

Supporting information

H₂O₂ Oxidation by Fe^{III}-OOH Intermediates and its Impact on Catalytic Efficiency

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Contents

1. Simulation of the EPR spectra.....	3
2. Colorimetric quantification of formaldehyde.....	3
3. Quantification of O ₂ by head space Raman spectroscopy.....	4
4. Raman spectroscopy for the second-order-rate constant determination of disproportionation reaction.....	7
5. Additional spectroscopic and electrochemical data.....	9
6. Supplementary data for DFT calculations.....	19
6.1 Absolute energies for all the structures.....	20
6.2 Optimized geometries for all the structures.....	22
References.....	34

1. Simulation of the EPR spectra

Simulation of the EPR spectra was performed using the EasySpin package (version 5.1., option pepper) based on the exact numerical solution of the spin Hamiltonian of the singlet spin state for singlet molecules oriented randomly in the solid phase.¹ The initial parameters for calculating the EPR spectrum of $[(\text{N4Py})\text{Fe}^{\text{III}}(\text{OOH})]^{2+}$ were $S = \frac{1}{2}$, $g = [2.1620, 2.1095, 1.983]$, line width $\Delta H = 0.85$ mT, of $[(\text{N4Py})\text{Fe}^{\text{III}}(\text{OCH}_3)]^{2+}$ were $S = \frac{1}{2}$, $g = [2.2929, 2.1246, 1.9638]$, $\Delta H = 1.3$ mT, and of $[(\text{N4Py})\text{Fe}^{\text{III}}(\text{OOX})]^{2+}$ were $S = \frac{1}{2}$, $g = [2.17903, 2.1288, 1.98]$, line width $\Delta H = 1.0$ mT. The temperature was 77 K, and the frequency $\nu_0 = 9.462846$ GHz.

2. Colorimetric quantification of formaldehyde

The formation of formaldehyde was quantified as described in literature.² The colorimetric reagent was prepared by dissolving NH_4OAc (15 g, 0.19 mol), acetic acid (0.3 mL, 5.4 mol) and pentane-2,4-dione (0.2 mL, 1.9 mol) in 100 mL water. Take 1 mL reaction solution, diluted 10 times (1 mL solution dissolved in 9 mL water, concentration of formaldehyde should not exceed 8 μg of formaldehyde per mL), then mixed with the other 10 mL of colorimetric reagent. The mixture was put into a 31 °C water bath. Every 2 min, 1 mL mixture was transferred to the cuvette and check the UV-vis absorbance at 420 nm, after around 35 min, the absorbance will reach to its maximum and stable for ca. 10 min. This maximum absorbance was used to calculate the concentration of formaldehyde using equation (1).

$$C = \frac{A_{420\text{nm}}}{L \times \epsilon_{420\text{nm}}} \times 20 \quad (1)$$

Where C is the concentration of formaldehyde in the reaction, $A_{420\text{nm}}$ is the maximum absorbance of the mixture at 420 nm, L is the pathlength of the cuvette, $\epsilon_{420\text{nm}}$ is the molar absorptivity of diacetyldihydro-lutidine (DDL), which was determined by calibration curve with solutions containing known amounts of formaldehyde.

3. Quantification of O₂ by head space Raman spectroscopy

The formation of oxygen was quantified by head space Raman spectroscopy as follows:

4 mL volume cuvette was used with 2 mL of the reaction mixture and hence the headspace volume was 2 mL. Under standard conditions and taking the mole fractions of oxygen and nitrogen in the atmosphere as ca. 0.21 and 0.78. The number of O₂ and N₂ molecules is

$$n_{O_2} = \frac{2 \times 10^{-3} L \times 21\%}{22.4 L} \times N_A = 0.1129 \times 10^{20}$$

$$n_{N_2} = \frac{2 \times 10^{-3} L \times 78\%}{22.4 L} \times N_A = 0.419 \times 10^{20}$$

Before addition of H₂O₂, the ratio of Raman intensity of O₂ (1553 cm⁻¹) and N₂ (2239 cm⁻¹) stretching modes is 3700/9095.

After addition of H₂O₂, O₂ is released continuously from the reaction mixture, manifested in an increase in relative intensity of the band at 1553 cm⁻¹ with respect to the band at 2239 cm⁻¹. The Raman scattering intensity changed from 3600 to ca. 13600 (with no change in the intensity of the N₂ band) and remained constant thereafter.

Hence the number of molecules of O₂ in the headspace after the reaction is

$$n'_{O_2} = 0.1129 \times 10^{20} \times \frac{13600}{3700} = 0.4041 \times 10^{20}$$

Which is an increase of

$$\Delta n_{O_2} = 0.4041 \times 10^{20} - 0.1129 \times 10^{20} = 0.2912 \times 10^{20}$$

Considering the solubility of O₂ in methanol changes with the increase partial pressure of O₂, the partial pressure is proportional to the molar fraction, so the final partial pressure of O₂ is

$$\frac{0.4041 \times 10^{20}}{0.419 \times 10^{20} + 0.4041 \times 10^{20}} = 0.491$$

Using Henry's law, the solubility of O₂ is proportional to the partial pressure of O₂, and at 20 °C, and the molar fraction solubility of O₂ in methanol is ^{3,4}

$$x_1 = \frac{n_{O_2}}{n_{O_2} + n_{CH_3OH}} = 4.15 \times 10^{-4}$$

([dx.doi.org/10.1021/jie502386t](https://doi.org/10.1021/jie502386t); J. Phys. Chem. Ref. Data, Vol. 12, No. 2, 1983)

$$C_{[mL/L]} = \frac{x_1 \times 4.689 \times 10^{20}}{V_T^\circ}$$

x_1 , molar fraction

V_T° , molar volume of a pure solvent at room temperature T, at room temperature, for methanol,

$$V_T^\circ = 40.7403 \text{ cm}^3/\text{mol}$$

$C_{[mL/L]}$, number of mL of gas at STP from air dissolved in 1 L of solvent

therefore,

$$C = 47.76 \text{ mL/L}, \text{ and then } C = 0.04776 \text{ mL/mL},$$

And at the end of the reaction, due to the increase in the mole fraction of O₂, from 0.21 to 0.491, solubility increased to

$$C = 0.04776 \text{ mL/mL} \times \frac{0.491}{0.21} = 0.116 \text{ mL/mL}$$

the dissolved O₂ in methanol is

$$x = \frac{(0.116 - 0.04776) \times 2 \times 10^{-3} \text{ L}}{22.4 \text{ L}} \times N_A = 0.0367 \times 10^{20}$$

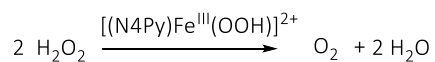
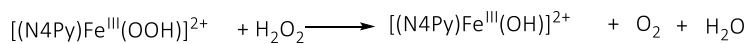
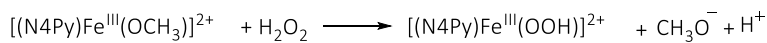
Together with the consideration of solubility changes, the actually released number of O₂ molecules is

$$0.2912 \times 10^{20} + 0.0367 \times 10^{20} = 0.3279 \times 10^{20}$$

And hence corresponds to 28% of the H₂O₂ undergoing disproportionation.

Since the concentration of H₂O₂ was 200 mM, if all H₂O₂ is consumed by disproportionation will generate

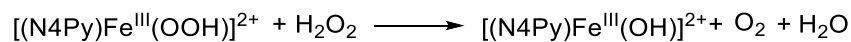
$$n = 100 \times 10^{-3} \frac{\text{mole}}{\text{L}} \times 2 \times 10^{-3} \text{ L} \times N_A = 1.205 \times 10^{20}$$



So the efficiency was calculated as

$$\frac{0.3279 \times 10^{20}}{1.205 \times 10^{20}} = 27.21\%$$

4. Raman spectroscopy for the second-order-rate constant determination of disproportionation reaction.



This reaction rate was determined by Raman spectroscopy. H_2O_2 (200 mM) was added to **1** (0.125 to 1.0 mM) in methanol at 21 °C, at first 1000 to 7000 s (depended on the concentration of **1**), the concentration of Fe^{III} -OOH is almost constant, and decay of H_2O_2 was monitored by Raman spectroscopy.

$$-\frac{d[H_2O_2]}{dt} = k[Fe^{III}(OOH)][H_2O_2]$$

in which, $[Fe^{III}$ -OOH] is almost constant during the decay region of H_2O_2 , note the detection limitation of H_2O_2 is around 25 - 50 mM, even at the end of the decay from Raman spectra, the concentration of H_2O_2 remains above 25 mM, which is far more than the concentration of Fe^{III} -OOH, so the pseudo-first-order condition is satisfied during the measurement time region.

so

$$-\frac{d[H_2O_2]}{dt} = \{k[Fe^{III}(OOH)]\}[H_2O_2]$$

$$-\frac{d[H_2O_2]}{dt} = k_{obs}[H_2O_2]$$

rearrangement

$$-\frac{d[H_2O_2]}{[H_2O_2]} = k_{obs}dt$$

integrate

$$-\frac{d[H_2O_2]}{[H_2O_2]} = k_{obs}dt$$

$$-\int_{[H_2O_2]_0}^{[H_2O_2]_t} \frac{d[H_2O_2]}{[H_2O_2]} = \int_0^t k_{obs}dt$$

$$-\ln \frac{[H_2O_2]_t}{[H_2O_2]_0} = k_{obs} dt$$

so

$$[H_2O_2]_t = [H_2O_2]_0 e^{-k_{obs} dt}$$

since,

$$k_{obs} = k [Fe^{III}(OOH)]$$

The second order rate constant can be obtained by the linear plot of k_{obs} with concentration of Fe^{III} -OOH.

5. Additional spectroscopic and electrochemical data

Dissolution of **1** in methanol results in large changes to spectroscopic properties, consistent with substitution of the CH₃CN ligand for methanol or methoxide. As in water, the acidity of the bound methanol is expected to be such that a mixture of methoxido and methanol bound complexes are formed, however, for simplicity, only the Fe(II)-OMe complex is referred to in the text as complex **2**.

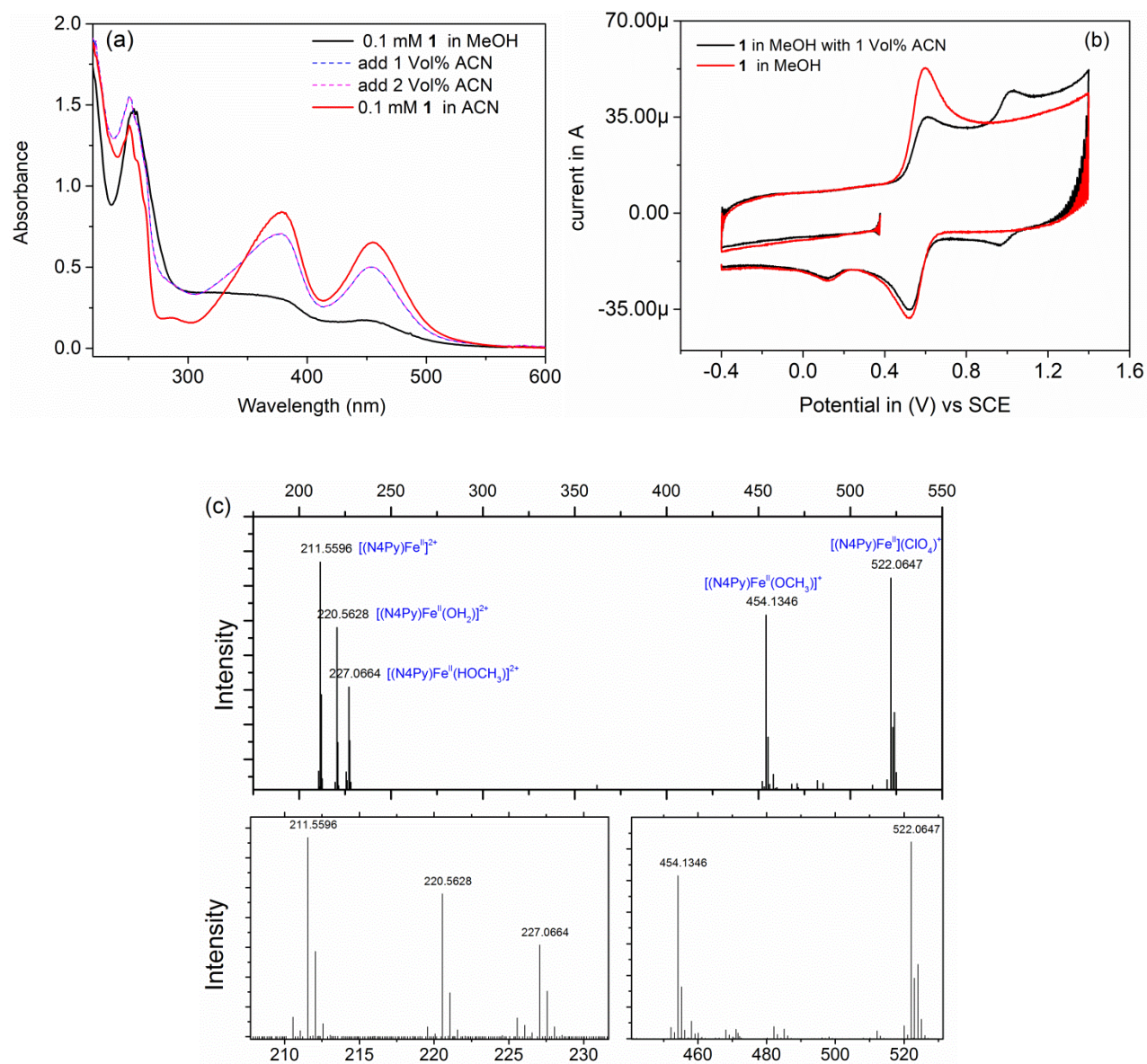


Figure S 1. (a) UV-vis absorption spectrum of **1** (0.1 mM) in methanol and in acetonitrile and after addition of acetonitrile to a solution of **1** in methanol (dash lines); (b) Cyclic voltammetry of **1** (1 mM) in methanol (0.1 M TBAOTf, tetrabutylammonium triflate) (red line) and after addition of 1 vol % acetonitrile (black line). Scan rate 100 mV/s. (c) ESI-Mass spectrum of complex **1** in methanol.

