Supporting Information

[OSSO]-Type Iron(III) Complexes for the Low-Pressure Reaction of Carbon Dioxide with Epoxides: Catalytic Activity, Reaction Kinetics and Computational Study

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Summary

General Considerations

All manipulation involving air- and/or moisture-sensitive compounds were performed under nitrogen atmosphere using standard Schlenk technique and a MBraun glovebox. Toluene (99.5%; Sigma-Aldrich) and THF (99%; Sigma-Aldrich) were used as received or refluxed for 48 h over sodium or sodium ketyls and distilled before use for moisture- and oxygen-sensitive reactions. All other reagents were used as received (TCI or Sigma-Aldrich) or distilled under reduced pressure over calcium hydride. Deuterated solvents were purchased from Euriso-Top or Sigma-Aldrich and used as received. NMR spectra were collected on Bruker Avance spectrometers (600, 400, 300 or 250 MHz for ^{1}H): the chemical shifts were referenced to tetramethylsilane (TMS) as external reference using the residual protio signal of the deuterated solvents. 2-mercapto-4-metyl-6-trithylphenol was prepared as reported in reference 19. Measurements of effective magnetic moments were performed on a Bruker Avance 400 MHz spectrometer in toluene-d_8 using a 5 mm Wilmad coaxial insert NMR tube. High resolution Electrospray Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry (ESI FT-ICR MS) measurements of complexes were performed on a Bruker Solaris XR instrument. The effective magnetic moment (μ_{eff}) was calculated from $\mu_{eff} = 8\chi_g MwT$, where χ_g ($cm^3\ g^{-1}$) is the corrected molar susceptibility derived from $\chi_g = 3\Delta f/4\pi f_o CMw + \chi_o$. Δf is the shift in frequency (Hz) of the residual protio signal of the solvent in the presence of the complex from the value of the pure solvent, C and Mw are respectively the concentration (mol cm^{-3}) and the molecular weight of the complex (g mol^{-1}), f_0 is the operating frequency of the spectrometer (Hz), and χ_0 is the mass susceptibility of the pure solvent (-0.6179×10^{-6} $cm^3\ g^{-1}$ for toluene-d_8). $4\pi/3$ is the shape factor for a cylindrical sample in a superconducting magnet. Elemental analysis was performed on a CHNS Thermo Scientific Flash EA 1112 equipped with a thermal conductivity detector. FT-IR measurements were carried out on a Bruker Vertex 70 spectrometer equipped with DTGS detector and a Ge/KBr beam splitter. The samples were analyzed in the solid state as KBr disks. UV-Vis spectra were collected on a PerkinElmer Lambda EZ 201 spectrophotometer. The molecular weights (Mn and Mw) and the molecular weights distributions (Mw/Mn) of polymer samples were measured by gel permeation chromatography (GPC) at 30 °C using THF as the solvent, a flow rate of the eluent of 1 mL/min, and narrow polystyrene standards as the references. The measurements were performed on a Waters 1525 binary system equipped with a Waters 2414 RI detector using four Styragel columns (range 1000–1 000 000 Å). Differential scanning calorimetry (DSC) thermograms were recorded using a DSC 2920 (TA Instruments) in nitrogen flow with a heating and cooling rate of 10 °C min^{-1} in the range from 20 to 150 °C.

Synthesis of the [OSSO]-type ligand L1

A 100 mL two-neck round-bottom flask equipped with condenser and magnetic stirring bar was charged with 6.32 g of 2-mercapto-4-metyl-6-trithylphenol (16.5 mmol) dissolved in 15 mL of ethanol, 0.67 g of NaOH (16.8 mmol) and the mixture was refluxed about 1 hour until complete dissolution of the hydroxide. 1.56 g of 1,2-dibromomethane (8.3 mmol) were slowly added at 0 °C and the mixture heated to the reflux of the solvent that was kept overnight. The solvent was distilled off, water was added until dissolution of NaBr by-product and the aqueous phase extracted twice with CH_2Cl_2. The combined organic phases were dried with MgSO4, after evaporation of the solvent the product was purified by crystallization from acetonitrile and recovered as a pale yellow solid. Yield: 5.16 g, 79%. ^{1}H-NMR (400 MHz, CD_2Cl_2, 25 °C): δ 2.15 (6H, s); 2.51 (4H, s); 6.37 (2H, s, -OH); 7.01-7.23 (32H, overlapped signals, Ar-H). ^{13}C-NMR (400 MHz, CD_2Cl_2, 25 °C): δ 16.47; 20.34; 31.27; 34.08; 37.17; 117.18; 124.04; 124.20; 127.55; 129.60; 133.75; 134.12; 143.46; 150.09; 153.56. EA for $C_{28}H_{34}O_3S_2$ calc.: C, 69.67; H, 7.10; S 13.29; found: C, 69.55; H, 7.09; S, 13.18. Mass spectrum: 505.0 m/z (MNa^+).

