3.907279	376.24	0.0764
C	-0.33883	-3.77724	3.950002	374.79	0.329
C	0.434773	-2.70882	3.368798	373.08	0.2293
C	1.807669	-2.71152	3.216962	370.2	0.0339
H	2.270067	-3.4655	3.561207	369.47	0.0574
C	2.58157	-1.73614	2.619352	365.57	0.0183
C	4.014445	-1.84151	2.423902	359.33	0.2037
C	4.391756	-0.71794	1.741777	357.38	0.15
C	3.209416	0.107644	1.583044	356.53	0.1065
C	3.166961	1.42364	1.106539	354.93	0.1451
C	3.458016	4.568182	1.217441	352.73	0.0474
H	3.22882	5.498913	0.969842	350.2	0.073
H	4.038944	4.199016	0.505879	348.89	0.4197
C	4.220159	4.574018	2.531293	348.18	0.05
H	4.990537	5.173819	2.458704	345.39	0.0174
H	4.530438	3.667099	2.734038	343.44	0.0102
H	3.629594	4.885412	3.248963	343.32	0.0057
C	0.516185	5.645094	1.656221	341.96	0.0093
H	-0.32843	5.789893	1.160129	340.62	0.007
H	1.205846	6.229857	1.254605	340.23	0.0005
C	0.312571	6.051444	3.09623	338.94	0.0001
H	0.03571	6.990217	3.133898	337.68	0.0009
H	1.150694	5.935912	3.5905	332.57	0.0103

H	-0.38313	5.488954	3.498702	331.49	0.0319
C	-4.3369	3.403284	2.493047	330.87	0.0196
H	-5.2985	3.189374	2.393008	330.03	0.0095
H	-4.07869	4.001727	1.7465	329.54	0.002
C	-4.12315	4.135037	3.815839	329.39	0.0018
H	-4.57901	5.002375	3.786471	328.72	0.0159
H	-3.16291	4.275108	3.960198	327.69	0.0076
H	-4.48731	3.598492	4.550963	326.47	0.017
C	-5.37792	0.459418	2.998571	325.88	0.0157
H	-5.83291	1.145625	3.544873	325.03	0.0556
H	-5.36425	-0.38382	3.519037	324.56	0.0751
C	-6.16218	0.242393	1.711623	324.15	0.0078
H	-7.06089	-0.08493	1.925793	322.33	0.0429
H	-5.69844	-0.41814	1.154278	321.39	0.0256
H	-6.23211	1.089958	1.224323	319.5	0.047
C	-2.83498	-4.15507	4.396631	318.97	0.1301
H	-3.58053	-3.52077	4.554801	318.75	0.0472
H	-2.61162	-4.58072	5.262369	318.3	0.0335
C	-3.29866	-5.23338	3.413622	317.41	0.0099
H	-4.07397	-5.70045	3.786311	316.51	0.1331
H	-2.57181	-5.8748	3.264168	314.98	0.0041
H	-3.54362	-4.81524	2.560693	314.77	0.052
C	0.232101	-5.06832	4.436077	313.97	0.0145
H	-0.43931	-5.52354	5.004679	313.9	0.0097
H	1.023947	-4.87625	4.998489	313.52	0.0787
C	0.645468	-6.00534	3.311188	312.5	0.1337
H	1.016879	-6.82917	3.690271	312.19	0.0077
H	1.321198	-5.56939	2.753898	311.79	0.0594
H	-0.13815	-6.22456	2.766341	310.32	0.0326
C	4.827659	-3.00534	2.891511	308.88	0.0336
H	4.517439	-3.2728	3.792957	308.2	0.0314
H	5.774954	-2.72606	2.968987	307.9	0.0948
C	4.739303	-4.2193	1.95703	306.68	0.2127

H	5.238556	-4.96659	2.347212	306.05	0.0955
H	5.123627	-3.98868	1.08678	305.02	0.0702
H	3.800731	-4.47521	1.842696	303.23	0.018
C	5.81312	-0.35943	1.425197	302.9	0.0016
H	5.834427	0.180672	0.596071	302.2	0.0238
H	6.327247	-1.18876	1.260229	301.55	0.0183
C	6.467125	0.418324	2.540727	300.68	0.0052
H	7.377112	0.668566	2.278156	300.44	0.0198
H	6.50396	-0.13395	3.351414	300.04	0.0177
H	5.946797	1.229152	2.722224	298.51	0.0725
H	-1.7607	4.06643	1.690324	297.84	0.0124
H	-2.23209	3.782937	-1.27446	296.49	0.0322
				295.03	0.0065
				294.37	0.0123
				293.99	0.0894
				293.47	0.0263
				292.21	0.2375
				291.63	0.0046
				290.73	0.0518
				289.72	0.1201
				282.13	0.0033
				279.96	0.0312
				279.49	0.0047
				279.06	0.0074
				278.73	0.0001
				277.27	0.0015
				276.66	0.0075
				276.53	0.0044
				274.36	0.0205
				273.64	0.0128
				272.6	0.0363
				272.38	0.0542
				271.88	0.0068

				271.23	0.0238
				270.94	0.0118
				270.49	0.0173
				270.01	0.0023
				269.11	0.0034
				268.93	0.1182
P3	X-ray xyz coordinates			Excites state energies	Oscillator strength
Fe	0.164138	0.145877	1.840688	2388.74	0.0001
O	0.074812	0.752655	-0.004759	2089.01	0.0005
N	1.553854	1.393016	2.515627	1735.26	0.0001
N	-1.251849	1.398533	2.54193	1621.54	0.0032
N	-1.237312	-1.28499	1.835641	1556.43	0.0276
N	1.566573	-1.302101	1.857279	1249.43	0
C	2.894803	1.318542	2.198794	1168.59	0.0001
C	3.547443	2.569856	2.555085	1158.31	0
C	2.646907	3.326044	3.168712	1126.63	0.0006
C	1.385166	2.634657	3.087925	1086.69	0.0001
C	0.165176	3.15936	3.448231	1067.77	0.0036
H	0.175485	3.977586	3.932389	946.29	0.0002
C	-1.073362	2.611209	3.17459	942.53	0
C	-2.346036	3.281719	3.291497	927.79	0.0069
C	-3.276438	2.522131	2.680397	850.54	0.0005
C	-2.604479	1.308249	2.235076	834.09	0.0006
C	-3.206091	0.183266	1.721688	829.07	0.0005
C	-2.591199	-1.06417	1.694345	754.04	0.0001
C	-3.278612	-2.34103	1.598025	740.22	0.0002
C	-2.329038	-3.318176	1.672401	737.46	0.0016
C	-1.054697	-2.651675	1.786605	730.88	0.0001
C	0.173059	-3.295815	1.794631	720.62	0.0004
H	0.16968	-4.244533	1.763115	704.7	0.0048
C	1.411491	-2.66086	1.842061	694.89	0.0008
C	2.676566	-3.312119	1.829792	644.82	0.0005