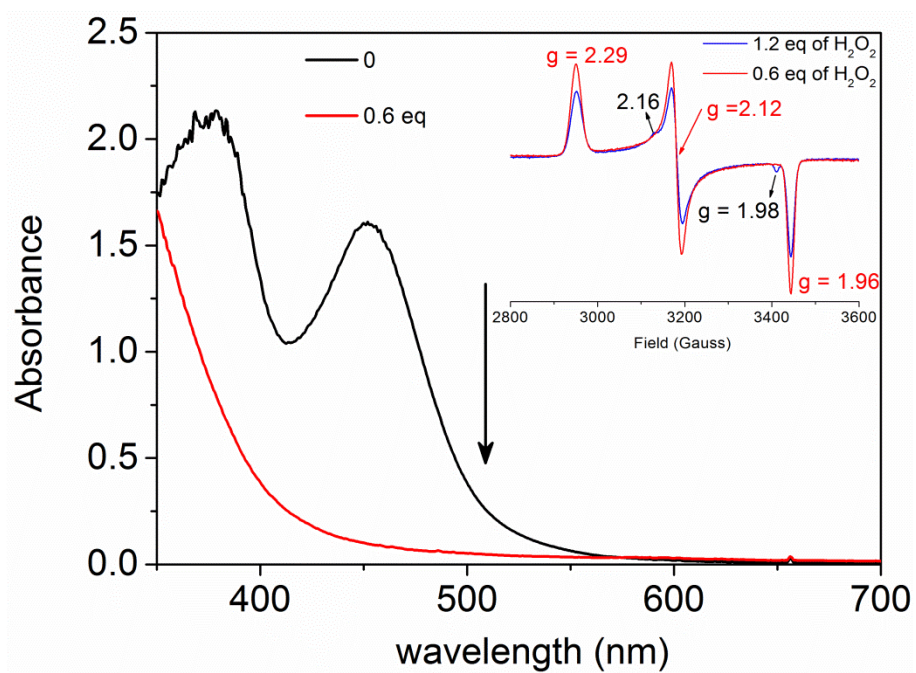


Figure S 2. UV-vis absorption spectrum of **1** (1 mM) in methanol (black) after addition of 0.6 equiv. H₂O₂ (red); Inset shows the X-band EPR spectra for the flash frozen sample of corresponding reaction solution at 77 K.

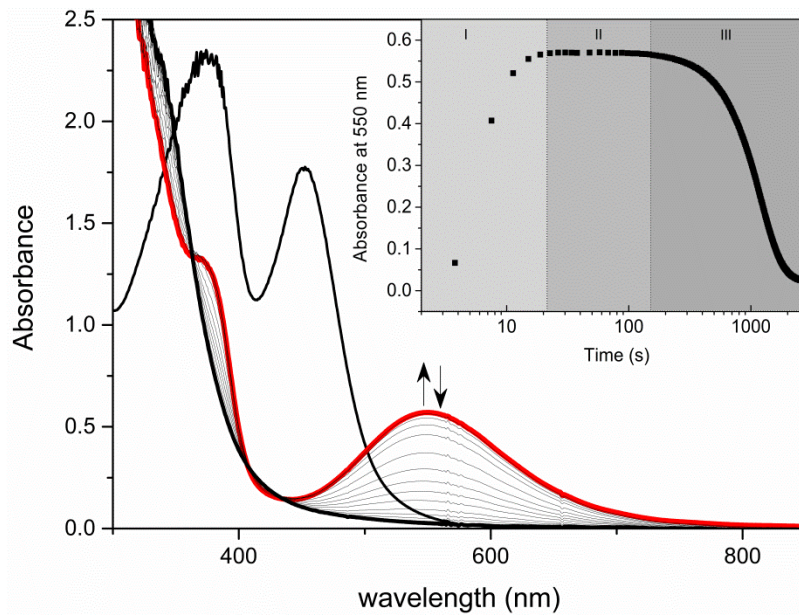


Figure S 3. UV-vis absorption spectrum of **1** (0.5 mM) upon addition of 50 equiv. H₂O₂. Inset is the corresponding absorbance at 550 nm over time.

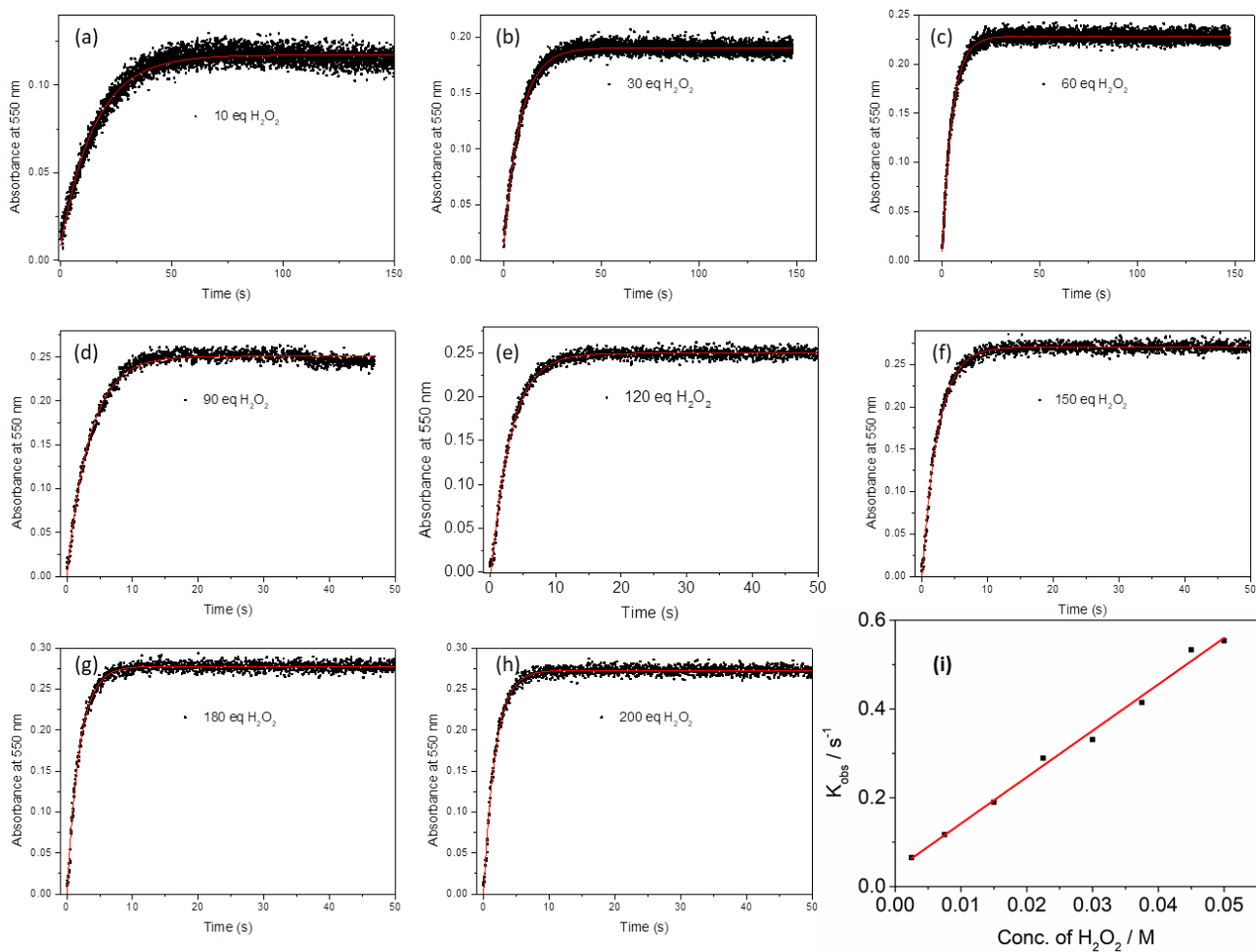


Figure S 4. (a) Absorbance at 550 nm over time after addition of H₂O₂ (2.5 mM to 50 mM) to **1** (0.25 mM) in methanol. (a) 2.5 mM; (b) 7.5 mM; (c) 15 mM; (d) 22.5 mM; (e) 30 mM; (f) 37.5 mM; (g) 45 mM; (h) 50 mM; and (i) k_{obs} vs [H₂O₂].

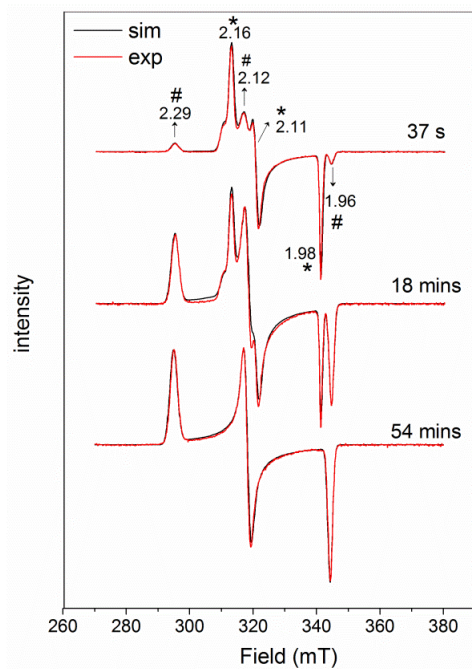


Figure S 5. X-band EPR spectra (recorded at 77 K) of the reaction mixture of **1** (1 mM) with 50 equiv. H₂O₂ in methanol. (top) EPR spectrum 37 s after addition of H₂O₂, (middle) 18 min after addition, (bottom) after complete decay of Fe^{III}-OOH (54 min). Experimental data is shown as red lines and simulations as black lines. Microwave Frequency 9.46 GHz, Power 63.5 mW.

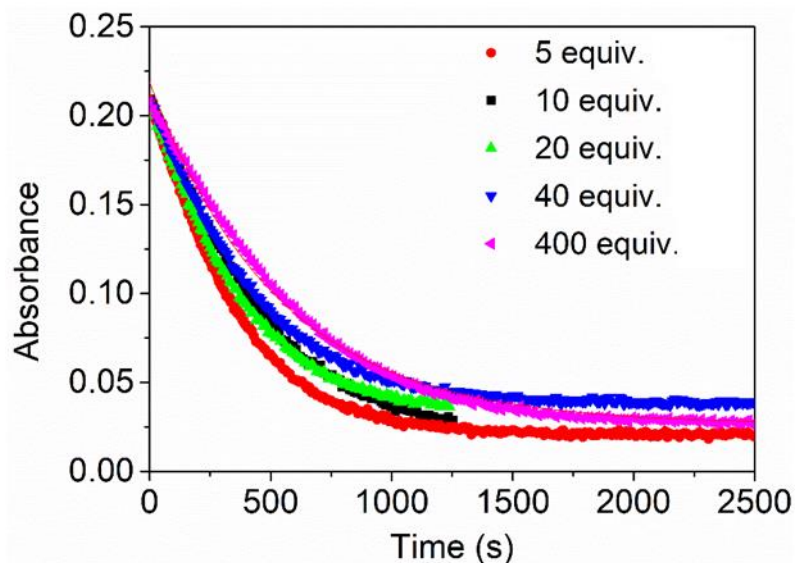


Figure S 6. The decay of $[(\text{N4Py})\text{Fe}^{\text{III}}(\text{OOH})]^{2+}$ after the absorbance at 550 nm decrease to 0.2, of the reaction of **1** (0.56 mM) with H_2O_2 (2.5 to 50 mM, see legend) in methanol at 21 °C.

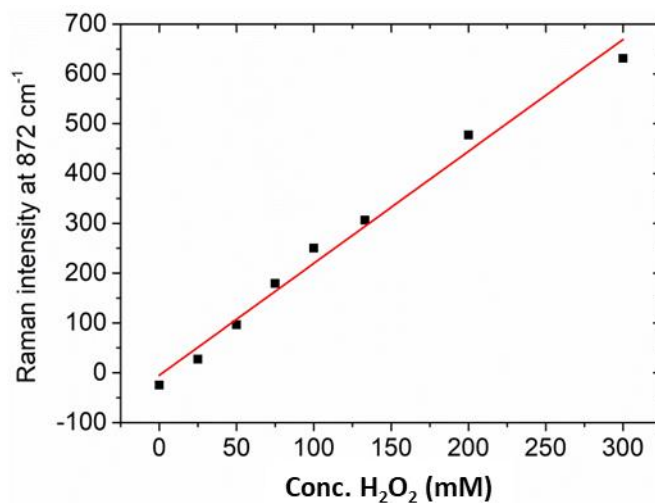


Figure S 7. Calibration curve for Raman intensity at 872 cm^{-1} ($\lambda_{\text{exc}} 785\text{ nm}$, at 21 °C) with respect to concentration of H_2O_2 . Commercially available H_2O_2 (50 wt% in water, verified by iodometric titration) was diluted in methanol as appropriate. Raman intensity is relative to solvent (methanol) bands and stability of the solutions verified by continuous monitoring over > 30 min.

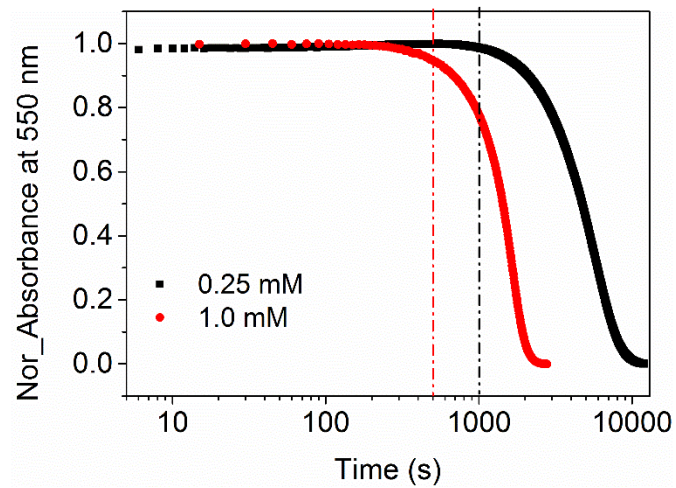


Figure S 8. Normalized UV-vis absorbance at 550 nm of reaction of **1** (1 mM in red, 0.25 mM in black) with H₂O₂ (200 mM) at 21 °C.