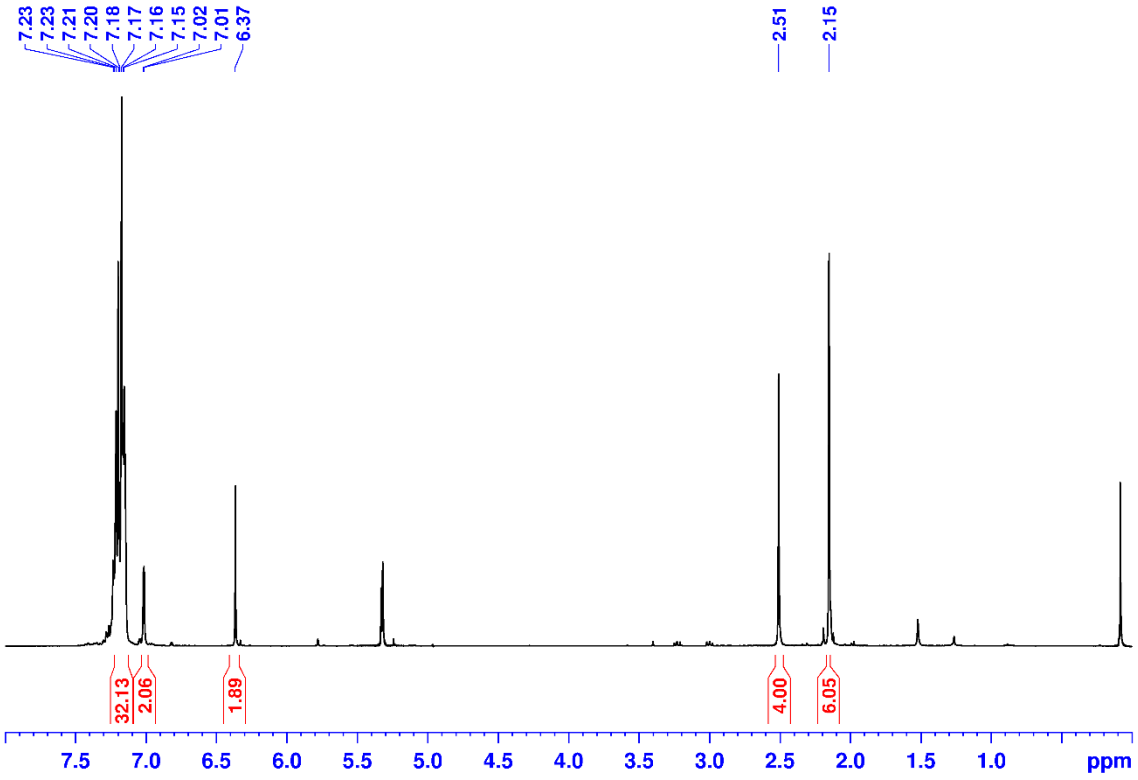


Figure S1 ^{1}H NMR spectra of pro-ligand **L1** (CD_2Cl_2, 400 MHz).

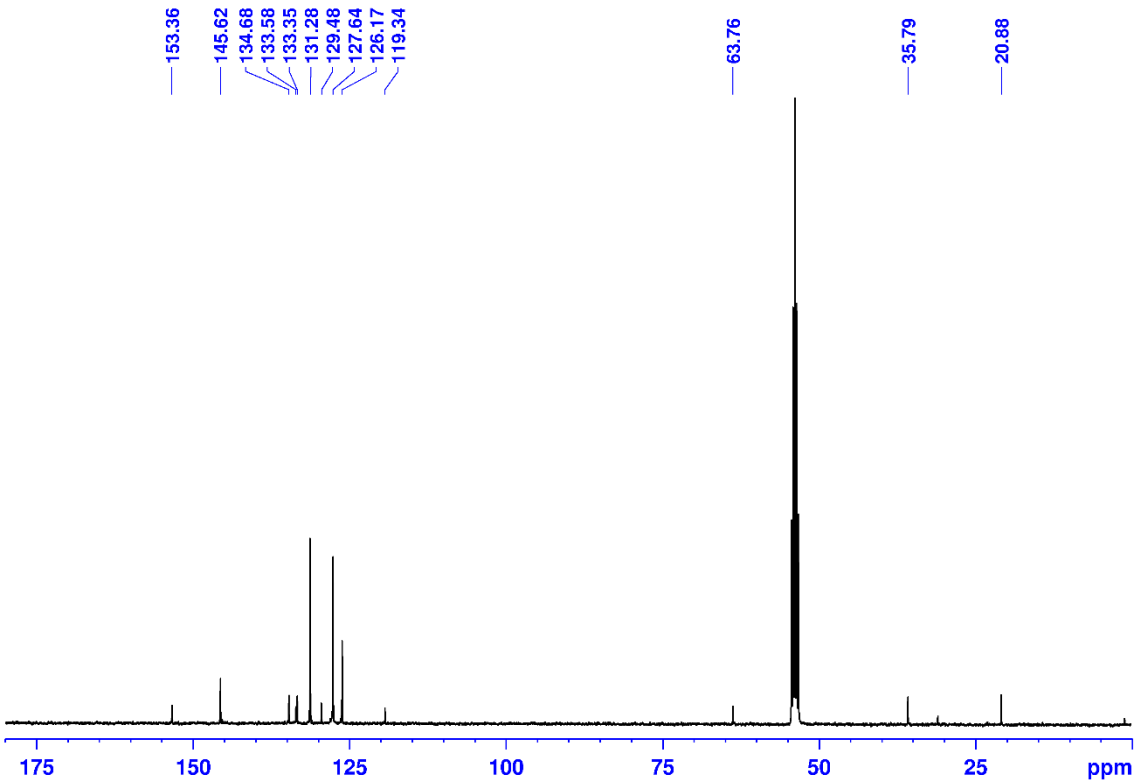


Figure S2 ^{13}C NMR spectra of pro-ligand **L1** (CD_2Cl_2, 400 MHz).

Synthesis of the iron(III) complex 1

Pro-ligand **L1** (0.530 g; 0.67 mmol) was dissolved in THF (20 mL). The solution was added to a suspension of sodium hydride (0.035 g; 1.47 mmol) in THF (10 mL) and the mixture stirred at room temperature overnight. The resulting suspension was filtered through celite and slowly added at room temperature to 0.106 g of anhydrous iron(III) chloride (0.66 mmol) dissolved in 20 mL of THF. The rapid change of the color to the deep purple was observed and the reaction kept overnight. The mixture was then filtered through celite and the solvent removed under reduced pressure affording a deep purple crystalline solid. Yield: 0.566 g, 90.0 %. Elemental analysis calcd. for $C_{58}H_{52}ClFeO_3S_2$: C, 73.14; H, 5.50; S, 6.73; found: C, 73.01; H, 5.43; S, 6.68. Mass spectrum: 844.2146 m/z (LFe^+, calc: 844.21267).