C	3.609773	-2.348091	1.762626	639.88	0.0039
C	2.924651	-1.103772	1.760689	629.96	0.0034
C	3.499041	0.149886	1.730236	622.48	0.0752
C	4.962375	2.996816	1.972216	603.97	0.02
H	5.10837	2.643611	1.05975	589.32	0.0093
H	5.079706	3.980059	1.971154	574.37	0.0096
C	5.833223	2.345361	2.955523	570.47	0.0533
H	6.770539	2.519775	2.72964	562.09	0.0007
H	5.641344	2.700788	3.849096	548.05	0.0011
H	5.669683	1.378848	2.947598	542.79	0.0027
C	2.737976	4.80181	3.586301	537.47	0.0015
H	3.522361	5.24369	3.176046	532.24	0.0009
H	1.917438	5.296858	3.337594	529.08	0.0013
C	2.883401	4.702684	5.074117	521.28	0.0014
H	2.952275	5.602268	5.456531	519.14	0.0014
H	2.102096	4.246464	5.450211	498.65	0.0025
H	3.693498	4.193747	5.290031	490.09	0.0002
C	-2.550492	4.602067	4.029193	487.42	0.0037
H	-1.778075	5.194546	3.853013	478.64	0.0051
H	-3.361309	5.047781	3.675406	477.7	0.0028
C	-2.698731	4.422704	5.499854	474.74	0.01
H	-2.828265	5.295696	5.924718	469.84	0.0002
H	-3.475901	3.852444	5.682589	463.34	0.001
H	-1.892261	3.999255	5.860239	460.94	0.0097
C	-4.76266	2.792921	2.556108	456.24	0.0148
H	-4.9232	3.767619	2.619429	453.91	0.0026
H	-5.076647	2.489532	1.667038	450.16	0.0071
C	-5.552714	2.086852	3.630883	447.1	0.006
H	-6.50531	2.283337	3.520051	445.7	0.0059
H	-5.408008	1.119169	3.560204	440.71	0.012
H	-5.254649	2.396481	4.512042	436.23	0.0136
C	-4.749773	-2.541267	1.645808	433.85	0.0133
H	-4.967373	-3.429626	1.266412	430.62	0.0002

H	-5.18693	-1.856092	1.078952	429.08	0.0368
C	-5.318234	-2.451392	3.062129	426.77	0.0192
H	-6.28661	-2.58974	3.035101	421.64	0.0014
H	-4.903744	-3.140271	3.62294	418.02	0.0239
H	-5.123364	-1.566215	3.435416	416.41	0.0444
C	-2.525859	-4.797387	1.687683	411.82	0.0521
H	-1.810614	-5.224446	1.153368	406.16	0.0173
H	-3.392695	-5.012399	1.260585	405.49	0.0173
C	-2.508624	-5.381657	3.095599	401.87	0.032
H	-2.641963	-6.350588	3.049789	400.91	0.0119
H	-1.645438	-5.189408	3.518458	399.7	0.0015
H	-3.228003	-4.977311	3.625713	398.07	0.002
C	2.864781	-4.786818	1.916847	394.61	0.0215
H	3.749011	-5.020225	1.539742	392.86	0.1324
H	2.173818	-5.231053	1.362828	391.42	0.0184
C	2.776039	-5.324546	3.338364	391.33	0.0084
H	2.90704	-6.295918	3.329989	388.58	0.0076
H	3.47049	-4.906683	3.889987	386.61	0.0304
H	1.894059	-5.117667	3.71294	382.16	0.0172
C	5.099247	-2.553149	1.876409	381.33	0.0845
H	5.55805	-1.864863	1.333739	380.72	0.1123
H	5.329234	-3.438642	1.49786	379.37	0.0006
C	5.617665	-2.479963	3.308319	377.79	0.0267
H	6.587934	-2.620462	3.311263	376.61	0.0043
H	5.414713	-1.598079	3.684475	375.89	0.0459
H	5.18567	-3.173388	3.848763	373.67	0.0117
N	-1.424657	1.340623	-2.525841	370.68	0.086
N	1.379313	1.439398	-2.552204	369.16	0.0486
N	1.453998	-1.242321	-1.842871	368.08	0.1748
N	-1.347768	-1.352678	-1.864437	366.61	0.0025
C	-2.762393	1.221963	-2.208899	364.89	0.0711
C	-3.456274	2.45048	-2.566598	362.77	0.0074
C	-2.581367	3.235495	-3.181099	360.61	0.0194

C	-1.297336	2.586537	-3.099552	359.02	0.0618
C	-0.09546	3.151105	-3.460475	358.52	0.3947
H	-0.13296	3.967986	-3.945561	357.03	0.2362
C	1.160614	2.64475	-3.186236	355.92	0.0396
C	2.410292	3.357073	-3.303928	354.52	0.0055
C	3.365424	2.629535	-2.691984	350.64	0.0526
C	2.73419	1.394488	-2.245273	347.61	0.0314
C	3.372866	0.290714	-1.730621	346.5	0.109
C	2.79979	-0.976446	-1.70185	345.62	0.0104
C	3.529278	-2.229633	-1.604095	342.55	0.0376
C	2.612722	-3.237896	-1.677345	342.13	0.0333
C	1.316926	-2.614267	-1.792281	340.74	0.2738
C	0.111267	-3.298883	-1.799552	339.89	0.3246
H	0.146188	-4.246927	-1.766959	338.32	0.0926
C	-1.147592	-2.705511	-1.847679	336.4	0.1032
C	-2.390313	-3.398459	-1.834647	335.33	0.1505
C	-3.355059	-2.465919	-1.768558	335.14	0.0293
C	-2.711691	-1.199506	-1.768045	334.4	0.0518
C	-3.327448	0.034394	-1.739004	332.85	0.0035
C	-4.88463	2.830817	-1.984187	330.59	0.0558
H	-5.018817	2.473988	-1.071318	329.74	0.127
H	-5.034591	3.809616	-1.984238	328.29	0.0209
C	-5.733317	2.149651	-2.966737	326.87	0.021
H	-6.675917	2.293058	-2.741034	325.41	0.0264
H	-5.553346	2.510247	-3.860716	322.97	0.0078
H	-5.53773	1.18912	-2.957719	322.28	0.0143
C	-2.721447	4.706943	-3.600361	321	0.0097
H	-3.520099	5.122962	-3.190592	319.24	0.0233
H	-1.917829	5.229282	-3.352231	318.63	0.0201
C	-2.863469	4.601347	-5.08806	316.76	0.0024
H	-2.962208	5.49771	-5.471493	316.46	0.1115
H	-2.067418	4.170932	-5.463651	315.22	0.0074
H	-3.65619	4.065511	-5.303382	312.91	0.0106