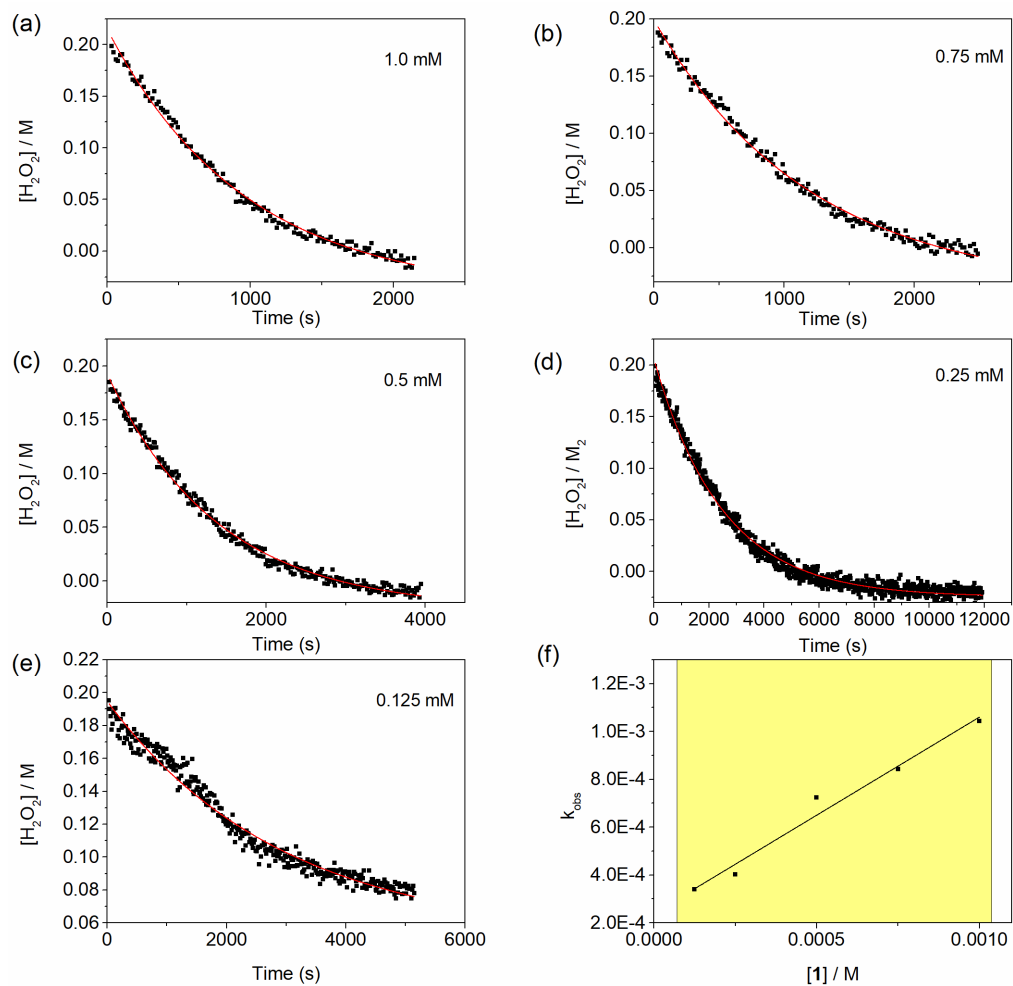


Figure S 9. (a-e) Decrease in the concentration of H₂O₂ in methanol with time following addition of H₂O₂ (200 mM) to **1** (0.25 mM) at 21 °C, (see Figure S10 for calibration curve). (f) Plot of the pseudo-first-order rate k_{obs} versus concentration of **1** in M.

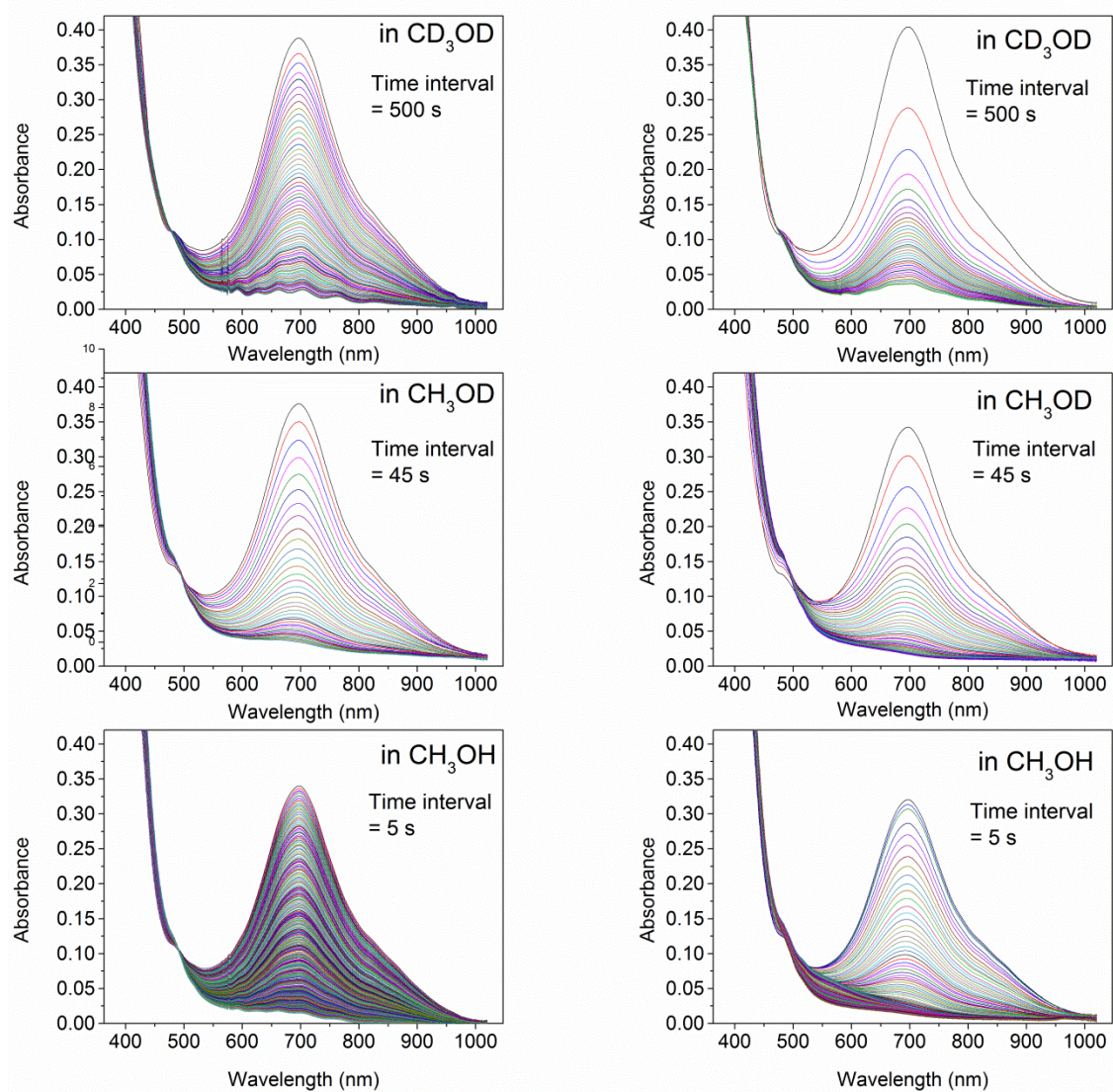


Figure S 10. (Left) UV-vis absorption spectra of **4** (1 mM) in CH₃OH, CH₃OD, and CD₃OD. (Right) UV-vis absorption spectra of **4** (1 mM) after addition of 1 equiv. H₂O₂ in CH₃OH, CH₃OD, and CD₃OD.

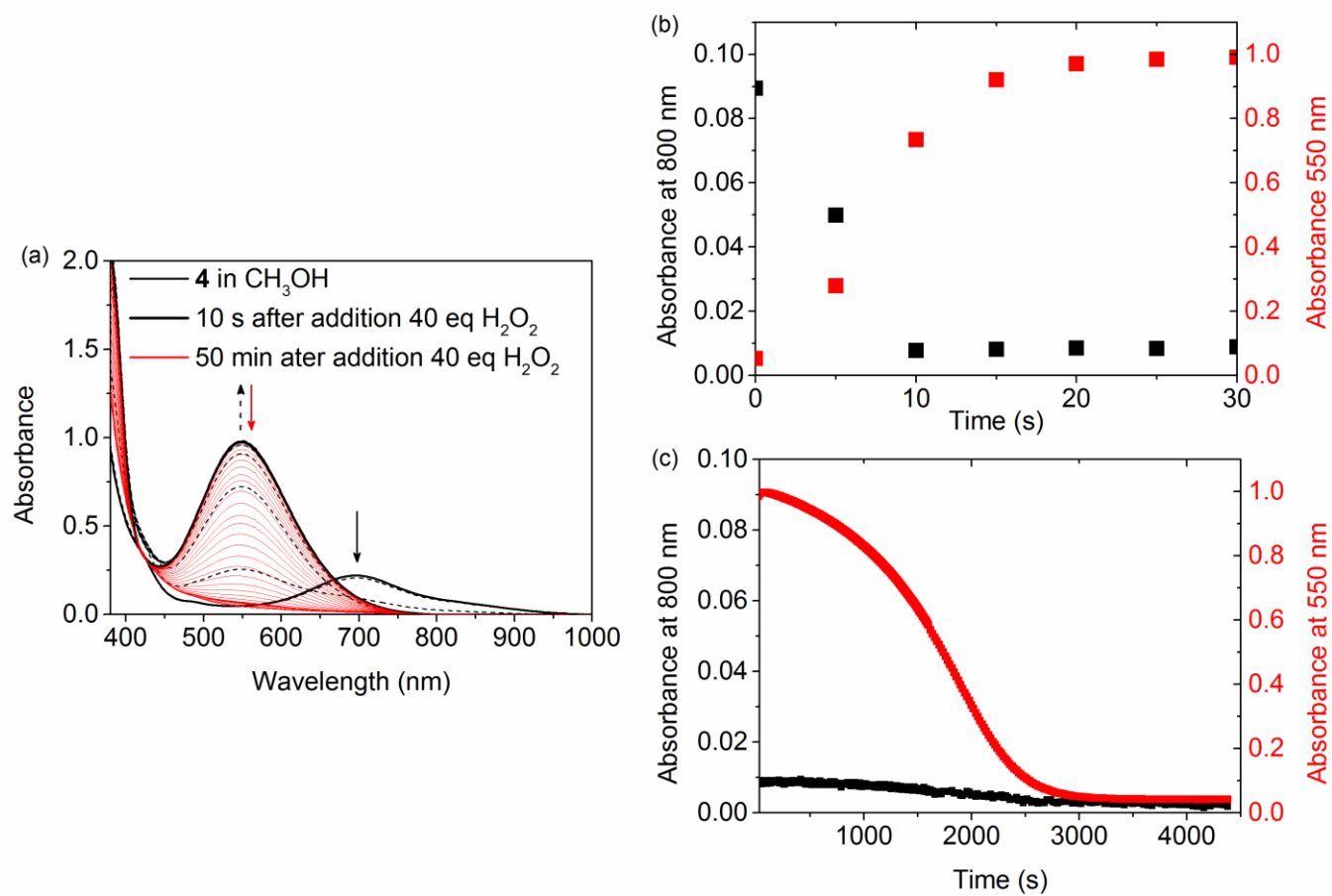


Figure S 11. (a) UV-vis absorption spectrum of **4** (0.5 mM) after addition of 40 equiv. H_2O_2 in CH_3OH . The change in absorbance at 550 nm (black) and 800 nm (red) between 0 ~150 s (b) and the change after 150 s (c) are shown separately.

6. Supplementary data for DFT calculations

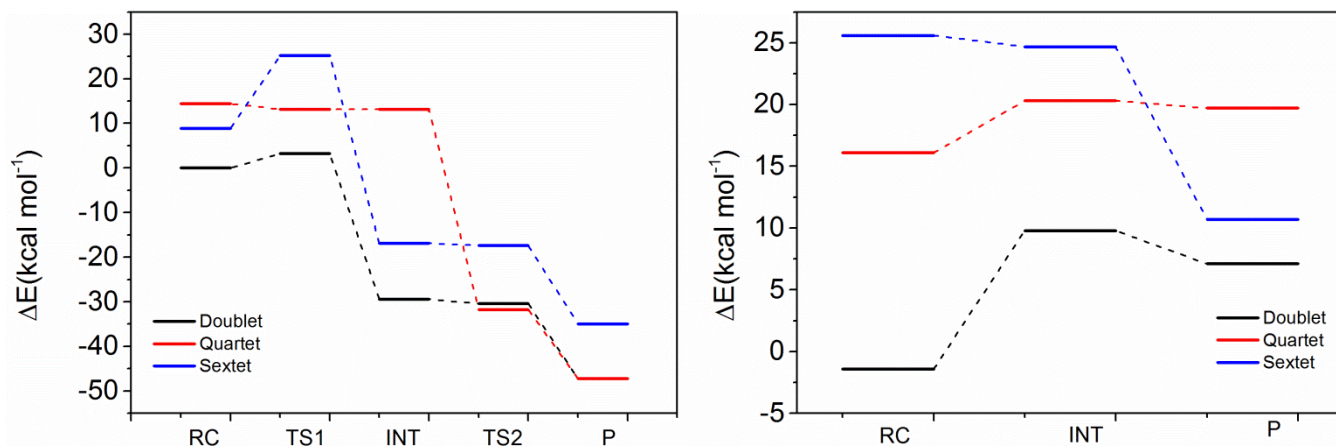


Figure S 12. Comparison of energy profiles (in kcal mol⁻¹) of pathway a (left) and pathway b (right) in different spin states: doublet (black), quartet (red) and sextet (blue), as obtained at the S12g/TZ2P//BP86-D₃/TDZP level.

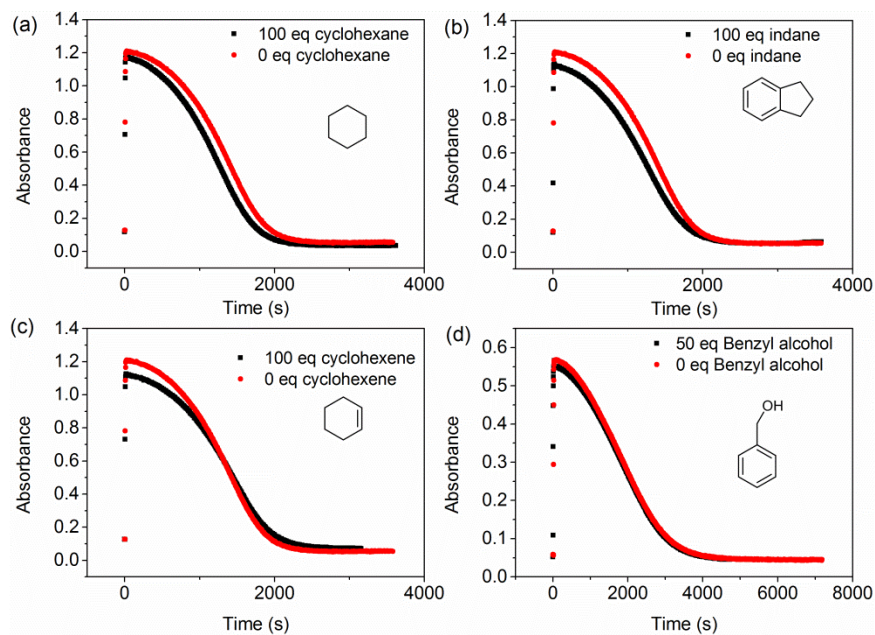


Figure S 13. Time-dependence of absorbance at 550 nm in the reaction of **1** (1 mM) with 50 equiv. H₂O₂ in methanol (red traces) at 21 °C: and (black traces) (a) with 100 equiv. cyclohexane added prior to H₂O₂, (b) with 100 equiv. indane added prior to H₂O₂, (c) with 100 equiv. cyclohexene added prior to H₂O₂, and (d) with 50 equiv. benzyl alcohol added immediately after maximum absorbance at 550 nm was reached.

If there is a reaction between Fe^{III}-OOH with substrates, the rate of decay is expected to be influenced (increased rate), however, as shown here, the rate of decay of the Fe^{III}-OOH is insensitive to the addition of a range of substrates. We note in Figure S 13, that benzyl alcohol has no effect while it reacts rapidly with the Fe(IV)=O complex.⁵ Hence we confirm that the direct reaction between Fe^{III}-OOH and other substrates does not take place.

6.1 Absolute energies for all the structures.

Table S 1. Absolute S12g/TZ2P//BP86-D₃/TDZP level energies (kcal mol⁻¹) of optimized geometry for pathway a (catalase) in ADF.