Synthesis of the iron(III) complex 2

Pro-ligand **L2** (7.170 g; 9.55 mmol) was dissolved in THF (150 mL). The solution was added to a suspension of sodium hydride (0.50 g; 21.0 mmol) in THF (50 mL) and the mixture stirred at room temperature overnight. The resulting suspension was filtered through celite and slowly added at room temperature to 1.117 g of anhydrous iron(III) chloride (9.36 mmol) dissolved in 150 mL of THF. The rapid change of the color to the deep purple was observed and the reaction kept overnight. The mixture was then filtered through celite and the solvent removed under reduced pressure affording a deep purple crystalline solid. Yield: 7.76 g, 90.9 %. Elemental analysis calcd. for $C_{54}H_{60}ClFeO_3S_2$: C, 71.08; H, 6.63; S, 7.03; found: C, 71.02 H, 6.66; S, 6.97. Mass spectrum: 804.2775 m/z (LFe^+, calc: 844.27527).

Synthesis of the iron(III) complex 3

Pro-ligand **L3** (1.256 g; 3.75 mmol) was dissolved in THF (100 mL). The solution was added to a suspension of sodium hydride (0.198 g; 8.26 mmol) in THF (45 mL) and the mixture stirred at room temperature overnight. The resulting suspension was filtered through celite and slowly added at room temperature to 0.597 g of anhydrous iron(III) chloride (3.68 mmol) dissolved in 100 mL of THF. The rapid change of the color to the deep purple was observed and the reaction kept overnight. The mixture was then filtered through celite and the solvent removed under reduced pressure affording a deep purple crystalline solid. Yield: 1.70 g, 93.2 %. Elemental analysis calcd. for $C_{22}H_{28}ClFeO_3S_2$: C, 53.29; H, 5.69; S, 12.93; found: C, 53.18 H, 5.61; S, 12.86. Mass spectrum: 610.26009 m/z (LFe^+, calc: 610.25962).

Synthesis of the iron(III) complex 4

Pro-ligand **L4** (2.000 g; 3.59 mmol) was dissolved in THF (100 mL). The solution was added to a suspension of sodium hydride (0.190 g; 7.92 mmol) in THF (45 mL) and the mixture stirred at room temperature overnight. The resulting suspension was filtered through celite and slowly added at room temperature to 0.571 g of anhydrous iron(III) chloride (3.52 mmol) dissolved in 100 mL of THF. The rapid change of the color to the deep purple was observed and the reaction kept overnight. The mixture was then filtered through celite and the solvent removed under reduced pressure affording a deep purple crystalline solid. Yield: 2.45 g, 96.9 %. Elemental analysis calcd. for $C_{38}H_{58}ClFeO_3S_2$: C, 63.54; H, 8.14; S, 8.93; found: C, 63.50 H, 8.22; S, 8.88. Mass spectrum: 388.02484 m/z (LFe^+, calc: 388.02486).

ESI FT-ICR MS Analysis

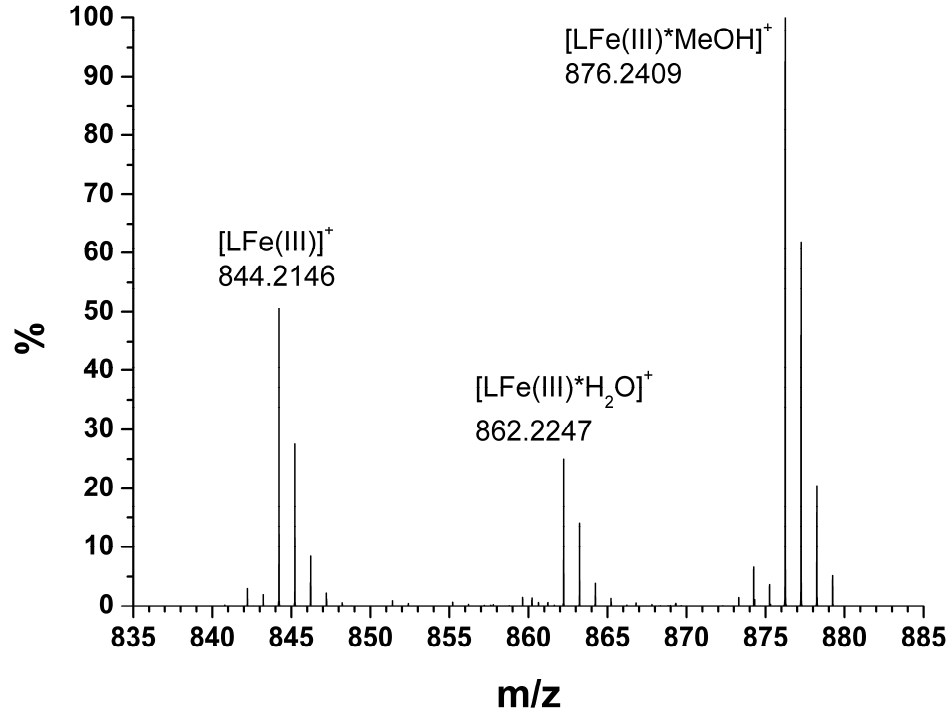


Figure S3. ESI FT-ICR MS of complex **1**. Calcd.: $[LFe(III)]^+$ = 844.2132 uma; $[LFe(III)*H2O]^+$ = 862.22378 uma; $[LFe(III)*MeOH]^+$ = 876.23943 uma.