C	2.570747	4.682651	-4.043125	311.01	0.0243
H	1.779053	5.249319	-3.867603	310.47	0.016
H	3.366289	5.15548	-3.68986	309.47	0.0081
C	2.724895	4.506648	-5.513584	308.62	0.0216
H	2.825337	5.382981	-5.939441	307.32	0.0064
H	3.520599	3.962337	-5.695687	306.57	0.0302
H	1.932958	4.056209	-5.873474	306.13	0.0146
C	4.841818	2.949733	-2.56803	304.1	0.0192
H	4.969861	3.929158	-2.63246	302.58	0.0011
H	5.165703	2.657962	-1.678623	301.57	0.0073
C	5.654933	2.269106	-3.642018	300.51	0.0449
H	6.600466	2.497282	-3.531427	299.3	0.005
H	5.542481	1.297227	-3.570238	298.72	0.0018
H	5.346754	2.567653	-4.523522	298.22	0.0229
C	5.006284	-2.380897	-1.651679	296.86	0.002
H	5.253297	-3.261099	-1.271278	296.45	0.0359
H	5.420408	-1.680922	-1.085608	296.34	0.0116
C	5.571469	-2.273777	-3.068112	293.82	0.0267
H	6.54391	-2.379819	-3.040944	292.65	0.0112
H	5.180125	-2.976693	-3.628132	291.97	0.0109
H	5.347282	-1.395994	-3.442398	290.88	0.0099
C	2.858619	-4.709762	-1.690951	289.93	0.0125
H	2.157958	-5.15976	-1.156139	289.61	0.0202
H	3.732116	-4.895347	-1.263626	289.09	0.0246
C	2.860847	-5.295878	-3.098203	287.47	0.0127
H	3.026328	-6.259787	-3.051296	286.76	0.0108
H	1.991754	-5.132917	-3.521264	286.6	0.0059
H	3.566394	-4.868439	-3.628789	286.33	0.0077
C	-2.529388	-4.878699	-1.920026	285.1	0.003
H	-3.405375	-5.14095	-1.542639	284.93	0.0053
H	-1.824047	-5.299085	-1.365516	282.63	0.0366
C	-2.422788	-5.414792	-3.340934	282.27	0.026
H	-2.521419	-6.389973	-3.331453	282.04	0.0478

H	-3.130739	-5.020877	-3.893017	281.4	0.0236
H	-1.548169	-5.179126	-3.715761	280.55	0.0244
C	-4.836891	-2.720518	-1.88208	279.86	0.0103
H	-5.318335	-2.047253	-1.340183	279.09	0.016
H	-5.037313	-3.612739	-1.502522	278.43	0.0072
C	-5.357427	-2.666235	-3.314062	278.19	0.0646
H	-6.322488	-2.838921	-3.316828	277.63	0.0005
H	-5.183903	-1.778517	-3.691223	277.23	0.0196
H	-4.902605	-3.345525	-3.853727	276.75	0.0418
C	-4.484189	0.189737	-0.484718	276.54	0.0164
H	-5.36984	0.281152	-0.814205	275.16	0.0329
C	-4.430184	0.214579	0.857648	274.18	0.007
H	-5.262753	0.255662	1.310578	273.88	0.0037
Fe	0.005747	0.141149	-1.849514	273.25	0.01
H	4.37126	0.335061	-1.695367	272.82	0.0189
H	4.498493	0.151087	1.697134	271.96	0.0112
				270.88	0.0129
				270.44	0.0896
				269.9	0.0033
				269.22	0.0107
				268.92	0.0537
				268.48	0.0107
				267.56	0.0422
				267.24	0.0128
				267.01	0.0258
				266.61	0.0487
				266.36	0.0614
				266.05	0.0076
				265.6	0.0251
				265.31	0.0337
				264.48	0.0079
				263.61	0.0335
				263.22	0.034

				263.02	0.0025
				262.3	0.0175
				262.16	0.0169
				262.13	0.0054
				261.5	0.0008
				260.84	0.011
				260.51	0.0041
				260.38	0.0025
				260.3	0.0033
				259.38	0.0084
P4	DFT Optimised xyz coordinates			Excites state energies	Oscillator strength
Fe	0.091761	0.817686	1.546323	-1836.65	-0.0001
O	0.132562	0.595076	-0.211497	-2702.59	0
N	0.84196	2.735678	1.917049	3224.32	0.0006
N	-1.833211	1.571134	1.885954	2157.71	0.0001
N	-0.699931	-1.016304	2.168491	1941.79	0
N	1.98262	0.123258	2.122991	1759.86	0.0005
C	2.167484	3.100954	1.884562	1650.15	0.0011
C	2.29241	4.565108	1.914073	1439.78	0.0002
C	1.017807	5.058823	1.985048	1332.1	0.0001
C	0.12464	3.893139	1.972423	1064.6	0
C	-1.275442	3.96818	1.988034	1042.22	0.0001
H	-1.708184	4.966807	2.01903	1030.39	0.0001
C	-2.166784	2.903744	1.948794	885.17	0.0001
C	-3.62307	3.058482	1.923431	835.55	0.0146
C	-4.150685	1.800451	1.803488	828.3	0.0061
C	-2.999296	0.869917	1.76804	814.99	0.0003
C	-3.073223	-0.550338	1.669936	788.11	0.003
C	-2.015611	-1.405267	2.033324	782.32	0.0102
C	-2.130604	-2.85099	2.327195	735.65	0.0005
C	-0.85989	-3.299425	2.566183	710.92	0.0031
C	0.024678	-2.143276	2.432774	707.48	0.0034

C	1.423698	-2.225163	2.51234	693.18	0.0015
H	1.84192	-3.212847	2.699303	675.94	0.0046
C	2.327278	-1.18216	2.36129	669.33	0.002
C	3.790581	-1.317773	2.419828	655.51	0.0076
C	4.302628	-0.069605	2.189485	650.95	0.0045
C	3.149828	0.824617	2.029095	647.35	0.0037
C	3.238877	2.21547	1.873822	641.22	0.0091
C	3.590554	5.311973	1.959375	634.36	0.0117
H	4.303764	4.859167	1.249871	632.83	0.0039
H	3.427577	6.341848	1.606456	617.16	0.0028
C	4.213946	5.347044	3.36701	602.76	0.005
H	5.162919	5.903944	3.357886	593.35	0.0016
H	3.537265	5.836752	4.08377	588.7	0.0052
H	4.417204	4.331702	3.742807	573.67	0.0024
C	0.56837	6.481704	2.125031	570.25	0.0002
H	1.367922	7.150284	1.771154	568.58	0.0009
H	-0.293265	6.665363	1.46071	563.59	0.0023
C	0.193537	6.852709	3.57137	545.49	0.0016
H	-0.132192	7.901989	3.631684	543.77	0.0007
H	-0.624145	6.219805	3.951542	531.43	0.0045
H	1.053916	6.722682	4.245531	525.01	0.0039
C	-4.33845	4.364223	2.097299	511.98	0.0118
H	-3.845224	5.13787	1.485087	507.12	0.01
H	-5.361192	4.27853	1.700855	502.04	0.0101
C	-4.394167	4.826892	3.564736	483.03	0.0007
H	-4.92075	5.78935	3.648566	475.64	0.0034
H	-4.924876	4.091894	4.188954	464.38	0.0069
H	-3.3839	4.952387	3.985088	460.46	0.0231
C	-5.611226	1.461099	1.901711	457.88	0.0047
H	-6.195917	2.371885	1.705016	455.13	0.0222
H	-5.903923	0.749623	1.11852	451.47	0.0182
C	-5.999041	0.909194	3.284686	444.92	0.0523
H	-7.070456	0.66032	3.32041	440.1	0.0142