	E_el_BP86-D3	G_el_BP86-D3	Free energy corrections	E_el_S12g	G_S12g	
² RC	-8169.24	-7928.98	240.26	-8374.53	-8134.27	0.0
⁴ RC	-8143.06	-7904.60	238.46	-8358.37	-8119.91	14.36
⁶ RC	-8136.42	-7899.73	236.69	-8362.09	-8125.40	8.87
² TS1	-8163.88	-7925.41	238.47	-8369.55	-8131.07	3.2
⁴ TS1	-8140.12	-7901.49	238.63	-8359.69	-8121.06	13.21
⁶ TS1	-8129.73	-7893.17	236.56	-8345.60	-8109.04	25.23
² INT	-8189.12	-7951.36	237.76	-8401.27	-8163.51	-29.4
⁴ INT	-8150.58	-7913.54	237.04	-8358.11	-8121.07	13.21
⁶ INT	-8165.03	-7930.27	234.76	-8385.94	-8151.18	-16.91
² TS2	-8187.69	-7952.25	235.44	-8400.12	-8164.68	-30.41
⁴ TS2	-8189.33	-7953.65	235.68	-8401.60	-8165.92	-31.65
⁶ TS2	-8127.60	-7892.99	234.61	-8386.26	-8151.65	-17.38
² P	-8203.20	-7965.73	237.47	-8418.88	-8181.41	-47.41
⁴ P	-8202.85	-7965.52	237.33	-8418.81	-8181.48	-47.21
⁶ P	-8178.64	-7943.76	234.88	-8404.08	-8169.20	-34.93

Table S 2. Absolute S12g/TZ2P//BP86-D₃/TDZP level energies (kcal mol⁻¹) of optimized geometry for pathway b (homolysis) in ADF.

	E_el_BP86-D3	G_el_BP86-D3	Free energy corrections	E_el_S12g	G_S12g	
² RC _{homo}	-8169.54	-7929.46	240.08	-8375.78	-8135.70	0.0
⁴ RC _{homo}	-8140.70	-7902.72	237.98	-8356.12	-8118.14	16.13
⁶ RC _{homo}	-8126.49	-7892.01	234.48	-8343.12	-8108.64	25.63
² TSI _{homo}	-8154.59	-7917.22	237.37	-8362.39	-8125.02	10.68
⁴ TSI _{homo}	-8138.63	-7901.29	237.34	-8351.28	-8113.94	20.33
⁶ TSI _{homo}	-8124.93	-7889.47	235.46	-8345.06	-8109.60	24.67
² P _{homo}	-8159.70	-7921.72	237.98	-8365.11	-8127.13	8.57
⁴ P _{homo}	-8144.34	-7904.96	239.38	-8358.15	-8118.77	19.70
⁶ P _{homo}	-8136.27	-7899.43	236.84	-8360.45	-8123.61	10.66

6.2 Optimized geometries for all the structures

Table S 3. XYZ coordinates of optimized geometries.

² RC				⁴ RC			
C	1.021800000	2.520500000	1.505600000	C	1.750500000	-2.190200000	-1.695000000
C	1.719600000	3.722300000	1.454800000	C	2.687200000	-3.215200000	-1.635200000
C	2.325100000	4.111500000	0.262600000	C	3.251000000	-3.549700000	-0.406600000
C	2.216900000	3.293000000	-0.863200000	C	2.863300000	-2.856200000	0.741900000
C	1.509100000	2.111400000	-0.742300000	C	1.921700000	-1.852200000	0.613300000
N	0.934700000	1.732500000	0.424100000	N	1.384200000	-1.523700000	-0.589400000
C	1.274700000	1.096300000	-1.832500000	C	1.419900000	-0.983500000	1.740200000
C	2.101800000	-0.117700000	-1.490200000	C	2.083100000	0.371400000	1.597100000
C	3.238500000	-0.542700000	-2.152300000	C	3.085100000	0.847800000	2.425100000
C	3.867100000	-1.703800000	-1.698200000	C	3.603300000	2.117200000	2.156100000
C	3.327500000	-2.398300000	-0.618300000	C	3.097700000	2.853000000	1.087300000
C	2.177900000	-1.918200000	0.000100000	C	2.086500000	2.303000000	0.302000000
N	1.598300000	-0.784500000	-0.423200000	N	1.603800000	1.079300000	0.554900000
N	-0.163400000	0.652000000	-1.649200000	N	-0.053400000	-0.775100000	1.473300000
C	-0.540700000	-0.516300000	-2.509600000	C	-0.676700000	0.262000000	2.360300000
C	-1.148200000	1.777500000	-1.748200000	C	-0.823900000	-2.063100000	1.518900000
C	-2.175600000	1.637700000	-0.668300000	C	-2.020900000	-1.939700000	0.623700000
C	-1.287800000	-1.533900000	-1.700600000	C	-1.611000000	1.131800000	1.576200000
C	-2.090400000	-2.501600000	-2.289100000	C	-2.677100000	1.784600000	2.178400000
C	-2.678700000	-3.475600000	-1.487300000	C	-3.466600000	2.643400000	1.417600000
C	-2.452200000	-3.448300000	-0.113700000	C	-3.167100000	2.823200000	0.069800000
C	-1.658100000	-2.443900000	0.421300000	C	-2.101700000	2.126000000	-0.481300000
N	-1.085100000	-1.507000000	-0.358700000	N	-1.336700000	1.294000000	0.252600000
N	-1.783900000	0.945000000	0.429700000	N	-1.761800000	-1.335200000	-0.556500000
C	-2.616300000	0.820500000	1.479600000	C	-2.747400000	-1.165800000	-1.451300000
C	-3.875100000	1.404800000	1.476300000	C	-4.042500000	-1.606000000	-1.199600000
C	-4.292100000	2.112200000	0.351500000	C	-4.316200000	-2.225700000	0.018200000
C	-3.430900000	2.224700000	-0.737300000	C	-3.289400000	-2.396200000	0.948700000
Fe	-0.063500000	0.035300000	0.265900000	Fe	-0.014600000	-0.071200000	-0.443200000
O	0.326800000	-0.287900000	1.925100000	O	0.250500000	0.272600000	-2.157800000
O	-0.648600000	-1.077500000	2.924400000	O	-0.763300000	1.102200000	-2.940700000
H	0.524300000	2.160800000	2.403600000	H	1.271700000	-1.881100000	-2.622800000
H	1.780000000	4.342500000	2.348000000	H	2.963700000	-3.742800000	-2.547100000
H	2.870100000	5.053600000	0.202600000	H	3.984900000	-4.352600000	-0.337200000
H	2.658300000	3.570500000	-1.819100000	H	3.275100000	-3.096800000	1.720700000
H	3.611100000	0.013500000	-3.011200000	H	3.441900000	0.250800000	3.263200000
H	4.763300000	-2.070800000	-2.198300000	H	4.389600000	2.530500000	2.788000000
H	3.786700000	-3.314900000	-0.250000000	H	3.474900000	3.849300000	0.859700000
H	1.708800000	-2.427200000	0.842600000	H	1.644900000	2.833400000	-0.542800000
H	-1.120300000	-0.180300000	-3.378100000	H	-1.186600000	-0.218900000	3.205000000
H	0.379800000	-0.984900000	-2.887900000	H	0.119400000	0.898200000	2.773700000
H	-0.612500000	2.725900000	-1.595300000	H	-0.177200000	-2.863400000	1.131800000
H	-1.598800000	1.807900000	-2.747800000	H	-1.089800000	-2.307800000	2.555500000
H	-2.243500000	-2.487200000	-3.367600000	H	-2.883400000	1.616600000	3.234800000
H	-3.311100000	-4.244300000	-1.931500000	H	-4.311500000	3.159700000	1.873200000
H	-2.893600000	-4.188600000	0.552100000	H	-3.758700000	3.482900000	-0.563200000
H	-1.477000000	-2.357100000	1.487300000	H	-1.855900000	2.195800000	-1.535400000
H	-2.248700000	0.223800000	2.310200000	H	-2.478800000	-0.641200000	-2.367300000
H	-4.519500000	1.286600000	2.346400000	H	-4.822500000	-1.449200000	-1.943700000
H	-5.282500000	2.566000000	0.316800000	H	-5.326400000	-2.563100000	0.251200000
H	-3.722700000	2.764000000	-1.637600000	H	-3.472100000	-2.866200000	1.914300000
H	-0.472400000	-0.517100000	3.724500000	H	-0.708600000	0.620000000	-3.807000000
H	1.470400000	1.485800000	-2.840100000	H	1.594600000	-1.431400000	2.728300000
O	1.473400000	-2.829800000	2.987500000	O	1.121900000	3.116300000	-2.660500000
O	2.329500000	-1.628600000	3.228700000	O	2.149500000	2.078400000	-2.978500000
H	0.568800000	-2.422600000	3.140500000	H	0.296500000	2.634800000	-2.958800000
H	1.865000000	-0.963800000	2.642900000	H	1.725600000	1.280200000	-2.549300000

⁶ RC				² TS1			
C	-1.884800000	2.033100000	-1.924400000	C	2.102500000	1.346500000	1.924500000
C	-2.898300000	2.984900000	-1.961100000	C	3.389300000	1.825200000	2.144100000
C	-3.605200000	3.263200000	-0.793800000	C	4.356800000	1.662800000	1.155700000
C	-3.281900000	2.588500000	0.385300000	C	4.022000000	1.028200000	-0.042400000
C	-2.258500000	1.657300000	0.347700000	C	2.725500000	0.574900000	-0.197100000
N	-1.581900000	1.384200000	-0.789700000	N	1.797300000	0.729200000	0.775400000
C	-1.806200000	0.836800000	1.540400000	C	2.159600000	-0.125500000	-1.408200000
C	-2.287200000	-0.581500000	1.318000000	C	1.915200000	-1.564700000	-1.034300000
C	-3.321800000	-1.162200000	2.030800000	C	2.617800000	-2.656000000	-1.508300000
C	-3.677600000	-2.478000000	1.729300000	C	2.210800000	-3.927900000	-1.102300000
C	-2.984500000	-3.160300000	0.734100000	C	1.112000000	-4.058100000	-0.257600000
C	-1.956200000	-2.511100000	0.057600000	C	0.450800000	-2.917900000	0.185400000
N	-1.622300000	-1.241900000	0.342300000	N	0.868900000	-1.698800000	-0.184400000
N	-0.314100000	0.805900000	1.512700000	N	0.776400000	0.463800000	-1.588700000
C	0.295500000	-0.129100000	2.490300000	C	-0.062200000	-0.244600000	-2.610700000
C	0.303700000	2.152000000	1.562000000	C	0.792000000	1.948300000	-1.785200000
C	1.517600000	2.204500000	0.677900000	C	-0.282100000	2.572000000	-0.951900000
C	1.502400000	-0.800000000	1.890900000	C	-1.440300000	-0.484100000	-2.069000000
C	2.625400000	-1.125600000	2.640400000	C	-2.535600000	-0.742300000	-2.881400000
C	3.683300000	-1.789200000	2.020600000	C	-3.761000000	-1.042000000	-2.292400000
C	3.587100000	-2.116100000	0.669500000	C	-3.863400000	-1.069400000	-0.903000000
C	2.439200000	-1.755300000	-0.023300000	C	-2.743000000	-0.783200000	-0.137700000
N	1.422300000	-1.110000000	0.576900000	N	-1.561000000	-0.504900000	-0.719400000
N	1.445400000	1.504100000	-0.476200000	N	-0.678000000	1.864200000	0.134400000
C	2.462300000	1.565800000	-1.354300000	C	-1.605500000	2.357200000	0.974100000
C	3.599300000	2.326400000	-1.110300000	C	-2.160400000	3.612500000	0.763300000
C	3.689800000	3.031700000	0.087200000	C	-1.767100000	4.353700000	-0.348100000
C	2.631500000	2.972000000	0.992500000	C	-0.819600000	3.822700000	-1.219200000
Fe	-0.049100000	-0.076000000	-0.566900000	Fe	0.021900000	0.038400000	0.272400000
O	0.156400000	-0.693200000	-2.331300000	O	-0.350800000	-0.394300000	1.822000000
O	1.462500000	-0.878200000	-2.954200000	O	-2.080400000	0.141600000	2.971000000
H	-1.292900000	1.773100000	-2.801000000	H	1.298700000	1.439900000	2.651200000
H	-3.122100000	3.499000000	-2.894700000	H	3.619400000	2.322200000	3.085400000
H	-4.400500000	4.008900000	-0.795000000	H	5.368100000	2.039400000	1.308500000
H	-3.804500000	2.791700000	1.319300000	H	4.745100000	0.900200000	-0.846200000
H	-3.828500000	-0.600400000	2.814400000	H	3.447300000	-2.510700000	-2.198600000
H	-4.483600000	-2.966000000	2.277500000	H	2.737000000	-4.811000000	-1.464100000
H	-3.229200000	-4.190100000	0.476500000	H	0.754000000	-5.036100000	0.060400000
H	-1.389300000	-3.001000000	-0.731100000	H	-0.423600000	-2.967200000	0.830500000
H	0.549500000	0.386500000	3.428000000	H	-0.086000000	0.326700000	-3.546700000
H	-0.434800000	-0.915000000	2.734200000	H	0.396600000	-1.219400000	-2.831400000
H	-0.418300000	2.886200000	1.173500000	H	1.764000000	2.338100000	-1.449700000
H	0.544900000	2.441700000	2.594800000	H	0.685100000	2.195900000	-2.848600000
H	2.671100000	-0.854500000	3.694800000	H	-2.419000000	-0.711400000	-3.964100000
H	4.579500000	-2.040600000	2.588500000	H	-4.631400000	-1.247800000	-2.915100000
H	4.393000000	-2.632700000	0.149100000	H	-4.804100000	-1.299000000	-0.404400000
H	2.312200000	-1.964800000	-1.082800000	H	-2.761600000	-0.763300000	0.947700000
H	2.352100000	0.966700000	-2.256500000	H	-1.893600000	1.708300000	1.805100000
H	4.402800000	2.346500000	-1.845800000	H	-2.905500000	3.987100000	1.463600000
H	4.578800000	3.618400000	0.319900000	H	-2.201800000	5.334000000	-0.543500000
H	2.666900000	3.512600000	1.937800000	H	-0.493100000	4.367500000	-2.104300000
H	1.200100000	-0.864400000	-3.912300000	H	-1.422100000	0.328400000	3.683800000
H	-2.202500000	1.249100000	2.481100000	H	2.784200000	-0.013500000	-2.303900000
O	0.646600000	-3.768500000	-1.907700000	O	-2.616900000	-2.290700000	3.191600000
O	-0.472600000	-3.288800000	-2.761100000	O	-1.209500000	-2.684100000	3.020700000
H	1.375300000	-3.806100000	-2.577900000	H	-2.497100000	-1.228000000	3.166800000
H	-0.359600000	-2.295700000	-2.635900000	H	-0.821900000	-1.861300000	2.583100000