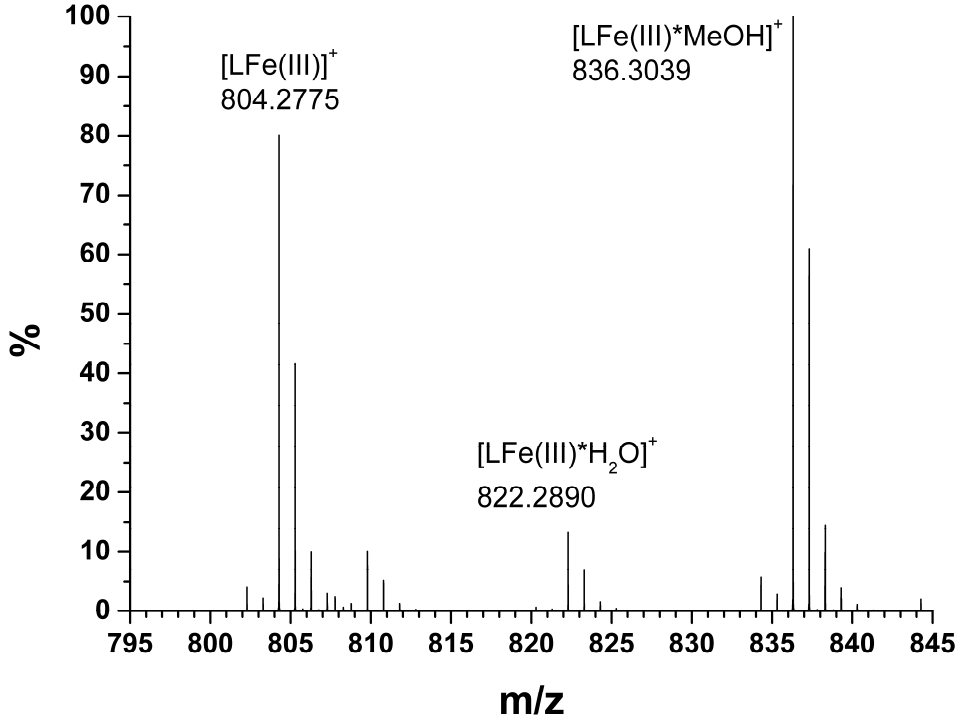


Figure S4. ESI FT-ICR MS of complex **2**. Calcd.: $[LFe(III)]^+$ = 804.27527 uma; $[LFe(III)*H_2O]^+$ = 822.28583 uma; $[LFe(III)*MeOH]^+$ = 836.30148 uma.

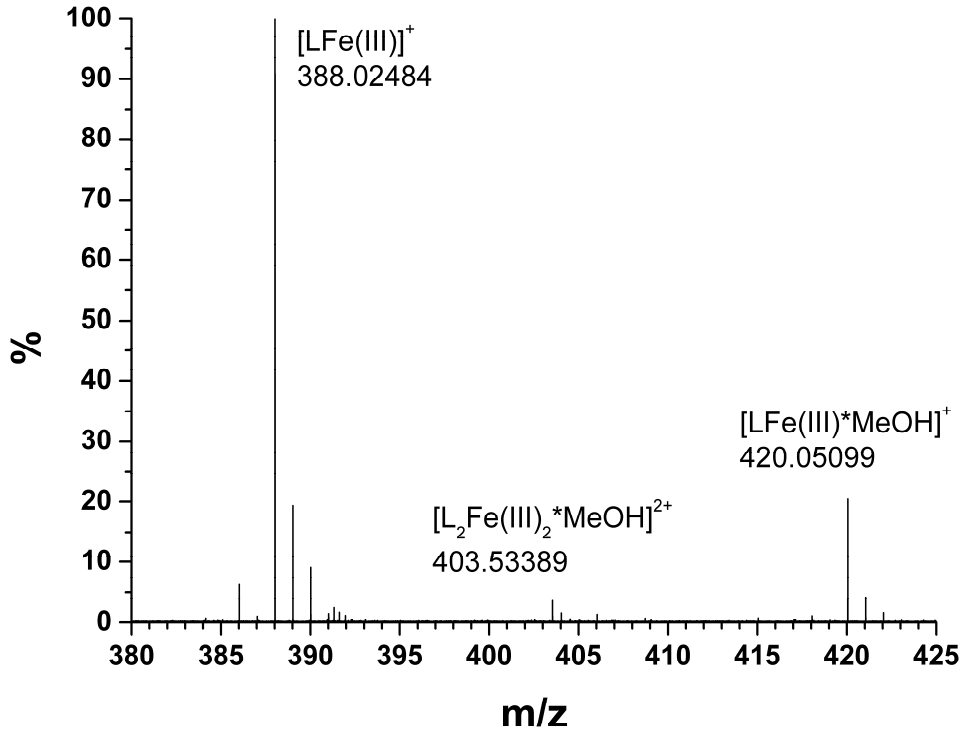


Figure S5. ESI FT-ICR MS of complex **3**. Calcd.: $[LFe(III)]^+$ = 388.02541 uma; $[L_2Fe_2*MeOH]^{2+}$ = 403.53461 uma; $[LFe*MeOH]^+$ = 420.05108 uma.

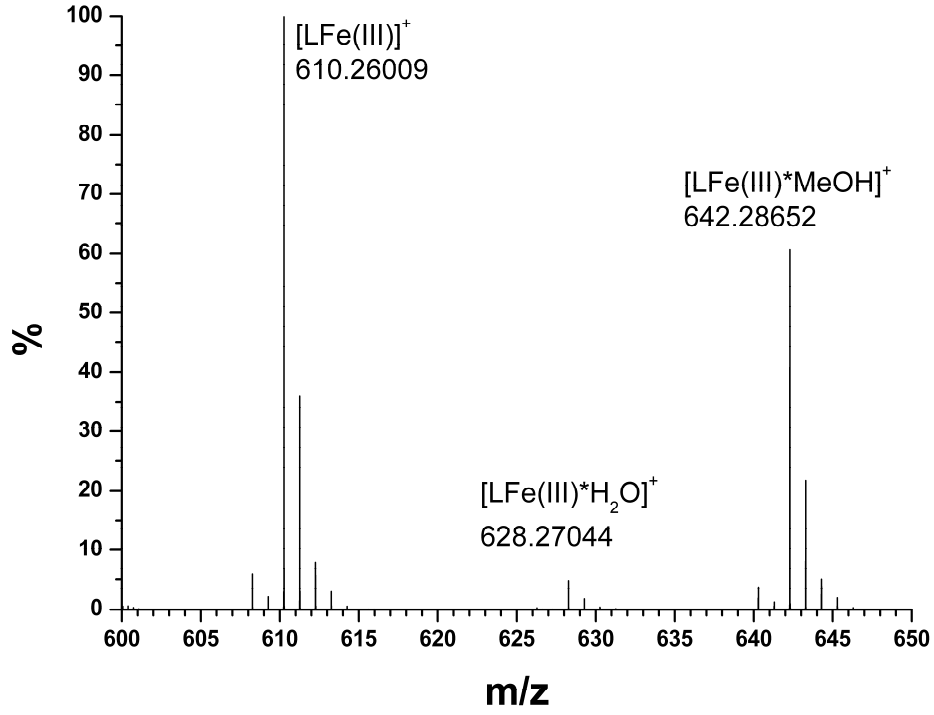
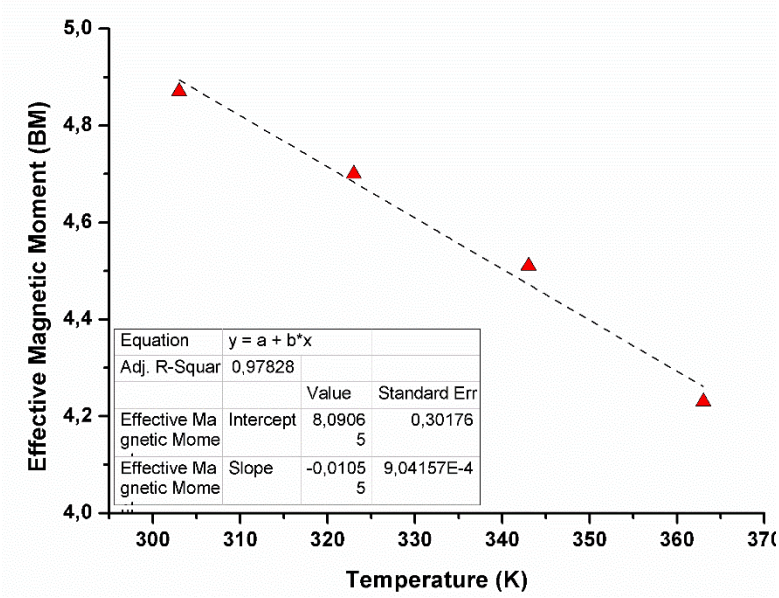