H	-5.428929	0.001279	3.537525	431.17	0.0188
H	-5.794607	1.650091	4.072245	430.11	0.0071
C	-3.394531	-3.62902	2.54062	427.49	0.0704
H	-3.153707	-4.70255	2.550725	425.03	0.044
H	-4.085508	-3.483636	1.702841	421.68	0.0441
C	-4.096899	-3.252275	3.857022	415.85	0.0178
H	-5.017271	-3.840859	3.989535	411.59	0.0063
H	-3.443073	-3.440169	4.722142	411.43	0.0029
H	-4.368824	-2.185113	3.875672	406.14	0.0317
C	-0.41207	-4.673117	2.966518	405.17	0.0313
H	0.503645	-4.934379	2.408571	401.97	0.0093
H	-1.168643	-5.407997	2.653023	401.03	0.0157
C	-0.152103	-4.810637	4.476364	397.24	0.0583
H	0.181314	-5.829312	4.725587	395.16	0.0104
H	0.622351	-4.104596	4.815431	394.18	0.0501
H	-1.066729	-4.600618	5.051569	391.69	0.1228
C	4.520438	-2.577819	2.76697	391.45	0.0044
H	5.544661	-2.527307	2.365468	390.21	0.0175
H	4.040934	-3.433189	2.267073	388.4	0.0102
C	4.573339	-2.837392	4.283566	387.59	0.0125
H	5.110415	-3.773157	4.500133	385.19	0.1081
H	5.089719	-2.018123	4.806092	384.32	0.0401
H	3.560786	-2.917472	4.709663	382.83	0.0535
C	5.736551	0.367998	2.181798	379.78	0.0015
H	5.894538	1.095169	1.366887	379.28	0.008
H	6.375029	-0.496214	1.941038	377.87	0.015
C	6.192209	0.983625	3.517041	375.6	0.0221
H	7.246588	1.293842	3.46379	373.28	0.0175
H	5.589765	1.867492	3.779533	372.66	0.0143
H	6.090558	0.258336	4.338465	370.84	0.0396
N	-1.716653	0.148846	-2.515465	370.47	0.0155
N	1.090192	0.781624	-3.025431	369.32	0.0423
N	1.879942	-1.538907	-1.559411	368.4	0.0096

N	-0.890882	-2.212718	-1.168577	367.05	0.02
C	-2.949167	-0.136385	-1.921717	366.33	0.1071
C	-3.92568	0.886216	-2.323032	364.73	0.0158
C	-3.267448	1.733667	-3.180579	364.23	0.0215
C	-1.883276	1.272254	-3.242545	361.97	0.2461
C	-0.849526	1.971905	-3.921787	360.52	0.0065
H	-1.163629	2.813829	-4.538217	360.32	0.1522
C	0.50887	1.752436	-3.821811	359.08	0.049
C	1.550938	2.570454	-4.447335	357.88	0.04
C	2.749527	2.098186	-3.970832	357.2	0.0941
C	2.427031	0.982039	-3.082921	355.23	0.048
C	3.386033	0.20037	-2.390929	354.39	0.1102
C	3.138513	-0.980473	-1.715245	351.83	0.0594
C	4.155512	-1.90045	-1.208622	350.7	0.1068
C	3.487405	-3.04085	-0.828444	349.78	0.0844
C	2.0692	-2.776788	-1.048352	348.01	0.0024
C	1.024779	-3.700894	-0.800145	344.82	0.042
H	1.322147	-4.705687	-0.500303	343.89	0.0654
C	-0.32668	-3.459356	-0.914547	342.78	0.0064
C	-1.383208	-4.446609	-0.733779	340.78	0.3329
C	-2.575543	-3.773311	-0.85406	339.98	0.0258
C	-2.225685	-2.364892	-1.074717	338.59	0.1301
C	-3.170324	-1.267936	-1.149295	338.22	0.0218
C	-5.390941	0.915259	-2.00225	337.56	0.0378
H	-5.548656	0.666261	-0.944801	336.2	0.109
H	-5.759942	1.944835	-2.126211	335.88	0.0687
C	-6.21961	-0.025272	-2.894503	334.26	0.1069
H	-7.283301	0.003379	-2.613391	332.5	0.0824
H	-6.138854	0.266605	-3.952386	330.74	0.0444
H	-5.873521	-1.068009	-2.818033	329.29	0.0416
C	-3.823289	2.88195	-3.969771	327.86	0.0862
H	-4.766126	3.217669	-3.512283	327.55	0.1001
H	-3.135999	3.742575	-3.902915	327.12	0.0106

C	-4.06917	2.533126	-5.448572	324.59	0.0637
H	-4.470207	3.401488	-5.992537	322.98	0.0093
H	-3.14022	2.217647	-5.949846	321.95	0.0611
H	-4.791174	1.707738	-5.543298	320.86	0.0346
C	1.305194	3.654544	-5.451987	319.78	0.0555
H	0.463248	4.285413	-5.119654	318.84	0.0448
H	2.181597	4.319423	-5.490584	317.82	0.0097
C	1.01312	3.107736	-6.861196	314.97	0.0071
H	0.839749	3.931628	-7.569701	314.75	0.0391
H	1.858516	2.509054	-7.233656	314.19	0.0053
H	0.121192	2.461369	-6.863131	313.44	0.0097
C	4.138328	2.539504	-4.325602	312.96	0.0669
H	4.104704	3.572098	-4.705463	311.81	0.0037
H	4.760553	2.576101	-3.414772	310.3	0.0404
C	4.808128	1.631092	-5.371839	308.8	0.0059
H	5.822661	1.986907	-5.606612	308.24	0.017
H	4.885841	0.592304	-5.012271	306.9	0.0089
H	4.226908	1.614484	-6.306478	305.93	0.0039
C	5.631829	-1.641459	-1.213339	304.85	0.021
H	6.103857	-2.252405	-0.427516	303.74	0.0702
H	5.818799	-0.591862	-0.93046	303.06	0.0072
C	6.303946	-1.94217	-2.565063	302.33	0.0358
H	7.383602	-1.734732	-2.518536	301.49	0.0001
H	6.171503	-2.998222	-2.844462	301.02	0.0024
H	5.873258	-1.329791	-3.372729	300.37	0.0405
C	4.0578	-4.353241	-0.378112	299.91	0.0048
H	3.439913	-4.769706	0.435758	298.99	0.0028
H	5.055603	-4.187007	0.055736	298.53	0.0031
C	4.160304	-5.38426	-1.516406	298.16	0.008
H	4.577447	-6.333609	-1.147967	297.16	0.0414
H	3.173734	-5.594181	-1.959351	296.23	0.0228
H	4.811381	-5.015054	-2.323009	295.46	0.0314
C	-1.155229	-5.916367	-0.548838	295.33	0.031

H	-2.029758	-6.361324	-0.049739	295.01	0.0016
H	-0.308739	-6.072124	0.140654	294.55	0.0382
C	-0.884973	-6.654041	-1.871963	294.32	0.0294
H	-0.720346	-7.727461	-1.69428	292.78	0.0009
H	-1.736637	-6.548573	-2.561378	292.08	0.0276
H	0.005394	-6.249031	-2.378212	290.85	0.0145
C	-3.944178	-4.387128	-0.944245	289.73	0.017
H	-4.631748	-3.927294	-0.220271	289.35	0.0272
H	-3.876693	-5.4465	-0.655267	289.18	0.0029
C	-4.544517	-4.282988	-2.356118	288.56	0.0076
H	-5.540122	-4.750367	-2.393131	288.18	0.0132
H	-4.650056	-3.233071	-2.673787	287.66	0.008
H	-3.902846	-4.786246	-3.095466	287.21	0.0172
C	-4.369417	-1.407665	-0.265155	286.74	0.0075
H	-5.308368	-1.777034	-0.688166	285.65	0.0212
C	-4.30728	-1.134714	1.049252	284.92	0.0162
H	-5.197391	-1.300762	1.661902	284.6	0.0013
Fe	0.106558	-0.429183	-1.649349	284.32	0.0079
H	4.425717	0.515764	-2.475785	283.2	0.0085
H	4.238033	2.645169	1.820908	282.32	0.0836
				282.15	0.01
				281.29	0.0266
				280.58	0.0134
				279.31	0.0066
				279.03	0.001
				278.35	0.0043
				277.89	0.0062
				277.37	0.0242
				277.2	0.1434
				276.99	0.0304
				276.01	0.0286
				275.52	0.0021
				275.04	0.0094

				274.67	0.0162
				274.57	0.0326
				273.28	0.0257
				272.68	0.0018
				272.39	0.0345
				270.89	0.0144
				270.48	0.0172
				269.32	0.0145
				269.06	0.0493
				268.13	0.0068
				267.98	0.0116
				267.35	0.0037
				266.92	0.0238
				266.45	0.0165

Table S16. The energies of spin ladders in P2, P3 and P4 are given in the Table.