⁴ TS1				⁶ TS1			
C	2.181900000	1.397400000	1.805100000	C	-1.891500000	1.969100000	-1.898600000
C	3.469100000	1.905900000	1.940300000	C	-2.977400000	2.833700000	-1.972100000
C	4.376500000	1.754900000	0.894600000	C	-3.748100000	3.053200000	-0.832800000
C	3.981900000	1.100300000	-0.273900000	C	-3.419700000	2.408100000	0.362300000
C	2.689800000	0.614600000	-0.342400000	C	-2.326900000	1.562200000	0.366800000
N	1.818100000	0.758700000	0.684800000	N	-1.585800000	1.350300000	-0.749000000
C	2.072900000	-0.124900000	-1.505100000	C	-1.866200000	0.739300000	1.548100000
C	1.882500000	-1.556800000	-1.070700000	C	-2.289600000	-0.692700000	1.297100000
C	2.583400000	-2.648900000	-1.545600000	C	-3.296300000	-1.347700000	1.983600000
C	2.257900000	-3.909600000	-1.041300000	C	-3.562300000	-2.676400000	1.642000000
C	1.243200000	-4.028000000	-0.096400000	C	-2.818000000	-3.289400000	0.638100000
C	0.573700000	-2.888600000	0.337800000	C	-1.824600000	-2.561200000	-0.012600000
N	0.906500000	-1.679500000	-0.136800000	N	-1.578100000	-1.286000000	0.314300000
N	0.670600000	0.436500000	-1.635700000	N	-0.354300000	0.751300000	1.507100000
C	-0.199600000	-0.322000000	-2.591400000	C	0.275300000	-0.206800000	2.479900000
C	0.639400000	1.913000000	-1.873500000	C	0.210900000	2.133700000	1.651700000
C	-0.398600000	2.539000000	-0.994300000	C	1.493600000	2.218100000	0.881100000
C	-1.550500000	-0.544200000	-1.979000000	C	1.436600000	-0.912000000	1.846100000
C	-2.688500000	-0.806500000	-2.728600000	C	2.510200000	-1.404100000	2.573700000
C	-3.886900000	-1.071300000	-2.070200000	C	3.505700000	-2.117000000	1.906600000
C	-3.917900000	-1.054600000	-0.677200000	C	3.406900000	-2.313600000	0.529900000
C	-2.753900000	-0.769400000	0.020500000	C	2.321100000	-1.778800000	-0.147200000
N	-1.596500000	-0.534200000	-0.625000000	N	1.359600000	-1.100500000	0.505700000
N	-0.693300000	1.865800000	0.144300000	N	1.478000000	1.556600000	-0.297800000
C	-1.557700000	2.384700000	1.036500000	C	2.553100000	1.574200000	-1.102500000
C	-2.156700000	3.617800000	0.818000000	C	3.701300000	2.273700000	-0.750400000
C	-1.874800000	4.314700000	-0.354500000	C	3.731300000	2.952200000	0.466700000
C	-0.984800000	3.765200000	-1.273800000	C	2.610200000	2.926600000	1.297900000
Fe	0.041400000	0.043800000	0.271300000	Fe	-0.032400000	0.064100000	-0.425400000
O	-0.462300000	-0.231400000	1.842800000	O	0.307900000	-0.375200000	-2.000200000
O	-1.657300000	0.442700000	3.661700000	O	1.520300000	-0.268200000	-3.791800000
H	1.421400000	1.484900000	2.577500000	H	-1.246100000	1.753900000	-2.747600000
H	3.746900000	2.416900000	2.860900000	H	-3.208800000	3.326300000	-2.915300000
H	5.386700000	2.155000000	0.980400000	H	-4.601800000	3.730100000	-0.868100000
H	4.656400000	0.979300000	-1.120000000	H	-3.996800000	2.563800000	1.272700000
H	3.352600000	-2.515100000	-2.304100000	H	-3.846200000	-0.839700000	2.774700000
H	2.786200000	-4.793500000	-1.397800000	H	-4.340300000	-3.229300000	2.168700000
H	0.957900000	-4.997600000	0.309500000	H	-2.997100000	-4.326100000	0.355200000
H	-0.223200000	-2.922800000	1.075200000	H	-1.217900000	-2.984300000	-0.812200000
H	-0.267400000	0.206700000	-3.550200000	H	0.568700000	0.324100000	3.394000000
H	0.259900000	-1.302500000	-2.784400000	H	-0.472000000	-0.964100000	2.759000000
H	1.619600000	2.333500000	-1.603600000	H	-0.504200000	2.845600000	1.214300000
H	0.466200000	2.129000000	-2.934900000	H	0.335500000	2.382700000	2.713300000
H	-2.628100000	-0.801700000	-3.816400000	H	2.561900000	-1.231600000	3.648000000
H	-4.791200000	-1.278800000	-2.642100000	H	4.359000000	-2.508800000	2.460100000
H	-4.837300000	-1.247600000	-0.126000000	H	4.168600000	-2.862800000	-0.021900000
H	-2.711200000	-0.724800000	1.105000000	H	2.187300000	-1.873600000	-1.222600000
H	-1.749100000	1.783600000	1.925800000	H	2.468600000	0.995900000	-2.024100000
H	-2.847300000	4.012500000	1.562500000	H	4.562200000	2.269500000	-1.417800000
H	-2.347000000	5.276500000	-0.556400000	H	4.627000000	3.491100000	0.775700000
H	-0.738000000	4.278100000	-2.202800000	H	2.604800000	3.440700000	2.258100000
H	-0.751500000	0.692400000	3.981100000	H	0.902100000	0.469900000	-4.030900000
H	2.650100000	-0.028600000	-2.434400000	H	-2.246100000	1.126200000	2.504100000
O	-2.319300000	-2.910900000	2.311100000	O	0.801000000	-3.550900000	-2.367900000
O	-1.125700000	-2.561300000	3.124300000	O	-0.345100000	-2.805300000	-2.946700000
H	-3.042500000	-2.677100000	2.946900000	H	1.387600000	-3.620700000	-3.163700000
H	-0.940100000	-1.636100000	2.774600000	H	-0.094300000	-1.866300000	-2.671800000

² INT				⁴ INT			
C	1.643100000	-1.877400000	-1.915700000	C	-1.591300000	2.293900000	-1.277600000
C	2.783400000	-2.625500000	-2.186400000	C	-2.661600000	3.179800000	-1.223400000
C	3.855300000	-2.584800000	-1.298000000	C	-3.589100000	3.069600000	-0.190500000
C	3.768300000	-1.802000000	-0.144700000	C	-3.431200000	2.077000000	0.779600000
C	2.607800000	-1.081200000	0.065000000	C	-2.349500000	1.224800000	0.666800000
N	1.578500000	-1.116800000	-0.814500000	N	-1.459500000	1.334000000	-0.349800000
C	2.314500000	-0.171800000	1.234600000	C	-2.009600000	0.079700000	1.592300000
C	2.340600000	1.243100000	0.712100000	C	-2.288400000	-1.194700000	0.829000000
C	3.298500000	2.197600000	0.997900000	C	-3.318400000	-2.084300000	1.066800000
C	3.149000000	3.468400000	0.440500000	C	-3.420500000	-3.206800000	0.241500000
C	2.044700000	3.738500000	-0.363200000	C	-2.492200000	-3.401400000	-0.778300000
C	1.115300000	2.733900000	-0.607200000	C	-1.476600000	-2.470200000	-0.963400000
N	1.280600000	1.507500000	-0.091500000	N	-1.396900000	-1.388800000	-0.173800000
N	0.862800000	-0.433300000	1.586400000	N	-0.504100000	0.128500000	1.744400000
C	0.296400000	0.530200000	2.585300000	C	0.072200000	-1.058600000	2.452800000
C	0.586500000	-1.863200000	1.937400000	C	0.009200000	1.429600000	2.281800000
C	-0.672300000	-2.309700000	1.259200000	C	1.207900000	1.862500000	1.490500000
C	-1.045900000	1.018000000	2.124500000	C	1.282900000	-1.550700000	1.716400000
C	-1.981900000	1.576300000	2.984600000	C	2.276100000	-2.309400000	2.319400000
C	-3.172300000	2.073300000	2.461200000	C	3.327900000	-2.789500000	1.543900000
C	-3.400200000	1.995800000	1.088500000	C	3.360600000	-2.494900000	0.182600000
C	-2.437700000	1.413300000	0.278600000	C	2.350400000	-1.718100000	-0.364800000
N	-1.285400000	0.943800000	0.793000000	N	1.333300000	-1.264600000	0.392000000
N	-1.006500000	-1.635900000	0.132300000	N	1.283900000	1.390400000	0.222400000
C	-2.092700000	-1.988000000	-0.580800000	C	2.296500000	1.754400000	-0.586200000
C	-2.882100000	-3.060900000	-0.189700000	C	3.275000000	2.635900000	-0.150300000
C	-2.552600000	-3.765600000	0.965900000	C	3.213200000	3.130200000	1.151000000
C	-1.434900000	-3.380800000	1.702300000	C	2.168500000	2.734600000	1.982500000
Fe	0.050300000	-0.031000000	-0.241800000	Fe	-0.013800000	0.006500000	-0.234800000
O	-0.559100000	0.262300000	-1.771800000	O	0.272700000	-0.071600000	-1.882600000
O	-3.386100000	-0.398500000	-3.103700000	O	-1.715000000	-0.254300000	-3.284400000
H	0.768700000	-1.861600000	-2.562900000	H	-0.833000000	2.314100000	-2.057600000
H	2.820000000	-3.233500000	-3.089200000	H	-2.757800000	3.947100000	-1.990300000
H	4.754900000	-3.168100000	-1.493500000	H	-4.431000000	3.759200000	-0.131500000
H	4.577100000	-1.760400000	0.583300000	H	-4.125900000	1.970800000	1.610900000
H	4.130700000	1.954200000	1.656600000	H	-4.015200000	-1.907500000	1.884300000
H	3.883400000	4.246300000	0.648500000	H	-4.219300000	-3.930300000	0.403500000
H	1.889500000	4.723700000	-0.800400000	H	-2.545400000	-4.269600000	-1.433600000
H	0.225800000	2.899800000	-1.208700000	H	-0.721700000	-2.553100000	-1.742400000
H	0.240700000	0.064900000	3.577100000	H	0.301300000	-0.809200000	3.496100000
H	0.971400000	1.395200000	2.663300000	H	-0.678200000	-1.863000000	2.460900000
H	1.417800000	-2.481900000	1.568900000	H	-0.775500000	2.191900000	2.169600000
H	0.536200000	-1.989700000	3.025900000	H	0.234300000	1.341500000	3.351800000
H	-1.771400000	1.617500000	4.052700000	H	2.218100000	-2.516500000	3.387300000
H	-3.919400000	2.513500000	3.121700000	H	4.119000000	-3.383400000	2.001300000
H	-4.319300000	2.370800000	0.640800000	H	4.167100000	-2.848600000	-0.458100000
H	-2.564300000	1.303200000	-0.795600000	H	2.335100000	-1.442900000	-1.416100000
H	-2.322800000	-1.381600000	-1.458100000	H	2.308200000	1.305700000	-1.578800000
H	-3.754200000	-3.324000000	-0.787000000	H	4.081200000	2.914900000	-0.827500000
H	-3.165700000	-4.602800000	1.299000000	H	3.979200000	3.811500000	1.521300000
H	-1.149000000	-3.901500000	2.615300000	H	2.092200000	3.093400000	3.008100000
H	-2.841300000	-0.823600000	-3.802200000	H	-2.166100000	-0.187500000	-2.404800000
H	2.988200000	-0.330800000	2.086700000	H	-2.533200000	0.131100000	2.555700000
O	-2.450900000	2.251300000	-3.114300000	O	3.032800000	0.049300000	-3.380100000
O	-1.103500000	2.272800000	-3.109600000	O	1.940300000	-0.893900000	-3.733300000
H	-3.029600000	0.529900000	-3.064400000	H	2.895700000	0.747300000	-4.070300000
H	-0.818300000	1.375600000	-2.576300000	H	1.228600000	-0.580500000	-3.081300000

⁶ INT			² TS2				
C	-1.867000000	1.740900000	-2.125300000	C	1.707700000	-1.856200000	-1.902200000
C	-2.970900000	2.559200000	-2.333800000	C	2.868200000	-2.579300000	-2.155900000
C	-3.852800000	2.792400000	-1.281400000	C	3.930600000	-2.506000000	-1.258300000
C	-3.617500000	2.206100000	-0.034900000	C	3.815900000	-1.713600000	-0.114100000
C	-2.500000000	1.407400000	0.107800000	C	2.637100000	-1.018100000	0.077400000
N	-1.648200000	1.184800000	-0.924600000	N	1.615500000	-1.087900000	-0.808700000
C	-2.113400000	0.653700000	1.358500000	C	2.308200000	-0.107400000	1.234500000
C	-2.449100000	-0.804400000	1.131400000	C	2.295800000	1.305300000	0.705900000
C	-3.506600000	-1.470400000	1.724200000	C	3.220500000	2.289000000	1.000700000
C	-3.688300000	-2.818900000	1.408400000	C	3.027700000	3.559500000	0.455600000
C	-2.810400000	-3.442200000	0.525800000	C	1.914500000	3.799200000	-0.344700000
C	-1.770400000	-2.702600000	-0.030700000	C	1.020700000	2.765400000	-0.600000000
N	-1.606900000	-1.406900000	0.264900000	N	1.228700000	1.538700000	-0.099300000
N	-0.605800000	0.739600000	1.440700000	N	0.859700000	-0.409000000	1.576000000
C	-0.012800000	-0.148200000	2.500700000	C	0.264300000	0.547600000	2.567500000
C	-0.127700000	2.156500000	1.578500000	C	0.624200000	-1.844200000	1.938500000
C	1.224100000	2.279700000	0.945100000	C	-0.615600000	-2.332800000	1.255200000
C	1.257700000	-0.765300000	2.001900000	C	-1.083000000	1.005900000	2.094600000
C	2.310200000	-1.111600000	2.835900000	C	-2.029100000	1.564400000	2.942800000
C	3.437000000	-1.720200000	2.285600000	C	-3.226700000	2.031700000	2.408900000
C	3.484500000	-1.966100000	0.914400000	C	-3.453300000	1.917800000	1.038600000
C	2.408100000	-1.584800000	0.129100000	C	-2.479800000	1.338000000	0.240400000
N	1.318300000	-1.004900000	0.666700000	N	-1.316500000	0.905300000	0.763800000
N	1.365800000	1.595000000	-0.213600000	N	-0.963600000	-1.674100000	0.123900000
C	2.532200000	1.641300000	-0.879000000	C	-2.040400000	-2.056600000	-0.556700000
C	3.605700000	2.389400000	-0.410500000	C	-2.801400000	-3.148700000	-0.194400000
C	3.468700000	3.090800000	0.785200000	C	-2.454400000	-3.840300000	0.964200000
C	2.257500000	3.036900000	1.475700000	C	-1.349400000	-3.422300000	1.701400000
Fe	-0.078400000	0.004300000	-0.411600000	Fe	0.053800000	-0.040800000	-0.248900000
O	0.288500000	-0.568800000	-1.952000000	O	-0.566300000	0.179200000	-1.819200000
O	2.408200000	-0.270100000	-3.693700000	O	-3.445500000	-0.383900000	-3.063800000
H	-1.139700000	1.514000000	-2.902400000	H	0.838800000	-1.867900000	-2.556700000
H	-3.129900000	3.004600000	-3.314500000	H	2.927200000	-3.194400000	-3.052400000
H	-4.722200000	3.434000000	-1.424300000	H	4.844200000	-3.072500000	-1.439100000
H	-4.284400000	2.372000000	0.809800000	H	4.616900000	-1.645600000	0.620500000
H	-4.161400000	-0.953500000	2.424000000	H	4.058200000	2.069100000	1.660600000
H	-4.505300000	-3.380000000	1.861600000	H	3.733600000	4.360600000	0.673400000
H	-2.919300000	-4.495200000	0.269100000	H	1.722800000	4.783400000	-0.769600000
H	-1.048900000	-3.147900000	-0.712900000	H	0.124900000	2.910300000	-1.197800000
H	0.144000000	0.423500000	3.424300000	H	0.211200000	0.083900000	3.560200000
H	-0.726000000	-0.954700000	2.723200000	H	0.921200000	1.426100000	2.647300000
H	-0.828400000	2.809400000	1.038200000	H	1.477300000	-2.440200000	1.582900000
H	-0.130100000	2.452200000	2.635400000	H	0.568700000	-1.960100000	3.027600000
H	2.248100000	-0.897100000	3.902000000	H	-1.820000000	1.630300000	4.009900000
H	4.278000000	-1.990500000	2.924300000	H	-3.980600000	2.474700000	3.059300000
H	4.351500000	-2.431600000	0.448100000	H	-4.380600000	2.262800000	0.583300000
H	2.405100000	-1.715600000	-0.950300000	H	-2.606900000	1.201500000	-0.829800000
H	2.603600000	1.043000000	-1.787000000	H	-2.285800000	-1.455800000	-1.464400000
H	4.538700000	2.401800000	-0.972300000	H	-3.665600000	-3.437300000	-0.791500000
H	4.302400000	3.666300000	1.187400000	H	-3.045300000	-4.692600000	1.299300000
H	2.118300000	3.565200000	2.418100000	H	-1.052500000	-3.930300000	2.618100000
H	1.545900000	-0.120100000	-3.231900000	H	-2.945100000	-0.848200000	-3.770700000
H	-2.589700000	1.058900000	2.261800000	H	2.974900000	-0.240700000	2.096400000
O	1.893700000	-3.044300000	-2.883900000	O	-2.395400000	2.229700000	-3.086900000
O	0.607900000	-2.953200000	-2.530100000	O	-1.070600000	2.226500000	-3.010500000
H	2.542600000	-1.234200000	-3.516700000	H	-3.045200000	0.526500000	-3.059700000
H	0.429700000	-1.895500000	-2.284900000	H	-0.758200000	1.168600000	-2.410800000