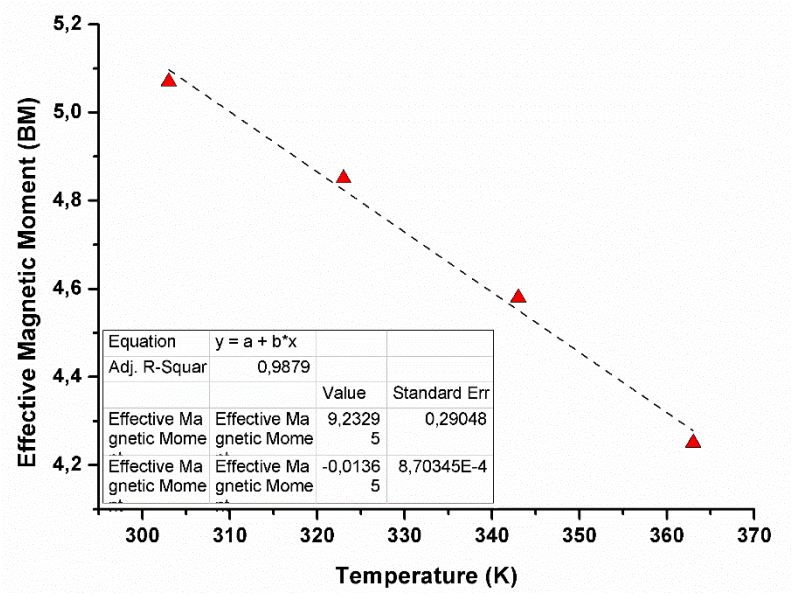
Figure S6. ESI FT-ICR MS of complex **4**. Calcd.: $[LFe(III)]^+$ = 610.25962 uma; $[LFe(III)*H_2O]^+$ = 628.27018 uma; $[LFe(III)*MeOH]^+$ = 642.28638 uma.

Evans Method Analysis



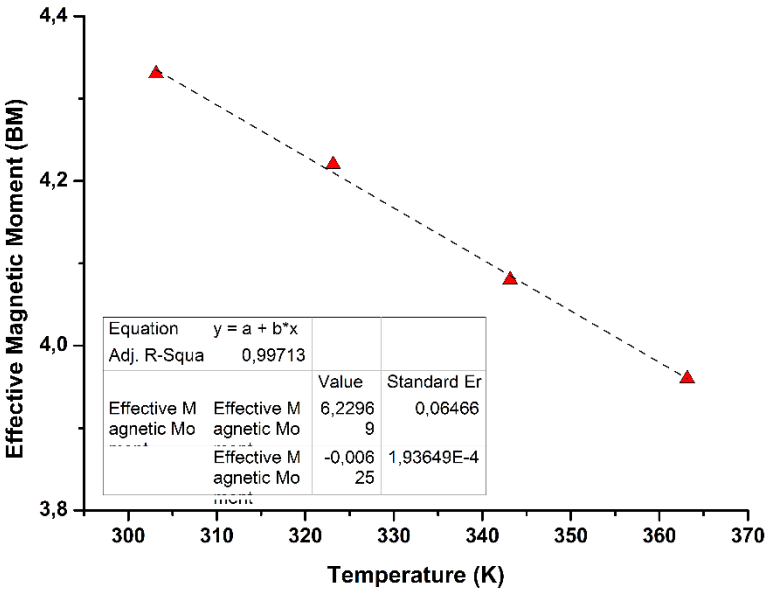
μ_{eff} (μ_B)	T (K)
4.87 ± 0.01	303
4.70 ± 0.01	323
4.51 ± 0.01	343
4.23 ± 0.01	363

Figure S7. Linear plot of effective magnetic moment μ_{eff} of complex **1** versus temperature.