Spin states	**P2** (in $kJmol^{-1}$)	Spin states	**P3** (in $kJmol^{-1}$)	Spin states	**P4** (in $kJmol^{-1}$)
S = 0	0.000	S = 1/2	0.000	S = 0	0.000-8.736
S = 1	2.520	S = 3/2	0.9072	S = 1	8.736-17.040
S = 2	7.560	S = 5/2	2.7216	S = 2	17.040-19.560
S = 3	15.120	S = 7/2	5.4432	S = 3	19.560-25.800
S = 4	25.200	S = 9/2	9.072	S = 4	25.800-28.200
S = 5	42.600	S = 11/2	13.608	S = 5	28.200-28.800
				S = 6	31.320

The coordinates of DFT optimised geometries are given below:-

P2

Fe	-0.343485000	-0.472727000	-1.541545000
Fe	0.045831000	0.395731000	1.785402000
O	-0.370359000	-0.332837000	0.223185000
N	0.980976000	1.099288000	-2.004125000
N	-1.979287000	0.773909000	-2.058325000
N	-1.621833000	-2.065443000	-2.060804000
N	1.298543000	-1.717625000	-2.004510000
N	1.574011000	1.824087000	1.475317000
N	-1.308826000	2.001164000	2.053739000
N	-1.236659000	-0.676717000	3.051089000
N	1.621460000	-0.870388000	2.363788000
C	2.346357000	1.091019000	-1.891002000
C	2.854012000	2.459773000	-2.011837000
C	1.755715000	3.281442000	-2.122839000
C	0.595180000	2.421138000	-2.099432000
C	-0.722708000	2.811066000	-2.130394000
C	-1.927588000	2.148402000	-2.120365000
C	-3.265777000	2.703941000	-2.193020000
C	-4.128032000	1.629265000	-2.176219000
C	-3.301821000	0.433352000	-2.081673000

C	-3.775979000	-0.881703000	-2.039406000
H	-4.857817000	-1.016572000	-2.045083000
C	-2.995168000	-2.037752000	-2.046877000
C	-3.520947000	-3.393216000	-2.120915000
C	-2.433558000	-4.231705000	-2.194808000
C	-1.254350000	-3.379472000	-2.168630000
C	0.061218000	-3.835690000	-2.258933000
H	0.193801000	-4.911652000	-2.371569000
C	1.228938000	-3.071589000	-2.208714000
C	2.564213000	-3.626301000	-2.311563000
C	3.443529000	-2.594219000	-2.076914000
C	2.629930000	-1.389063000	-1.891424000
C	3.119205000	-0.077811000	-1.682538000
C	4.281710000	2.885743000	-2.192928000
H	4.921031000	2.433225000	-1.427323000
H	4.352684000	3.974660000	-2.042612000
C	4.829590000	2.524650000	-3.583311000
H	5.877101000	2.848989000	-3.695441000
H	4.234662000	3.000755000	-4.378652000
H	4.788751000	1.436566000	-3.751962000
C	1.689307000	4.769665000	-2.291345000
H	0.864813000	5.154896000	-1.667182000
H	2.610870000	5.228338000	-1.899355000
C	1.468629000	5.207902000	-3.747648000
H	1.407555000	6.305331000	-3.829485000
H	0.532950000	4.782618000	-4.144214000
H	2.291479000	4.861162000	-4.393056000
C	-3.565313000	4.168127000	-2.314860000
H	-3.001497000	4.712403000	-1.538787000
H	-4.632245000	4.345819000	-2.103644000
C	-3.212975000	4.747351000	-3.694443000
H	-3.436457000	5.825478000	-3.741971000
H	-3.782262000	4.242354000	-4.491174000
H	-2.141806000	4.610919000	-3.912434000

C	-5.621113000	1.632313000	-2.329619000
H	-6.019147000	2.617445000	-2.041016000
H	-6.070358000	0.911574000	-1.624949000
C	-6.077101000	1.303105000	-3.760983000
H	-7.176484000	1.306163000	-3.839958000
H	-5.712642000	0.312387000	-4.074816000
H	-5.679235000	2.041000000	-4.475639000
C	-4.975122000	-3.763981000	-2.071833000
H	-5.113184000	-4.770424000	-2.498550000
H	-5.555410000	-3.083940000	-2.718815000
C	-5.551511000	-3.726334000	-0.646949000
H	-6.619720000	-3.997662000	-0.637936000
H	-5.447978000	-2.723371000	-0.206410000
H	-5.012804000	-4.427150000	0.010634000
C	-2.423136000	-5.726818000	-2.337302000
H	-3.358777000	-6.140043000	-1.926919000
H	-1.614132000	-6.152416000	-1.719448000
C	-2.254153000	-6.194222000	-3.792608000
H	-2.239876000	-7.294242000	-3.860377000
H	-1.315440000	-5.811529000	-4.223423000
H	-3.078727000	-5.821595000	-4.420828000
C	2.889398000	-5.059584000	-2.627490000
H	3.840871000	-5.106052000	-3.181642000
H	2.129656000	-5.466527000	-3.314789000
C	2.983516000	-5.955282000	-1.383341000
H	3.218464000	-6.996977000	-1.656238000
H	2.035181000	-5.952434000	-0.824310000
H	3.769607000	-5.593833000	-0.701596000
C	4.938427000	-2.701101000	-2.216409000
H	5.448212000	-2.186395000	-1.391739000
H	5.228217000	-3.759563000	-2.122584000
C	5.451123000	-2.156904000	-3.559683000
H	6.548201000	-2.235605000	-3.631510000
H	5.173365000	-1.099712000	-3.694559000