⁴ TS2				⁶ TS2			
C	1.676600000	-1.881700000	-1.897800000	C	1.805000000	-1.820900000	-2.084700000
C	2.826200000	-2.622000000	-2.151100000	C	2.884700000	-2.674400000	-2.278000000
C	3.890100000	-2.562700000	-1.254200000	C	3.766100000	-2.904300000	-1.224400000
C	3.787400000	-1.766700000	-0.111300000	C	3.555500000	-2.279000000	0.007700000
C	2.618700000	-1.053800000	0.079900000	C	2.459500000	-1.448300000	0.136600000
N	1.595600000	-1.110200000	-0.805500000	N	1.609300000	-1.228300000	-0.897500000
C	2.305400000	-0.135600000	1.235700000	C	2.089300000	-0.663200000	1.372800000
C	2.312400000	1.275600000	0.702200000	C	2.450900000	0.785700000	1.123300000
C	3.250700000	2.247100000	0.995500000	C	3.529300000	1.437400000	1.694800000
C	3.075300000	3.519500000	0.449100000	C	3.732300000	2.779100000	1.361900000
C	1.964600000	3.773600000	-0.350400000	C	2.851300000	3.411300000	0.488600000
C	1.057300000	2.751400000	-0.604100000	C	1.791800000	2.684800000	-0.047600000
N	1.248500000	1.522000000	-0.103200000	N	1.611600000	1.394100000	0.258600000
N	0.854500000	-0.415200000	1.582400000	N	0.578500000	-0.724900000	1.455600000
C	0.273200000	0.552700000	2.570200000	C	-0.003200000	0.191200000	2.498500000
C	0.598100000	-1.844700000	1.949100000	C	0.081800000	-2.131900000	1.618000000
C	-0.649300000	-2.317700000	1.267900000	C	-1.266500000	-2.255800000	0.976600000
C	-1.067000000	1.031400000	2.095600000	C	-1.251700000	0.837900000	1.981000000
C	-2.002300000	1.610300000	2.942200000	C	-2.296100000	1.232100000	2.803700000
C	-3.191700000	2.097300000	2.407400000	C	-3.399700000	1.868300000	2.237500000
C	-3.421000000	1.983200000	1.037500000	C	-3.433500000	2.092800000	0.862300000
C	-2.458500000	1.383000000	0.241200000	C	-2.367800000	1.661900000	0.087900000
N	-1.303600000	0.929800000	0.765500000	N	-1.301000000	1.054700000	0.641000000
N	-0.988800000	-1.658700000	0.134200000	N	-1.403100000	-1.575400000	-0.184900000
C	-2.069600000	-2.031700000	-0.576500000	C	-2.563700000	-1.631600000	-0.859800000
C	-2.845400000	-3.111500000	-0.178400000	C	-3.634100000	-2.390400000	-0.401500000
C	-2.508400000	-3.802000000	0.983900000	C	-3.500800000	-3.091200000	0.795200000
C	-1.397800000	-3.395400000	1.719000000	C	-2.297700000	-3.022500000	1.498500000
Fe	0.049500000	-0.040400000	-0.247700000	Fe	0.066500000	-0.009800000	-0.405300000
O	-0.569300000	0.183600000	-1.805200000	O	-0.279000000	0.540900000	-1.973700000
O	-3.453200000	-0.378700000	-3.064400000	O	-2.408600000	0.238000000	-3.687200000
H	0.806900000	-1.881600000	-2.551400000	H	1.078700000	-1.593700000	-2.863000000
H	2.875800000	-3.239300000	-3.046700000	H	3.024200000	-3.150700000	-3.247400000
H	4.795300000	-3.142500000	-1.434600000	H	4.616300000	-3.573800000	-1.355200000
H	4.589800000	-1.708800000	0.622600000	H	4.222400000	-2.442400000	0.852900000
H	4.085400000	2.016600000	1.655600000	H	4.185000000	0.915700000	2.390700000
H	3.792300000	4.311100000	0.665700000	H	4.568400000	3.328100000	1.795300000
H	1.785700000	4.760000000	-0.775600000	H	2.973400000	4.460500000	0.222300000
H	0.162600000	2.908500000	-1.199900000	H	1.068600000	3.135800000	-0.724500000
H	0.211500000	0.093300000	3.564400000	H	-0.187000000	-0.366500000	3.425500000
H	0.943200000	1.421500000	2.648900000	H	0.729300000	0.979700000	2.722600000
H	1.441800000	-2.454900000	1.595200000	H	0.778400000	-2.804600000	1.097200000
H	0.541000000	-1.957600000	3.038600000	H	0.073500000	-2.407100000	2.680700000
H	-1.791400000	1.676800000	4.008900000	H	-2.245300000	1.035000000	3.873700000
H	-3.937000000	2.556200000	3.056600000	H	-4.234000000	2.176500000	2.867500000
H	-4.342100000	2.343800000	0.581500000	H	-4.281600000	2.581300000	0.385000000
H	-2.586700000	1.245700000	-0.829100000	H	-2.353700000	1.777000000	-0.993800000
H	-2.306700000	-1.432500000	-1.456400000	H	-2.631400000	-1.038100000	-1.771200000
H	-3.713000000	-3.391400000	-0.774700000	H	-4.561600000	-2.413200000	-0.972400000
H	-3.111000000	-4.644500000	1.323000000	H	-4.331600000	-3.677900000	1.187800000
H	-1.107600000	-3.903300000	2.637900000	H	-2.162400000	-3.549100000	2.442500000
H	-2.971000000	-0.855100000	-3.776000000	H	-1.565500000	0.178600000	-3.168700000
H	2.974200000	-0.275100000	2.095000000	H	2.557600000	-1.061700000	2.283300000
O	-2.346000000	2.224100000	-3.137400000	O	-1.712900000	3.095800000	-2.863400000
O	-1.016400000	2.218200000	-3.057000000	O	-0.426900000	2.890400000	-2.617800000
H	-3.025800000	0.517700000	-3.059500000	H	-2.623600000	1.195600000	-3.600400000
H	-0.747700000	1.248100000	-2.474900000	H	-0.317900000	1.787800000	-2.307700000

²P				⁴P			
C	-2.423800000	0.982900000	-1.929000000	C	1.990600000	1.383100000	2.046200000
C	-3.778800000	1.228900000	-2.120200000	C	3.223200000	1.964900000	2.319700000
C	-4.686200000	0.872900000	-1.124600000	C	4.209200000	1.974600000	1.334900000
C	-4.221200000	0.280000000	0.051100000	C	3.942700000	1.406100000	0.087600000
C	-2.862300000	0.057000000	0.174400000	C	2.699400000	0.837000000	-0.116000000
N	-1.986100000	0.391200000	-0.806700000	N	1.750100000	0.816200000	0.853600000
C	-2.160100000	-0.567000000	1.356400000	C	2.215200000	0.167100000	-1.379700000
C	-1.670900000	-1.919200000	0.898400000	C	2.112500000	-1.306200000	-1.067900000
C	-2.155500000	-3.147900000	1.307100000	C	2.929200000	-2.308100000	-1.558700000
C	-1.572900000	-4.297400000	0.769500000	C	2.677200000	-3.620300000	-1.152900000
C	-0.528400000	-4.173400000	-0.144400000	C	1.613200000	-3.880000000	-0.291600000
C	-0.086200000	-2.906700000	-0.507300000	C	0.826700000	-2.826000000	0.157800000
N	-0.661400000	-1.804400000	-0.001900000	N	1.091800000	-1.563200000	-0.211500000
N	-0.897500000	0.261600000	1.544300000	N	0.775300000	0.633600000	-1.546300000
C	0.067100000	-0.322900000	2.533800000	C	0.024600000	-0.090300000	-2.624400000
C	-1.163400000	1.715400000	1.796600000	C	0.633800000	2.122400000	-1.652800000
C	-0.211200000	2.545800000	0.988000000	C	-0.513200000	2.581100000	-0.801200000
C	1.462500000	-0.225300000	1.990700000	C	-1.352800000	-0.429400000	-2.134000000
C	2.594100000	-0.228500000	2.794300000	C	-2.427800000	-0.657000000	-2.981600000
C	3.850700000	-0.206100000	2.192100000	C	-3.651400000	-1.036700000	-2.433500000
C	3.938500000	-0.172700000	0.802100000	C	-3.765300000	-1.173200000	-1.051700000
C	2.770300000	-0.155100000	0.053000000	C	-2.657600000	-0.916500000	-0.255200000
N	1.559900000	-0.187800000	0.638800000	N	-1.477300000	-0.556600000	-0.789800000
N	0.253400000	1.963600000	-0.145700000	N	-0.820800000	1.779900000	0.249400000
C	1.056900000	2.655200000	-0.974300000	C	-1.792100000	2.141800000	1.107400000
C	1.426400000	3.964900000	-0.697100000	C	-2.492800000	3.330200000	0.946100000
C	0.968200000	4.567200000	0.472100000	C	-2.192700000	4.155200000	-0.135200000
C	0.137700000	3.845200000	1.327000000	C	-1.188500000	3.772700000	-1.022500000
Fe	-0.141400000	0.053300000	-0.286100000	Fe	0.079800000	0.043900000	0.223600000
O	0.527300000	-0.179500000	-1.964700000	O	-0.517300000	-0.527200000	1.846100000
O	2.592200000	0.794100000	-3.398700000	O	-2.787800000	-0.308700000	3.286800000
H	-1.662400000	1.251500000	-2.659000000	H	1.172500000	1.357800000	2.763900000
H	-4.110500000	1.702500000	-3.043100000	H	3.398200000	2.409700000	3.298300000
H	-5.750700000	1.067900000	-1.253800000	H	5.177400000	2.435400000	1.529000000
H	-4.895600000	0.008600000	0.861800000	H	4.678600000	1.414500000	-0.715300000
H	-2.960300000	-3.202000000	2.038800000	H	3.733900000	-2.067100000	-2.251500000
H	-1.926200000	-5.282600000	1.073200000	H	3.300000000	-4.435100000	-1.521200000
H	-0.048700000	-5.050900000	-0.576400000	H	1.382900000	-4.894300000	0.032200000
H	0.727600000	-2.743100000	-1.208000000	H	-0.027500000	-2.963500000	0.815000000
H	-0.033100000	0.172000000	3.507800000	H	0.001200000	0.505500000	-3.545000000
H	-0.176600000	-1.386300000	2.673200000	H	0.552800000	-1.029100000	-2.847300000
H	-2.187300000	1.944300000	1.465800000	H	1.555000000	2.588100000	-1.272200000
H	-1.102000000	1.938800000	2.868800000	H	0.516300000	2.423900000	-2.701100000
H	2.485500000	-0.247900000	3.878100000	H	-2.301900000	-0.535500000	-4.056900000
H	4.752400000	-0.205400000	2.804700000	H	-4.509900000	-1.216000000	-3.080900000
H	4.901000000	-0.146100000	0.292500000	H	-4.706000000	-1.461600000	-0.584300000
H	2.776900000	-0.111100000	-1.031600000	H	-2.691400000	-0.986100000	0.828100000
H	1.410400000	2.131600000	-1.860100000	H	-2.006000000	1.450700000	1.920400000
H	2.081400000	4.492200000	-1.389600000	H	-3.275700000	3.588800000	1.658500000
H	1.259000000	5.587600000	0.721900000	H	-2.739400000	5.085000000	-0.293200000
H	-0.238600000	4.279800000	2.252600000	H	-0.927300000	4.388400000	-1.882500000
H	2.252400000	1.039900000	-4.286400000	H	-2.532900000	-0.051600000	4.199200000
H	-2.780100000	-0.609400000	2.261500000	H	2.838400000	0.386200000	-2.256900000
O	3.264300000	-2.759400000	-1.469100000	O	-2.172400000	-3.227700000	2.133100000
O	2.785200000	-2.278800000	-2.501400000	O	-1.311400000	-3.198000000	3.015600000
H	1.802300000	0.384000000	-2.944800000	H	-1.913700000	-0.449700000	2.826300000
H	-0.067300000	-0.751300000	-2.503700000	H	0.207800000	-0.961900000	2.351900000