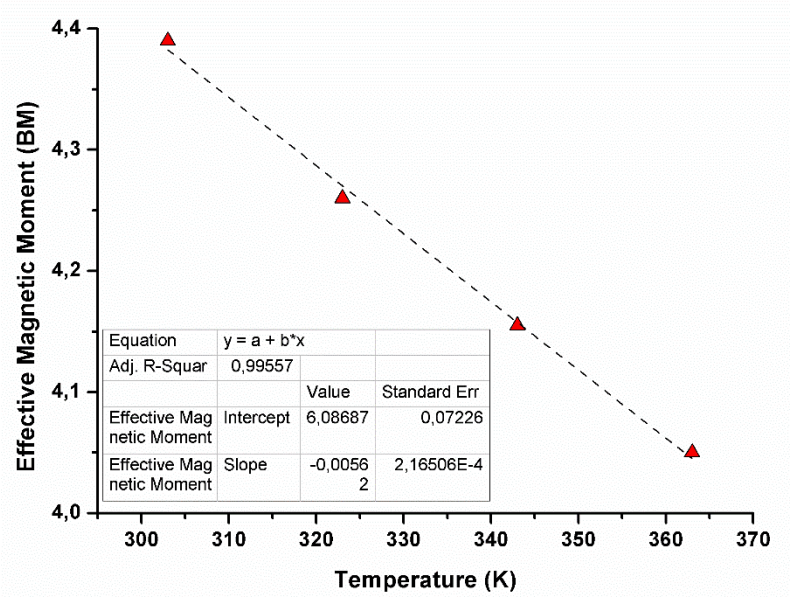
μ_{eff} (μ_B)	T (K)
5.07 ± 0.01	303
4.85 ± 0.01	323
4.58 ± 0.01	343
4.25 ± 0.01	363

Figure S8. Linear plot of effective magnetic moment μ_{eff} of complex **2** versus temperature.



μ_{eff} (μ_B)	T (K)
4.33 ± 0.01	303
4.22 ± 0.01	323
4.08 ± 0.01	343
3.96 ± 0.01	363

Figure S9 Linear plot of effective magnetic moment μ_{eff} of complex **3** versus temperature.



μ_{eff} (μ_B)	T (K)
4.39 ± 0.01	303
4.26 ± 0.01	323
4.16 ± 0.01	343
4.05 ± 0.01	363

Figure S10. Linear plot of effective magnetic moment μ_{eff} of complex **4** versus temperature.

FT-IR analysis

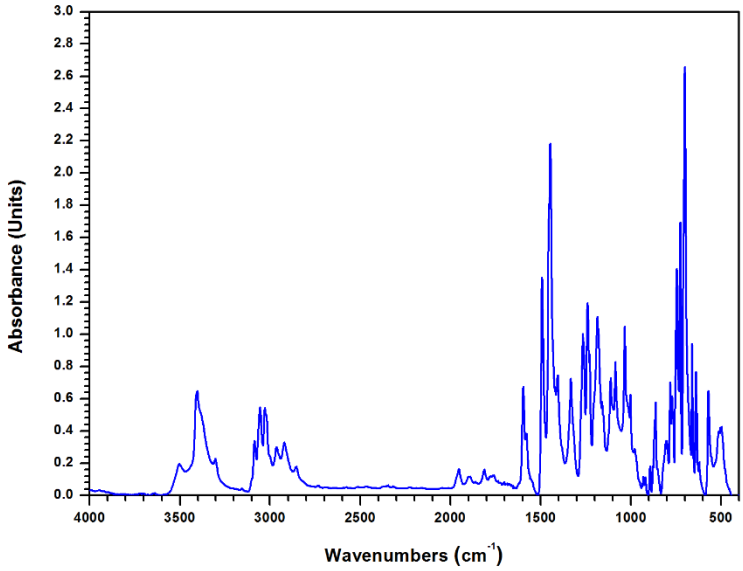


Figure S11 FT-IR spectrum of the pro-ligand **L1** (KBr disk).

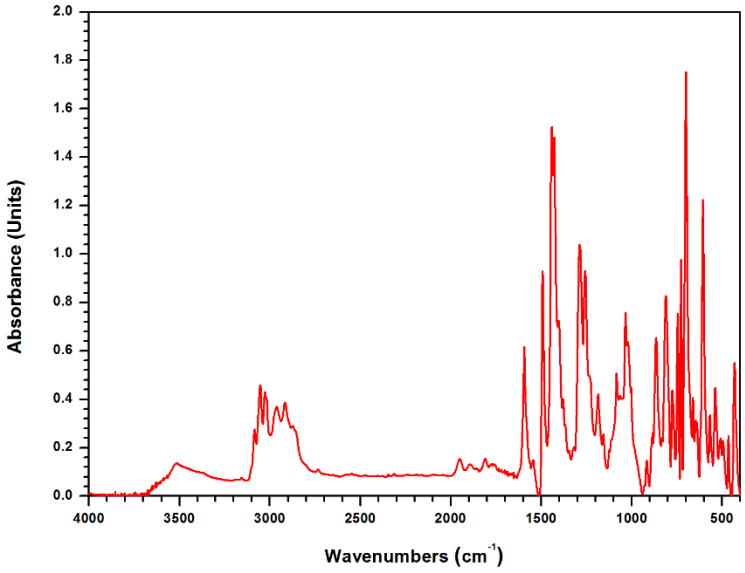


Figure S12 FT-IR spectrum of the iron(III) complex **1** (KBr disk).

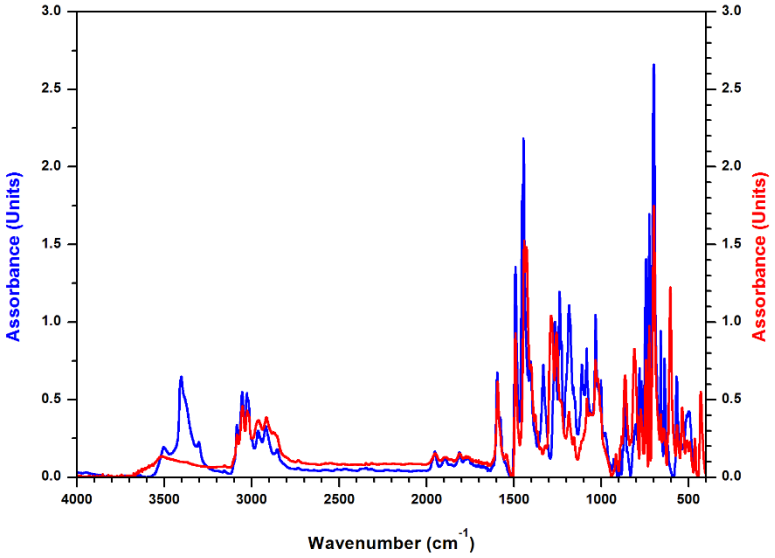


Figure S13 Comparison of the FT-IR spectra of the pro-ligand **L1** (blue curve) and of the iron(III) complex **1** (red curve)