H	5.010279000	-2.715687000	-4.400231000
C	4.477357000	0.054559000	-1.056074000
H	5.371895000	0.030983000	-1.686908000
C	4.638006000	0.147067000	0.276857000
H	5.656074000	0.176520000	0.680077000
C	2.902155000	1.576949000	1.291616000
C	3.631652000	2.837110000	1.178407000
C	2.688429000	3.842346000	1.230146000
C	1.408879000	3.195990000	1.387120000
C	0.164325000	3.777385000	1.406831000
C	-1.103099000	3.305434000	1.652107000
C	-2.356981000	4.027586000	1.617438000
C	-3.323008000	3.140511000	2.041897000
C	-2.644261000	1.882017000	2.310339000
C	-3.242376000	0.724553000	2.828236000
H	-4.318700000	0.760427000	2.997950000
C	-2.583874000	-0.448078000	3.190767000
C	-3.224585000	-1.615401000	3.784278000
C	-2.231973000	-2.541663000	3.996498000
C	-0.993503000	-1.936233000	3.520132000
C	0.246494000	-2.577616000	3.490172000
H	0.277318000	-3.587561000	3.897506000
C	1.432384000	-2.103849000	2.919949000
C	2.630751000	-2.910415000	2.757287000
C	3.512906000	-2.165709000	2.012008000
C	2.878404000	-0.861808000	1.794475000
C	3.461343000	0.268823000	1.197577000
C	5.122185000	3.035508000	1.228872000
H	5.345793000	4.095675000	1.029486000
H	5.626821000	2.470746000	0.432583000
C	5.726756000	2.635988000	2.584547000
H	6.815987000	2.803862000	2.600001000
H	5.540269000	1.572269000	2.801829000
H	5.276799000	3.219231000	3.403385000

C	2.885489000	5.329346000	1.211260000
H	2.012653000	5.796060000	0.725679000
H	3.757538000	5.581532000	0.585103000
C	3.066873000	5.930153000	2.614374000
H	3.192400000	7.024186000	2.567676000
H	3.952180000	5.504955000	3.113620000
H	2.191888000	5.711236000	3.246604000
C	-2.487755000	5.477254000	1.253669000
H	-3.520432000	5.686949000	0.930860000
H	-1.842463000	5.685627000	0.383065000
C	-2.099380000	6.422739000	2.402082000
H	-2.190037000	7.478314000	2.098158000
H	-1.058621000	6.244149000	2.715809000
H	-2.744206000	6.260596000	3.280461000
C	-4.799776000	3.374599000	2.174667000
H	-4.991736000	4.452627000	2.300273000
H	-5.169945000	2.895639000	3.097183000
C	-5.592697000	2.850679000	0.967949000
H	-6.675632000	3.011271000	1.095346000
H	-5.416115000	1.774553000	0.815452000
H	-5.270558000	3.359823000	0.048743000
C	-4.699270000	-1.759474000	4.022768000
H	-5.099285000	-0.826735000	4.455919000
H	-4.874897000	-2.541838000	4.778869000
C	-5.481277000	-2.103585000	2.743827000
H	-6.561858000	-2.185393000	2.944608000
H	-5.138078000	-3.059277000	2.319606000
H	-5.331856000	-1.333283000	1.970922000
C	-2.366988000	-3.948196000	4.502216000
H	-3.269308000	-4.028349000	5.130213000
H	-1.517804000	-4.192930000	5.162846000
C	-2.444580000	-4.983716000	3.366234000
H	-2.539599000	-6.007196000	3.763926000
H	-1.544593000	-4.942536000	2.732616000

H	-3.310664000	-4.785132000	2.715256000
C	2.805805000	-4.307540000	3.281321000
H	2.373649000	-4.375501000	4.294040000
H	3.879312000	-4.524067000	3.402631000
C	2.170634000	-5.377697000	2.379129000
H	2.301986000	-6.386791000	2.802501000
H	2.626913000	-5.361216000	1.379651000
H	1.092174000	-5.197659000	2.247167000
C	4.907684000	-2.580810000	1.640001000
H	5.140438000	-2.242008000	0.622935000
H	4.955371000	-3.681170000	1.605378000
C	5.971027000	-2.058967000	2.619602000
H	6.985240000	-2.354826000	2.305182000
H	5.796323000	-2.453492000	3.633095000
H	5.941975000	-0.960382000	2.691371000
H	0.186602569	4.833233313	1.180804342
H	-0.838293598	3.884049492	-2.172183906

P3

Fe	0.147172822	-0.521868941	-1.591026007
O	0.069815346	-0.708414304	0.138221704
N	1.525125049	-1.880610739	-2.035185088
N	-1.280619280	-1.868442827	-2.053686861
N	-1.243604511	0.897926674	-1.838789541
N	1.560232243	0.888606437	-1.869525126
C	2.867740611	-1.761336924	-1.739836217
C	3.509778088	-3.061342807	-1.868060838
C	2.601420309	-3.907896317	-2.334490654
C	1.345143203	-3.203201442	-2.375792462
C	0.119985976	-3.774167596	-2.633661948
H	0.122456372	-4.665842886	-2.963689378
C	-1.113444356	-3.176090539	-2.459654068
C	-2.391473159	-3.846561652	-2.451851354
C	-3.313974852	-2.982562714	-1.984345756
C	-2.631410007	-1.713990461	-1.764848893

C	-3.222782309	-0.510586194	-1.459581866
C	-2.598564583	0.716702806	-1.657193418
C	-3.276136621	1.995626677	-1.789236974
C	-2.319624388	2.936140749	-2.039345959
C	-1.050685630	2.249853639	-2.035401956
C	0.181773691	2.872395400	-2.161304024
H	0.185542589	3.811451846	-2.299973793
C	1.415283060	2.229371620	-2.097223375
C	2.685187203	2.862250220	-2.204516037
C	3.611462448	1.918388551	-1.968135243
C	2.917147461	0.699960658	-1.742113451
C	3.482336635	-0.532566320	-1.489233868
C	4.923631570	-3.388415015	-1.221449841
H	5.075581490	-2.878895401	-0.387205574
H	5.033674173	-4.356518405	-1.044811965
C	5.795677478	-2.930253462	-2.307399397
H	6.732495865	-3.068904299	-2.056098957
H	5.597897849	-3.438215782	-3.122553437
H	5.639336357	-1.976635381	-2.472097683
C	2.680017738	-5.435227481	-2.481600761
H	3.462603002	-5.802836425	-2.000715226
H	1.856749102	-5.871280040	-2.146492983
C	2.820723613	-5.604931102	-3.963482464
H	2.881526566	-6.558920375	-4.178988694
H	2.041449650	-5.217129110	-4.413329763
H	3.633774658	-5.149266390	-4.268786484
C	-2.608410944	-5.275882569	-2.941030461
H	-1.839766853	-5.833423431	-2.663481858
H	-3.421208383	-5.644683364	-2.511383262
C	-2.760701448	-5.361243311	-4.419715962
H	-2.898258069	-6.295084698	-4.681291855
H	-3.534287082	-4.826697030	-4.699728991
H	-1.952440064	-5.015493270	-4.851862591
C	-4.801698089	-3.214939061	-1.810243442