${}^6\text{P}$				${}^2\text{RC}_{\text{homo}}$			
C	2.143200000	-1.217900000	-2.025000000	C	0.127700000	-2.925600000	-0.243000000
C	3.456200000	-1.572200000	-2.311600000	C	0.598100000	-4.134900000	0.255100000
C	4.464200000	-1.232000000	-1.413100000	C	1.577300000	-4.133600000	1.246400000
C	4.138700000	-0.549300000	-0.239900000	C	2.062600000	-2.918500000	1.735500000
C	2.812900000	-0.224300000	-0.012000000	C	1.560200000	-1.750800000	1.193400000
N	1.843000000	-0.549400000	-0.900700000	N	0.625800000	-1.761300000	0.207700000
C	2.293400000	0.511800000	1.207300000	C	1.921800000	-0.343000000	1.602100000
C	1.854800000	1.881500000	0.735700000	C	2.703700000	0.270600000	0.468200000
C	2.486400000	3.072400000	1.049600000	C	4.041600000	0.618200000	0.487900000
C	1.945100000	4.259300000	0.552900000	C	4.581700000	1.217900000	-0.651600000
C	0.788700000	4.214400000	-0.222100000	C	3.764900000	1.458600000	-1.754500000
C	0.206800000	2.982000000	-0.498000000	C	2.426400000	1.087800000	-1.707200000
N	0.747300000	1.844900000	-0.037500000	N	1.919200000	0.486100000	-0.617900000
N	1.059000000	-0.205600000	1.635500000	N	0.597400000	0.410900000	1.613500000
C	0.195600000	0.494000000	2.608100000	C	0.741900000	1.893500000	1.792500000
C	1.231200000	-1.643700000	1.906700000	C	-0.415900000	-0.181900000	2.543900000
C	0.182100000	-2.461500000	1.196300000	C	-1.754100000	-0.196400000	1.869600000
C	-1.243700000	0.513200000	2.151600000	C	-0.128400000	2.612300000	0.802900000
C	-2.294200000	0.698600000	3.043700000	C	-0.553400000	3.921900000	0.977100000
C	-3.597700000	0.778700000	2.563400000	C	-1.289500000	4.534600000	-0.034700000
C	-3.827700000	0.659200000	1.193500000	C	-1.580100000	3.819800000	-1.194800000
C	-2.747000000	0.458000000	0.350500000	C	-1.142200000	2.507700000	-1.304700000
N	-1.487100000	0.398200000	0.824600000	N	-0.433000000	1.921700000	-0.322900000
N	-0.374000000	-1.933000000	0.083500000	N	-1.727000000	-0.235200000	0.513300000
C	-1.271900000	-2.640300000	-0.630700000	C	-2.884500000	-0.281600000	-0.171000000
C	-1.640800000	-3.924400000	-0.256900000	C	-4.113300000	-0.316300000	0.472900000
C	-1.082400000	-4.480800000	0.892400000	C	-4.149900000	-0.283100000	1.864700000
C	-0.163400000	-3.737600000	1.626400000	C	-2.951200000	-0.216000000	2.571100000
Fe	0.013700000	-0.018300000	-0.373800000	Fe	0.053300000	0.033900000	-0.271600000
O	-0.729500000	0.292400000	-2.068000000	O	-0.424300000	-0.301400000	-1.946100000
O	-2.371300000	-1.277300000	-3.476400000	O	0.550200000	-1.052000000	-2.826400000
H	1.308000000	-1.453500000	-2.682000000	H	-0.653600000	-2.852500000	-0.999700000
H	3.675000000	-2.113200000	-3.231200000	H	0.187400000	-5.066600000	-0.131800000
H	5.499400000	-1.506200000	-1.616000000	H	1.949800000	-5.073200000	1.654200000
H	4.896700000	-0.285200000	0.496200000	H	2.802600000	-2.876500000	2.533700000
H	3.372800000	3.068800000	1.682400000	H	4.639300000	0.440800000	1.380500000
H	2.416500000	5.214100000	0.785000000	H	5.631200000	1.511800000	-0.668700000
H	0.330900000	5.122800000	-0.611200000	H	4.153900000	1.939000000	-2.651400000
H	-0.701200000	2.879400000	-1.087700000	H	1.735300000	1.253300000	-2.530700000
H	0.273600000	0.038900000	3.605900000	H	0.511500000	2.179800000	2.826100000
H	0.529200000	1.538200000	2.707900000	H	1.788400000	2.170200000	1.597100000
H	2.214800000	-1.967200000	1.531600000	H	-0.124300000	-1.218800000	2.766600000
H	1.217600000	-1.850700000	2.986700000	H	-0.436800000	0.367400000	3.493500000
H	-2.080400000	0.780100000	4.109200000	H	-0.307300000	4.450300000	1.897500000
H	-4.428700000	0.923500000	3.253500000	H	-1.636700000	5.560800000	0.085100000
H	-4.832300000	0.708200000	0.775500000	H	-2.152800000	4.263100000	-2.008000000
H	-2.854600000	0.338200000	-0.724400000	H	-1.349700000	1.891500000	-2.177400000
H	-1.694500000	-2.159600000	-1.513800000	H	-2.812800000	-0.287000000	-1.254700000
H	-2.367400000	-4.468200000	-0.859400000	H	-5.025500000	-0.355300000	-0.121200000
H	-1.365800000	-5.481400000	1.218900000	H	-5.101300000	-0.296800000	2.396400000
H	0.291700000	-4.137600000	2.532500000	H	-2.936200000	-0.175500000	3.659600000
H	-1.781000000	-0.621300000	-2.994600000	H	1.214100000	-1.394700000	-2.174400000
H	3.057300000	0.580000000	1.996200000	H	2.443400000	-0.292800000	2.566800000
O	-3.581200000	1.618300000	-2.793500000	O	-2.546100000	-2.739100000	-2.314300000
O	-2.894100000	2.493700000	-2.262800000	O	-2.525100000	-1.546800000	-3.204800000
H	-3.273000000	-0.903500000	-3.382900000	H	-2.184200000	-3.420700000	-2.936000000
H	-0.333300000	0.960000000	-2.670300000	H	-1.723800000	-1.079000000	-2.826200000

$^4\text{RC}_{\text{homo}}$				$^6\text{RC}_{\text{homo}}$			
C	1.594500000	2.316000000	1.320700000	C	1.929400000	-2.286400000	-1.339500000
C	2.681200000	3.183200000	1.292700000	C	3.008400000	-3.150400000	-1.181400000
C	3.655700000	3.019900000	0.311600000	C	3.807800000	-3.034900000	-0.046700000
C	3.521300000	1.996700000	-0.629300000	C	3.511300000	-2.065400000	0.915200000
C	2.418700000	1.165900000	-0.542200000	C	2.421400000	-1.244100000	0.690300000
N	1.484200000	1.322600000	0.424600000	N	1.658100000	-1.350600000	-0.419200000
C	2.120800000	0.010000000	-1.476100000	C	1.960800000	-0.132300000	1.609200000
C	2.317900000	-1.259000000	-0.671000000	C	2.315200000	1.179000000	0.944900000
C	3.348100000	-2.164200000	-0.851300000	C	3.354500000	2.010200000	1.317600000
C	3.399200000	-3.285500000	-0.020500000	C	3.568600000	3.171100000	0.569600000
C	2.417000000	-3.467100000	0.949800000	C	2.742900000	3.458600000	-0.514400000
C	1.404600000	-2.522600000	1.074900000	C	1.718500000	2.577000000	-0.838100000
N	1.373000000	-1.438700000	0.283100000	N	1.522100000	1.462200000	-0.117700000
N	0.665400000	0.088900000	-1.791200000	N	0.449000000	-0.192600000	1.626900000
C	0.089600000	-1.091300000	-2.468500000	C	-0.161400000	0.931600000	2.412800000
C	0.189600000	1.383900000	-2.322800000	C	-0.084600000	-1.526200000	2.067200000
C	-1.023400000	1.874600000	-1.569800000	C	-1.299300000	-1.880000000	1.264700000
C	-1.168700000	-1.561700000	-1.779800000	C	-1.461500000	1.337700000	1.786000000
C	-2.120200000	-2.328400000	-2.442300000	C	-2.571300000	1.737800000	2.514900000
C	-3.227800000	-2.799600000	-1.744300000	C	-3.712000000	2.150400000	1.825600000
C	-3.361900000	-2.489700000	-0.392200000	C	-3.706000000	2.155600000	0.432200000
C	-2.391400000	-1.708800000	0.216200000	C	-2.565400000	1.728700000	-0.236200000
N	-1.318600000	-1.262300000	-0.467600000	N	-1.469800000	1.328500000	0.431900000
N	-1.213100000	1.414600000	-0.310300000	N	-1.316500000	-1.419700000	-0.011500000
C	-2.251900000	1.848500000	0.431200000	C	-2.336600000	-1.722900000	-0.834800000
C	-3.141500000	2.791500000	-0.060900000	C	-3.387300000	-2.522800000	-0.409500000
C	-2.962500000	3.276900000	-1.355100000	C	-3.386200000	-2.997100000	0.901300000
C	-1.896200000	2.807900000	-2.116600000	C	-2.330100000	-2.669600000	1.750900000
Fe	-0.024800000	-0.007400000	0.329300000	Fe	0.028200000	0.064000000	-0.390000000
O	-0.224500000	-0.072900000	2.214900000	O	-0.215800000	0.254300000	-2.028000000
O	0.857700000	-0.135800000	3.204400000	O	2.073200000	0.417300000	-3.127500000
H	0.798200000	2.387600000	2.059600000	H	1.268200000	-2.318100000	-2.204200000
H	2.751100000	3.978100000	2.034000000	H	3.212500000	-3.902400000	-1.942300000
H	4.512600000	3.692100000	0.268100000	H	4.657000000	-3.702700000	0.098100000
H	4.251100000	1.851900000	-1.424400000	H	4.106500000	-1.958400000	1.820900000
H	4.086800000	-1.999000000	-1.634100000	H	3.976100000	1.761100000	2.176100000
H	4.198000000	-4.017200000	-0.140500000	H	4.376900000	3.850200000	0.840200000
H	2.423700000	-4.335000000	1.607600000	H	2.885600000	4.358200000	-1.111400000
H	0.605900000	-2.604800000	1.810300000	H	1.043100000	2.732500000	-1.677100000
H	-0.108800000	-0.880100000	-3.529000000	H	-0.275000000	0.639700000	3.464500000
H	0.817000000	-1.916900000	-2.437300000	H	0.523000000	1.791600000	2.372300000
H	0.984300000	2.136700000	-2.209700000	H	0.684100000	-2.290000000	1.880700000
H	-0.030200000	1.311300000	-3.397500000	H	-0.289500000	-1.515900000	3.145300000
H	-1.984100000	-2.549900000	-3.500600000	H	-2.543300000	1.721100000	3.603700000
H	-3.983300000	-3.398000000	-2.253300000	H	-4.601300000	2.458300000	2.375700000
H	-4.212900000	-2.836000000	0.192300000	H	-4.578400000	2.472000000	-0.138100000
H	-2.455900000	-1.433100000	1.268100000	H	-2.513400000	1.687500000	-1.323400000
H	-2.361100000	1.412100000	1.424700000	H	-2.301300000	-1.279900000	-1.829800000
H	-3.968300000	3.124500000	0.564800000	H	-4.201200000	-2.751900000	-1.096000000
H	-3.654600000	4.008100000	-1.772900000	H	-4.209000000	-3.611800000	1.266600000
H	-1.732000000	3.159600000	-3.134800000	H	-2.305000000	-3.018300000	2.782400000
H	1.661800000	-0.196800000	2.626900000	H	2.455000000	0.245800000	-2.228100000
H	2.763400000	0.030800000	-2.368600000	H	2.382200000	-0.220800000	2.619900000
O	-3.282700000	0.205900000	3.106800000	O	-3.100400000	0.228200000	-3.386800000
O	-2.381500000	-0.900600000	3.527500000	O	-2.063200000	1.267700000	-3.603800000
H	-3.220300000	0.798900000	3.898700000	H	-2.977400000	-0.318100000	-4.204900000
H	-1.517400000	-0.584600000	3.100100000	H	-1.312100000	0.885600000	-3.037200000

$2^2\text{TS}_{\text{homo}}$				$4^4\text{TS}_{\text{homo}}$			
C	-1.760000000	2.242800000	0.069400000	C	1.588300000	-2.344900000	-1.253900000
C	-2.797100000	2.903400000	0.719400000	C	2.671000000	-3.217200000	-1.210100000
C	-3.430000000	2.292200000	1.798000000	C	3.643500000	-3.045400000	-0.228100000
C	-3.006400000	1.030500000	2.223900000	C	3.514200000	-2.007000000	0.696600000
C	-1.972300000	0.425800000	1.535600000	C	2.415100000	-1.173800000	0.593700000
N	-1.379200000	1.021400000	0.471500000	N	1.480900000	-1.342300000	-0.370100000
C	-1.371700000	-0.928300000	1.830100000	C	2.118900000	0.008100000	1.492700000
C	-1.810000000	-1.851900000	0.718000000	C	2.342900000	1.252800000	0.659700000
C	-2.715200000	-2.891100000	0.819600000	C	3.390600000	2.143000000	0.809900000
C	-3.000800000	-3.629500000	-0.330900000	C	3.462300000	3.232100000	-0.061400000
C	-2.366500000	-3.313900000	-1.530000000	C	2.486600000	3.394500000	-1.041600000
C	-1.459100000	-2.261800000	-1.564800000	C	1.456400000	2.465200000	-1.134900000
N	-1.210000000	-1.544600000	-0.458200000	N	1.402000000	1.417400000	-0.299900000
N	0.122300000	-0.750000000	1.635100000	N	0.648000000	-0.044300000	1.766600000
C	0.892300000	-2.034400000	1.670200000	C	0.087700000	1.162300000	2.425700000
C	0.723600000	0.310400000	2.507000000	C	0.157600000	-1.321600000	2.344400000
C	1.619500000	1.195000000	1.690800000	C	-1.065100000	-1.806400000	1.611400000
C	1.880200000	-2.058700000	0.542400000	C	-1.165700000	1.623400000	1.730000000
C	3.018500000	-2.852600000	0.544300000	C	-2.114600000	2.411100000	2.369200000
C	3.837400000	-2.864400000	-0.582100000	C	-3.213400000	2.874700000	1.652200000
C	3.497400000	-2.080400000	-1.682600000	C	-3.339600000	2.534700000	0.306800000
C	2.356800000	-1.294400000	-1.623600000	C	-2.372700000	1.731200000	-0.278000000
N	1.569600000	-1.294200000	-0.531700000	N	-1.307800000	1.293200000	0.423000000
N	1.378400000	1.225900000	0.358500000	N	-1.235500000	-1.378700000	0.336600000
C	2.092000000	2.033600000	-0.448300000	C	-2.279200000	-1.811600000	-0.397800000
C	3.077700000	2.864500000	0.061600000	C	-3.193300000	-2.717800000	0.118900000
C	3.341000000	2.842600000	1.429900000	C	-3.035200000	-3.166400000	1.428700000
C	2.605900000	1.994100000	2.252800000	C	-1.961700000	-2.700700000	2.182300000
Fe	0.069000000	-0.065300000	-0.290300000	Fe	-0.012400000	0.007400000	-0.292300000
O	-0.035700000	0.462700000	-1.856600000	O	-0.179800000	0.016200000	-2.085500000
O	-2.549900000	0.864200000	-2.547400000	O	0.726900000	-0.037900000	-3.418900000
H	-1.215600000	2.674400000	-0.768100000	H	0.794800000	-2.419100000	-1.995600000
H	-3.096000000	3.892300000	0.373700000	H	2.740600000	-4.021200000	-1.941400000
H	-4.242700000	2.798200000	2.319000000	H	4.496600000	-3.721600000	-0.173100000
H	-3.459500000	0.530800000	3.078800000	H	4.244700000	-1.852100000	1.489200000
H	-3.177000000	-3.121700000	1.778100000	H	4.126700000	1.991400000	1.598000000
H	-3.709700000	-4.455900000	-0.284900000	H	4.273600000	3.953500000	0.033400000
H	-2.564600000	-3.877000000	-2.440400000	H	2.512600000	4.235700000	-1.732900000
H	-0.925600000	-1.958900000	-2.463800000	H	0.662400000	2.531700000	-1.876600000
H	1.377900000	-2.167100000	2.644700000	H	-0.100400000	0.972900000	3.491500000
H	0.189800000	-2.870100000	1.533000000	H	0.825200000	1.977000000	2.365900000
H	-0.086100000	0.926000000	2.925400000	H	0.941500000	-2.086500000	2.240700000
H	1.260500000	-0.144400000	3.348400000	H	-0.046500000	-1.210600000	3.418100000
H	3.253500000	-3.451400000	1.423400000	H	-1.984000000	2.654400000	3.423200000
H	4.738000000	-3.478100000	-0.597500000	H	-3.967400000	3.491100000	2.141400000
H	4.112900000	-2.061100000	-2.580700000	H	-4.184100000	2.873800000	-0.291500000
H	2.042400000	-0.645800000	-2.438700000	H	-2.433900000	1.429300000	-1.322200000
H	1.847800000	1.990800000	-1.506200000	H	-2.371700000	-1.404500000	-1.404400000
H	3.634700000	3.510400000	-0.615700000	H	-4.023900000	-3.051200000	-0.502100000
H	4.119100000	3.477800000	1.853800000	H	-3.747900000	-3.867000000	1.864400000
H	2.786900000	1.946900000	3.325900000	H	-1.810200000	-3.024800000	3.211400000
H	-2.397700000	0.207100000	-1.828500000	H	1.601900000	0.064800000	-2.964600000
H	-1.623500000	-1.304900000	2.830100000	H	2.728900000	0.000900000	2.406800000
O	-0.022700000	3.542000000	-2.412200000	O	-3.276500000	-0.305800000	-3.118700000
O	-0.609700000	2.576400000	-3.358300000	O	-2.326500000	0.768600000	-3.510000000
H	-0.577700000	4.335800000	-2.627300000	H	-3.182700000	-0.917600000	-3.893100000
H	-0.465500000	1.726200000	-2.821100000	H	-1.502700000	0.462900000	-3.007700000