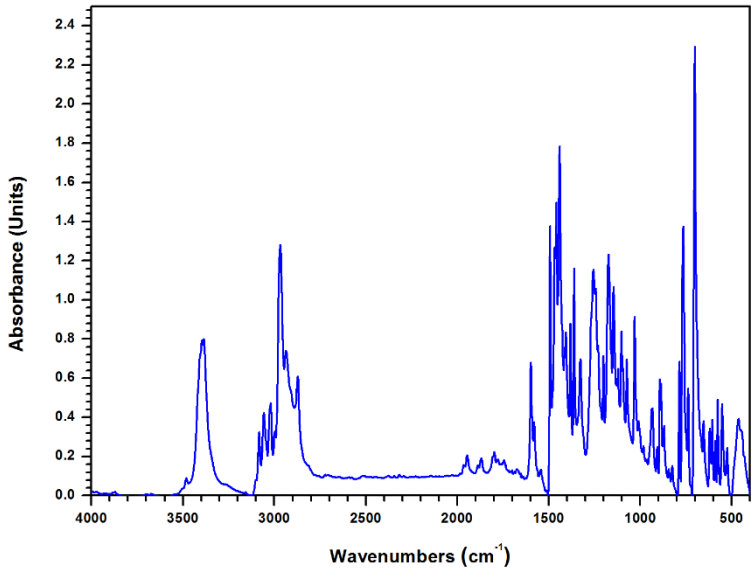


Figure S14 FT-IR spectrum of the pro-ligand **L2** (KBr disk).

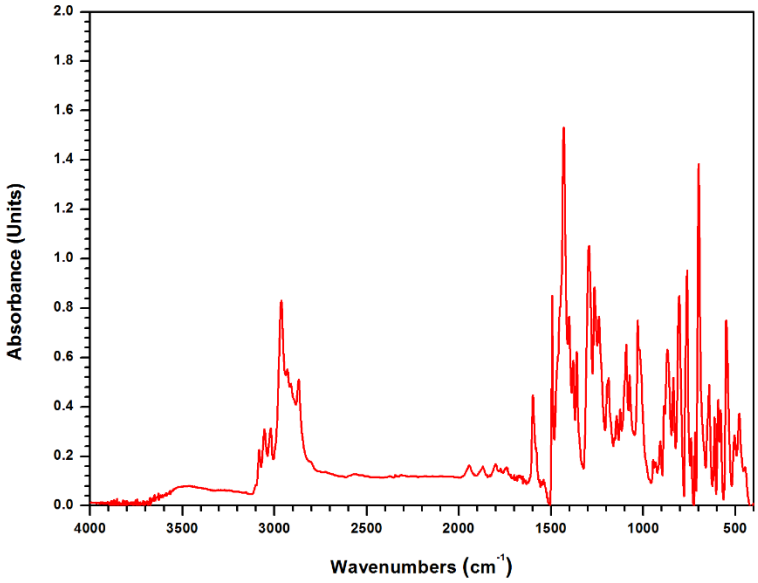


Figure S15 FT-IR spectrum of the iron(III) complex **2** (KBr disk).

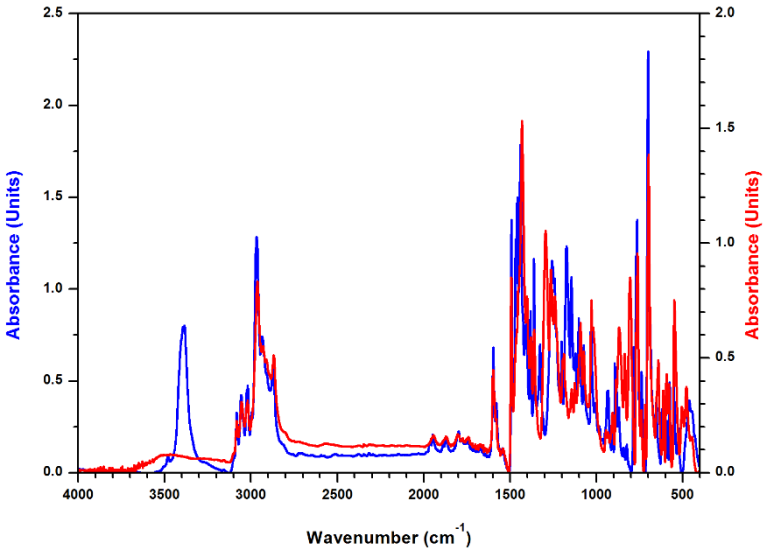


Figure S16 Comparison of the FT-IR spectra of the pro-ligand **L2** (blue curve) and of the iron(III) complex **2** (red curve)

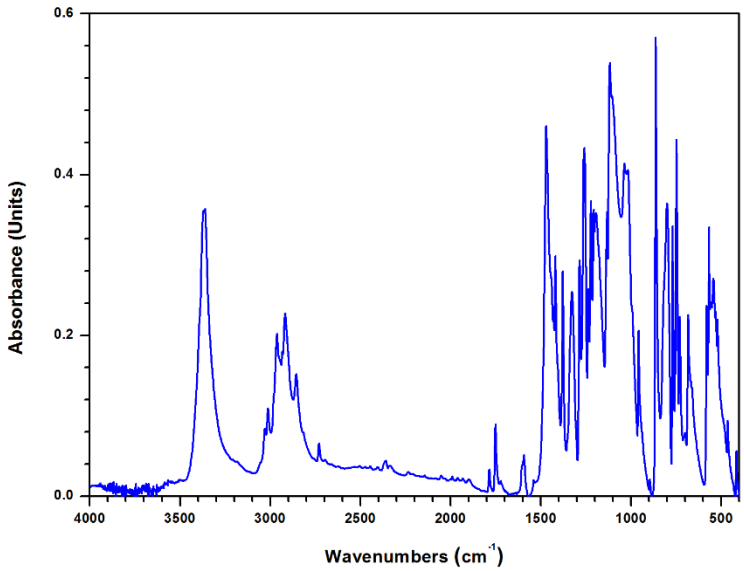


Figure S17 FT-IR spectrum of the pro-ligand **L3** (KBr disk).