H	-4.969689443	-4.183940856	-1.697845678
H	-5.110169392	-2.754958853	-0.989060240
C	-5.590427576	-2.706202485	-2.992171083
H	-6.544041552	-2.872121897	-2.845814121
H	-5.438294732	-1.742660665	-3.096038766
H	-5.297895010	-3.170780592	-3.804418536
C	-4.745938082	2.195776786	-1.868712492
H	-4.955556209	3.139364725	-1.653829177
H	-5.186082958	1.626517196	-1.187454277
C	-5.320232933	1.858584796	-3.244822075
H	-6.287451345	2.007228243	-3.240768957
H	-4.902704688	2.432749766	-3.920743643
H	-5.133298069	0.919400615	-3.454212269
C	-2.505529997	4.390289575	-2.318500976
H	-1.785187018	4.900319454	-1.870814887
H	-3.369178407	4.685097897	-1.934773221
C	-2.489120993	4.713201185	-3.808250880
H	-2.615105475	5.675733311	-3.936176424
H	-1.628938204	4.441575263	-4.191871016
H	-3.213414085	4.226301565	-4.255856693
C	2.884008129	4.296064191	-2.554356479
H	3.771319129	4.586112475	-2.227093764
H	2.198390651	4.837692896	-2.087153445
C	2.794048951	4.571595568	-4.048922280
H	2.932276428	5.527733631	-4.214717738
H	3.483358567	4.056313643	-4.518492727
H	1.909193775	4.308081169	-4.378446634
C	5.101988813	2.087947647	-2.120151749
H	5.557661676	1.504180947	-1.464173684
H	5.339918042	3.025006994	-1.906608592
C	5.614602428	1.755748737	-3.517059344
H	6.585868929	1.885740102	-3.547295026
H	5.403742791	0.822453171	-3.728955165
H	5.185782894	2.344756443	-4.171827514

N	-1.424657000	-1.340623000	2.525841000
N	1.379313000	-1.439398000	2.552204000
N	1.453998000	1.242321000	1.842871000
N	-1.347768000	1.352678000	1.864437000
C	-2.762393000	-1.221963000	2.208899000
C	-3.456274000	-2.450480000	2.566598000
C	-2.581367000	-3.235495000	3.181099000
C	-1.297336000	-2.586537000	3.099552000
C	-0.095460000	-3.151105000	3.460475000
H	-0.132960000	-3.967986000	3.945561000
C	1.160614000	-2.644750000	3.186236000
C	2.410292000	-3.357073000	3.303928000
C	3.365424000	-2.629535000	2.691984000
C	2.734190000	-1.394488000	2.245273000
C	3.372866000	-0.290714000	1.730621000
C	2.799790000	0.976446000	1.701850000
C	3.529278000	2.229633000	1.604095000
C	2.612722000	3.237896000	1.677345000
C	1.316926000	2.614267000	1.792281000
C	0.111267000	3.298883000	1.799552000
H	0.146188000	4.246927000	1.766959000
C	-1.147592000	2.705511000	1.847679000
C	-2.390313000	3.398459000	1.834647000
C	-3.355059000	2.465919000	1.768558000
C	-2.711691000	1.199506000	1.768045000
C	-3.327448000	-0.034394000	1.739004000
C	-4.884630000	-2.830817000	1.984187000
H	-5.018817000	-2.473988000	1.071318000
H	-5.034591000	-3.809616000	1.984238000
C	-5.733317000	-2.149651000	2.966737000
H	-6.675917000	-2.293058000	2.741034000
H	-5.553346000	-2.510247000	3.860716000
H	-5.537730000	-1.189120000	2.957719000
C	-2.721447000	-4.706943000	3.600361000

H	-3.520099000	-5.122962000	3.190592000
H	-1.917829000	-5.229282000	3.352231000
C	-2.863469000	-4.601347000	5.088060000
H	-2.962208000	-5.497710000	5.471493000
H	-2.067418000	-4.170932000	5.463651000
H	-3.656190000	-4.065511000	5.303382000
C	2.570747000	-4.682651000	4.043125000
H	1.779053000	-5.249319000	3.867603000
H	3.366289000	-5.155480000	3.689860000
C	2.724895000	-4.506648000	5.513584000
H	2.825337000	-5.382981000	5.939441000
H	3.520599000	-3.962337000	5.695687000
H	1.932958000	-4.056209000	5.873474000
C	4.841818000	-2.949733000	2.568030000
H	4.969861000	-3.929158000	2.632460000
H	5.165703000	-2.657962000	1.678623000
C	5.654933000	-2.269106000	3.642018000
H	6.600466000	-2.497282000	3.531427000
H	5.542481000	-1.297227000	3.570238000
H	5.346754000	-2.567653000	4.523522000
C	5.006284000	2.380897000	1.651679000
H	5.253297000	3.261099000	1.271278000
H	5.420408000	1.680922000	1.085608000
C	5.571469000	2.273777000	3.068112000
H	6.543910000	2.379819000	3.040944000
H	5.180125000	2.976693000	3.628132000
H	5.347282000	1.395994000	3.442398000
C	2.858619000	4.709762000	1.690951000
H	2.157958000	5.159760000	1.156139000
H	3.732116000	4.895347000	1.263626000
C	2.860847000	5.295878000	3.098203000
H	3.026328000	6.259787000	3.051296000
H	1.991754000	5.132917000	3.521264000
H	3.566394000	4.868439000	3.628789000

C	-2.529388000	4.878699000	1.920026000
H	-3.405375000	5.140950000	1.542639000
H	-1.824047000	5.299085000	1.365516000
C	-2.422788000	5.414792000	3.340934000
H	-2.521419000	6.389973000	3.331453000
H	-3.130739000	5.020877000	3.893017000
H	-1.548169000	5.179126000	3.715761000
C	-4.836891000	2.720518000	1.882080000
H	-5.318335000	2.047253000	1.340183000
H	-5.037313000	3.612739000	1.502522000
C	-5.357427000	2.666235000	3.314062000
H	-6.322488000	2.838921000	3.316828000
H	-5.183903000	1.778517000	3.691223000
H	-4.902605000	3.345525000	3.853727000
C	-4.484189000	-0.189737000	0.484718000
H	-5.369840000	-0.281152000	0.814205000
C	-4.430184000	-0.214579000	-0.857648000
H	-5.262753000	-0.255662000	-1.310578000
Fe	0.005747000	-0.141149000	1.849514000
H	4.371260000	-0.335061000	1.695367000
H	4.481866804	-0.535771772	-1.458727268

P4

Fe	-0.069897000	-0.274426000	1.829607000
O	0.165082000	0.370284000	0.174909000
N	1.076548000	1.126174000	2.726992000
N	-1.724026000	0.789048000	2.246190000
N	-1.274842000	-1.871911000	1.594440000
N	1.518778000	-1.508762000	1.868642000
C	2.444325000	1.192944000	2.649695000
C	2.919277000	2.463114000	3.171182000
C	1.804685000	3.159448000	3.573505000
C	0.661415000	2.322123000	3.245758000
C	-0.663199000	2.740407000	3.306848000
H	-0.851678000	3.737316000	3.703105000

C	-1.750923000	2.053187000	2.775958000
C	-3.061666000	2.644784000	2.599938000
C	-3.810046000	1.741645000	1.882725000
C	-2.965316000	0.566089000	1.686970000
C	-3.370990000	-0.659866000	1.136462000
C	-2.620286000	-1.841556000	1.325640000
C	-3.144534000	-3.200259000	1.249444000
C	-2.066146000	-4.040799000	1.403696000
C	-0.904200000	-3.197344000	1.570616000
C	0.403728000	-3.663323000	1.572975000
H	0.552816000	-4.734975000	1.446104000
C	1.535777000	-2.861716000	1.645500000
C	2.895826000	-3.330714000	1.467700000
C	3.703093000	-2.220510000	1.555532000
C	2.827611000	-1.099581000	1.841564000
C	3.264352000	0.181121000	2.165259000
C	4.361985000	2.858762000	3.290004000
H	4.901724000	2.567437000	2.372568000
H	4.435513000	3.957036000	3.344097000
C	5.061694000	2.241956000	4.512850000
H	6.117992000	2.551740000	4.567168000
H	4.564426000	2.552592000	5.445444000
H	5.028630000	1.141589000	4.473329000
C	1.731149000	4.501025000	4.241321000
H	2.673636000	5.045852000	4.070788000
H	0.942428000	5.110773000	3.767583000
C	1.462378000	4.408297000	5.752631000
H	1.408701000	5.409137000	6.210991000
H	0.512268000	3.888087000	5.952991000
H	2.260619000	3.841569000	6.257912000
C	-3.484665000	3.977306000	3.147147000
H	-2.700088000	4.726678000	2.945903000
H	-4.377481000	4.329116000	2.606731000
C	-3.782732000	3.946973000	4.655615000