${}^6\text{T}_{\text{homo}}$				${}^2\text{P}_{\text{homo}}$			
C	-1.887600000	2.334200000	-1.252600000	C	1.670300000	2.276900000	0.450300000
C	-2.971800000	3.193600000	-1.098800000	C	2.697700000	3.041400000	-0.090300000
C	-3.814900000	3.029200000	-0.001900000	C	3.180300000	2.734800000	-1.360600000
C	-3.561300000	2.010800000	0.920400000	C	2.619400000	1.674400000	-2.075600000
C	-2.464100000	1.196800000	0.700400000	C	1.608200000	0.947900000	-1.475600000
N	-1.652600000	1.360600000	-0.364900000	N	1.162500000	1.242900000	-0.233000000
C	-2.062200000	0.019000000	1.564200000	C	0.903100000	-0.255600000	-2.056900000
C	-2.426200000	-1.232800000	0.793700000	C	1.418000000	-1.454700000	-1.297000000
C	-3.508200000	-2.047900000	1.073500000	C	2.278100000	-2.422000000	-1.780600000
C	-3.746500000	-3.136200000	0.230500000	C	2.677500000	-3.439200000	-0.911800000
C	-2.902300000	-3.367800000	-0.852600000	C	2.195600000	-3.457800000	0.394200000
C	-1.832800000	-2.505700000	-1.071800000	C	1.325100000	-2.458900000	0.812900000
N	-1.609500000	-1.464300000	-0.258800000	N	0.963000000	-1.478500000	-0.024100000
N	-0.559000000	0.048600000	1.647900000	N	-0.548400000	-0.111000000	-1.640300000
C	0.013900000	-1.148800000	2.338400000	C	-1.382900000	-1.321800000	-1.921600000
C	-0.023900000	1.326900000	2.216200000	C	-1.190900000	1.157800000	-2.107700000
C	1.225500000	1.743700000	1.496400000	C	-1.960100000	1.782500000	-0.980500000
C	1.334900000	-1.509600000	1.725500000	C	-2.204400000	-1.670900000	-0.714800000
C	2.410900000	-1.976700000	2.465000000	C	-3.338500000	-2.468700000	-0.778500000
C	3.579500000	-2.343600000	1.797300000	C	-3.988600000	-2.817500000	0.402600000
C	3.632900000	-2.242800000	0.409100000	C	-3.491000000	-2.354400000	1.619200000
C	2.524500000	-1.756700000	-0.272300000	C	-2.364200000	-1.546200000	1.622700000
N	1.402200000	-1.392800000	0.375300000	N	-1.739700000	-1.221600000	0.475500000
N	1.298900000	1.406800000	0.186800000	N	-1.554600000	1.454400000	0.269500000
C	2.348500000	1.798700000	-0.558700000	C	-2.134400000	2.013400000	1.347800000
C	3.375500000	2.557800000	-0.015700000	C	-3.152200000	2.944900000	1.209800000
C	3.317500000	2.900100000	1.334500000	C	-3.588200000	3.287200000	-0.068700000
C	2.228800000	2.487600000	2.101300000	C	-2.985800000	2.696700000	-1.176800000
Fe	-0.034000000	-0.064300000	-0.403200000	Fe	-0.237700000	0.018800000	0.378200000
O	0.094900000	-0.034100000	-2.111300000	O	0.122700000	0.123300000	2.002800000
O	-0.558200000	0.262000000	-3.759300000	O	3.643900000	-0.362700000	0.526800000
H	-1.189300000	2.405000000	-2.086300000	H	1.249800000	2.457500000	1.436900000
H	-3.145400000	3.980200000	-1.831600000	H	3.110400000	3.866700000	0.488300000
H	-4.667000000	3.693800000	0.141600000	H	3.985700000	3.323400000	-1.800100000
H	-4.196000000	1.858600000	1.792400000	H	2.957200000	1.416600000	-3.078400000
H	-4.145600000	-1.841000000	1.932000000	H	2.620300000	-2.382300000	-2.813600000
H	-4.587600000	-3.801700000	0.425000000	H	3.355900000	-4.218100000	-1.259600000
H	-3.063200000	-4.208500000	-1.525900000	H	2.484600000	-4.241300000	1.093200000
H	-1.135000000	-2.632700000	-1.898300000	H	0.907000000	-2.416300000	1.816900000
H	0.093300000	-0.966200000	3.418200000	H	-2.009800000	-1.160600000	-2.807500000
H	-0.671800000	-1.995800000	2.189800000	H	-0.714100000	-2.167800000	-2.139500000
H	-0.776300000	2.116000000	2.071600000	H	-0.401600000	1.858500000	-2.417900000
H	0.143600000	1.221500000	3.296300000	H	-1.827100000	0.969600000	-2.981400000
H	2.334400000	-2.047500000	3.549300000	H	-3.698700000	-2.813100000	-1.747400000
H	4.442500000	-2.699200000	2.360200000	H	-4.880000000	-3.443600000	0.372000000
H	4.526200000	-2.522800000	-0.147700000	H	-3.971800000	-2.605100000	2.563700000
H	2.520100000	-1.641700000	-1.355400000	H	-1.929200000	-1.138100000	2.533100000
H	2.356400000	1.462100000	-1.594700000	H	-1.754600000	1.688100000	2.314300000
H	4.213500000	2.859000000	-0.642900000	H	-3.599200000	3.383900000	2.100700000
H	4.118800000	3.480300000	1.792300000	H	-4.396100000	4.006100000	-0.203400000
H	2.156600000	2.736700000	3.159300000	H	-3.301200000	2.940200000	-2.190700000
H	-1.485900000	0.096600000	-3.449300000	H	3.813300000	0.598100000	0.673800000
H	-2.529400000	0.048300000	2.558700000	H	1.024200000	-0.345800000	-3.144300000
O	3.236200000	-0.008100000	-3.119600000	O	2.911200000	1.208300000	3.104600000
O	2.237500000	-1.049500000	-3.475000000	O	2.663400000	-0.139000000	2.588800000
H	3.228300000	0.533100000	-3.950200000	H	3.736200000	1.027300000	3.626300000
H	1.417500000	-0.660700000	-3.041700000	H	1.676000000	-0.024200000	2.312000000

${}^4P_{\text{homo}}$				${}^6P_{\text{homo}}$			
C	-1.587900000	2.293800000	-1.277800000	C	1.919700000	-2.206100000	-1.519600000
C	-2.656900000	3.181000000	-1.223900000	C	2.984300000	-3.096600000	-1.423800000
C	-3.586000000	3.070900000	-0.192300000	C	3.779200000	-3.075200000	-0.280500000
C	-3.430800000	2.076900000	0.776700000	C	3.490200000	-2.171000000	0.744100000
C	-2.350200000	1.223200000	0.664200000	C	2.412700000	-1.318100000	0.578400000
N	-1.458600000	1.332400000	-0.351200000	N	1.650800000	-1.334200000	-0.536600000
C	-2.012200000	0.077000000	1.588800000	C	1.981900000	-0.273800000	1.591000000
C	-2.288900000	-1.196800000	0.824000000	C	2.361100000	1.080500000	1.023000000
C	-3.318400000	-2.087600000	1.060000000	C	3.410100000	1.856400000	1.485500000
C	-3.418200000	-3.209900000	0.234000000	C	3.663600000	3.072200000	0.846100000
C	-2.488100000	-3.403100000	-0.784400000	C	2.862700000	3.468300000	-0.222100000
C	-1.473100000	-2.471000000	-0.967600000	C	1.826700000	2.635000000	-0.630500000
N	-1.395600000	-1.389700000	-0.177500000	N	1.592400000	1.464100000	-0.019000000
N	-0.506800000	0.126200000	1.744200000	N	0.489300000	-0.321600000	1.650900000
C	0.068200000	-1.061200000	2.452900000	C	-0.122000000	0.764900000	2.460000000
C	0.004000000	1.427500000	2.283700000	C	-0.057800000	-1.658600000	2.001300000
C	1.201700000	1.864800000	1.493200000	C	-1.313800000	-1.946300000	1.222800000
C	1.279400000	-1.554200000	1.717700000	C	-1.409000000	1.233800000	1.834400000
C	2.270300000	-2.315400000	2.321500000	C	-2.508500000	1.619900000	2.588300000
C	3.322800000	-2.796000000	1.547200000	C	-3.642700000	2.101400000	1.935200000
C	3.358500000	-2.499600000	0.186400000	C	-3.643100000	2.195200000	0.545000000
C	2.350600000	-1.720400000	-0.361600000	C	-2.515200000	1.783200000	-0.151600000
N	1.333000000	-1.266100000	0.394000000	N	-1.426100000	1.306800000	0.481500000
N	1.282500000	1.390700000	0.226300000	N	-1.369700000	-1.456000000	-0.037400000
C	2.295500000	1.757000000	-0.580700000	C	-2.438800000	-1.712500000	-0.815200000
C	3.268900000	2.644100000	-0.144700000	C	-3.499200000	-2.485500000	-0.363700000
C	3.201400000	3.141800000	1.155100000	C	-3.453700000	-2.990100000	0.934900000
C	2.156700000	2.743100000	1.985200000	C	-2.348500000	-2.715300000	1.738700000
Fe	-0.013500000	0.005400000	-0.234700000	Fe	-0.011300000	0.079100000	-0.491600000
O	0.277800000	-0.071500000	-1.881600000	O	0.077800000	0.403900000	-2.331800000
O	-1.703400000	-0.247800000	-3.293200000	O	1.299000000	0.587700000	-3.101600000
H	-0.828400000	2.314000000	-2.056800000	H	1.262600000	-2.170400000	-2.388200000
H	-2.751000000	3.949500000	-1.989900000	H	3.178800000	-3.795300000	-2.236000000
H	-4.426900000	3.761800000	-0.133400000	H	4.617100000	-3.765100000	-0.178900000
H	-4.126500000	1.970700000	1.607200000	H	4.082400000	-2.137400000	1.657700000
H	-4.016400000	-1.911900000	1.876600000	H	4.009300000	1.522700000	2.331600000
H	-4.216400000	-3.934300000	0.394700000	H	4.479700000	3.708600000	1.188400000
H	-2.539500000	-4.271000000	-1.440300000	H	3.031100000	4.413000000	-0.737400000
H	-0.716800000	-2.552900000	-1.745300000	H	1.166300000	2.886000000	-1.460000000
H	0.296300000	-0.812500000	3.496600000	H	-0.275800000	0.441800000	3.499200000
H	-0.682700000	-1.865100000	2.460200000	H	0.568600000	1.621400000	2.478700000
H	-0.782500000	2.188300000	2.173600000	H	0.683100000	-2.426200000	1.732700000
H	0.229700000	1.337900000	3.353400000	H	-0.233900000	-1.737900000	3.083500000
H	2.210000000	-2.524200000	3.388900000	H	-2.476700000	1.538000000	3.674300000
H	4.112200000	-3.391800000	2.005200000	H	-4.521200000	2.395700000	2.509600000
H	4.165300000	-2.853700000	-0.453500000	H	-4.508100000	2.569500000	-0.000700000
H	2.337300000	-1.444000000	-1.412600000	H	-2.466500000	1.818900000	-1.239900000
H	2.311600000	1.306300000	-1.572300000	H	-2.433800000	-1.255600000	-1.805200000
H	4.075600000	2.924900000	-0.820400000	H	-4.349600000	-2.672300000	-1.017800000
H	3.962700000	3.828300000	1.525200000	H	-4.278800000	-3.586300000	1.325300000
H	2.076100000	3.104400000	3.009600000	H	-2.288200000	-3.089200000	2.760200000
H	-2.157500000	-0.186900000	-2.414700000	H	2.006000000	0.481300000	-2.412200000
H	-2.538000000	0.127000000	2.550900000	H	2.449700000	-0.444800000	2.571800000
O	3.041900000	0.052200000	-3.371200000	O	-2.939800000	0.473400000	-3.260500000
O	1.950100000	-0.889100000	-3.731700000	O	-2.000200000	1.593400000	-3.535100000
H	2.909800000	0.751200000	-4.061600000	H	-2.923000000	0.007400000	-4.135400000
H	1.236500000	-0.577300000	-3.081200000	H	-1.149900000	1.183300000	-3.176700000

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