H	-4.081894000	4.941999000	5.023051000
H	-4.596738000	3.239828000	4.880501000
H	-2.898867000	3.622303000	5.227147000
C	-5.260930000	1.895445000	1.528117000
H	-5.499463000	2.969194000	1.465179000
H	-5.449415000	1.490263000	0.527132000
C	-6.203583000	1.231966000	2.545192000
H	-7.257977000	1.340637000	2.242959000
H	-5.986951000	0.157219000	2.648945000
H	-6.084762000	1.683553000	3.542633000
C	-4.589113000	-3.619537000	1.247470000
H	-4.645235000	-4.702886000	1.057362000
H	-5.140786000	-3.145564000	0.425713000
C	-5.294970000	-3.302152000	2.575671000
H	-6.347342000	-3.629199000	2.555859000
H	-4.793941000	-3.805337000	3.417724000
H	-5.275745000	-2.220714000	2.784094000
C	-2.049016000	-5.540642000	1.447079000
H	-1.198658000	-5.914258000	0.851515000
H	-2.950073000	-5.932492000	0.949067000
C	-1.962273000	-6.107539000	2.873104000
H	-1.942266000	-7.209482000	2.865819000
H	-1.053282000	-5.750342000	3.382480000
H	-2.826089000	-5.784143000	3.475495000
C	3.299033000	-4.764212000	1.282460000
H	4.293949000	-4.804554000	0.811561000
H	2.611087000	-5.256204000	0.573662000
C	3.325282000	-5.560374000	2.598026000
H	3.618400000	-6.608636000	2.424926000
H	4.040130000	-5.117184000	3.309087000
H	2.336023000	-5.556343000	3.082362000
C	5.198064000	-2.147004000	1.462011000
H	5.486432000	-1.219820000	0.941339000
H	5.560054000	-2.969067000	0.823201000

C	5.902319000	-2.212303000	2.827164000
H	6.996960000	-2.149125000	2.715253000
H	5.576675000	-1.386360000	3.479316000
H	5.665105000	-3.153807000	3.347180000
N	-1.506432000	1.482884000	-2.080443000
N	1.345169000	2.189639000	-2.039462000
N	2.039313000	-0.606877000	-2.000994000
N	-0.816246000	-1.300243000	-2.055153000
C	-2.779227000	0.986266000	-1.968494000
C	-3.743050000	2.084517000	-2.103057000
C	-3.002323000	3.234544000	-2.257917000
C	-1.605595000	2.842281000	-2.213984000
C	-0.537963000	3.742619000	-2.245262000
H	-0.800101000	4.797749000	-2.324874000
C	0.823940000	3.448568000	-2.157110000
C	1.893362000	4.436717000	-2.158652000
C	3.070075000	3.735075000	-2.028791000
C	2.705378000	2.327185000	-1.965928000
C	3.613814000	1.268607000	-1.886630000
C	3.306227000	-0.092377000	-1.937801000
C	4.284435000	-1.170560000	-1.962127000
C	3.569078000	-2.342961000	-2.043298000
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C	1.091191000	-2.860604000	-2.111475000
H	1.347380000	-3.919939000	-2.129268000
C	-0.272212000	-2.555612000	-2.116687000
C	-1.328911000	-3.551533000	-2.131211000
C	-2.518461000	-2.868089000	-2.041233000
C	-2.176322000	-1.445834000	-1.949553000
C	-3.089389000	-0.380960000	-1.761678000
C	-5.234832000	1.990768000	-2.275707000
H	-5.692821000	1.401450000	-1.470308000
H	-5.667594000	2.999687000	-2.186320000
C	-5.637593000	1.394692000	-3.634803000

H	-6.733548000	1.331678000	-3.735139000
H	-5.251735000	2.011622000	-4.461554000
H	-5.222349000	0.382986000	-3.765782000
C	-3.492869000	4.630391000	-2.514324000
H	-4.524020000	4.735380000	-2.140848000
H	-2.891545000	5.346013000	-1.927982000
C	-3.445749000	5.025558000	-3.999665000
H	-3.801455000	6.057769000	-4.151182000
H	-2.419151000	4.954575000	-4.392551000
H	-4.076113000	4.353524000	-4.603424000
C	1.707108000	5.915491000	-2.336556000
H	0.851531000	6.258896000	-1.729806000
H	2.588253000	6.445907000	-1.939883000
C	1.486123000	6.325444000	-3.802528000
H	1.346919000	7.414799000	-3.896853000
H	2.347729000	6.034364000	-4.424086000
H	0.596710000	5.828402000	-4.221136000
C	4.474375000	4.265594000	-2.027875000
H	4.467883000	5.317687000	-1.698791000
H	5.076342000	3.721220000	-1.279825000
C	5.161242000	4.168622000	-3.400786000
H	6.190745000	4.560579000	-3.361991000
H	5.204615000	3.123931000	-3.747336000
H	4.603906000	4.742536000	-4.157970000
C	5.774067000	-0.986999000	-1.978532000
H	6.260314000	-1.907521000	-1.616784000
H	6.059819000	-0.196845000	-1.262718000
C	6.326950000	-0.631180000	-3.368862000
H	7.420830000	-0.497957000	-3.342666000
H	6.095099000	-1.424699000	-4.096584000
H	5.876375000	0.300935000	-3.744799000
C	4.091223000	-3.743514000	-2.166518000
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C	4.131057000	-4.250084000	-3.617827000
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H	4.781736000	-3.613961000	-4.238358000
C	-1.115310000	-5.030454000	-2.270731000
H	-1.993750000	-5.566394000	-1.877304000
H	-0.271285000	-5.337824000	-1.629242000
C	-0.846299000	-5.477564000	-3.716541000
H	-0.683161000	-6.566078000	-3.776685000
H	-1.696479000	-5.221778000	-4.368644000
H	0.044012000	-4.973475000	-4.124675000
C	-3.885245000	-3.463140000	-2.222557000
H	-4.577721000	-3.088440000	-1.460627000
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C	-4.470080000	-3.177942000	-3.615619000
H	-5.471747000	-3.624559000	-3.727208000
H	-4.557037000	-2.093882000	-3.791537000
H	-3.821389000	-3.585337000	-4.407141000
C	-4.412554000	-0.679792000	-1.119232000
H	-5.306746000	-0.800630000	-1.739933000
C	-4.550789000	-0.752317000	0.217177000
H	-5.551837000	-0.914965000	0.630432000
Fe	0.256311000	0.442121000	-1.569737000
H	4.669996000	1.531505000	-1.824176000
H	4.333806000	0.379064000	2.108676000