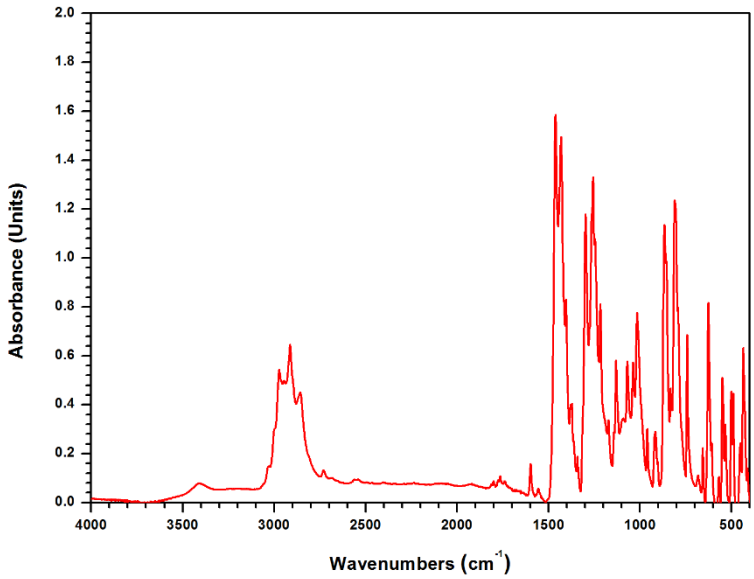


Figure S18 FT-IR spectrum of the iron(III) complex **3** (KBr disk).

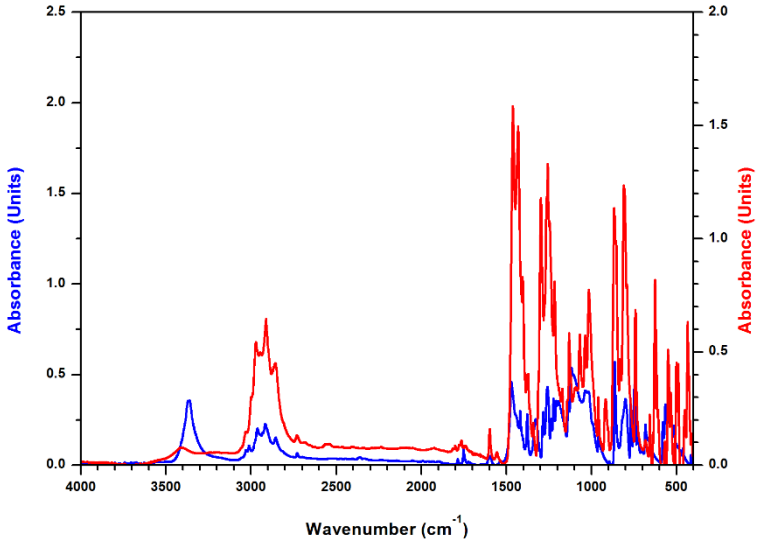


Figure S19 Comparison of the FT-IR spectra of the pro-ligand **L3** (blue curve) and of the iron(III) complex **3** (red curve)

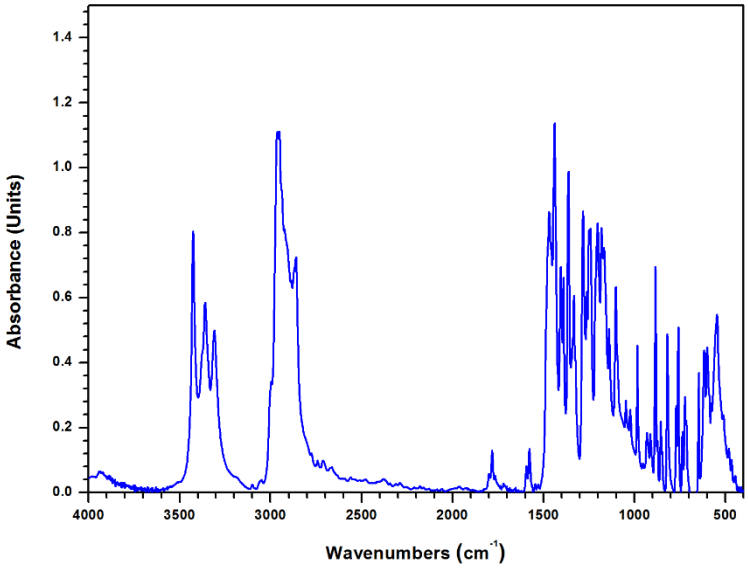


Figure S20 FT-IR spectrum of the pro-ligand **L4** (KBr disk).

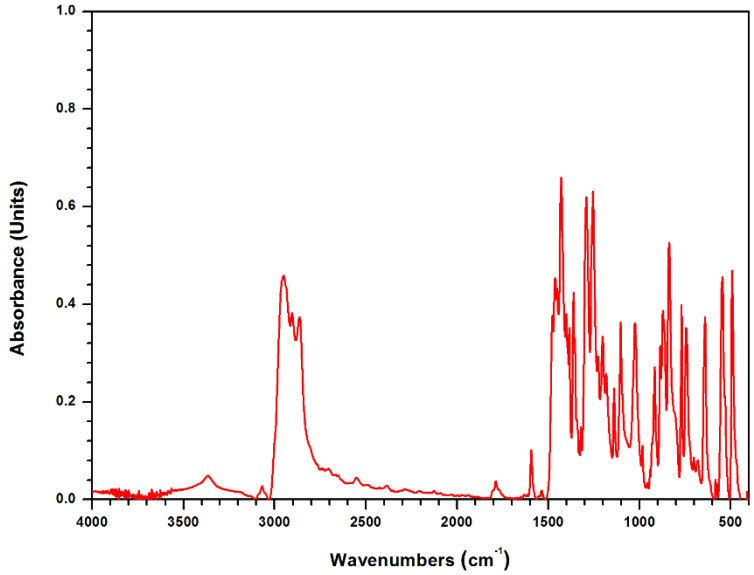


Figure S21 FT-IR spectrum of the iron(III) complex **4** (KBr disk).

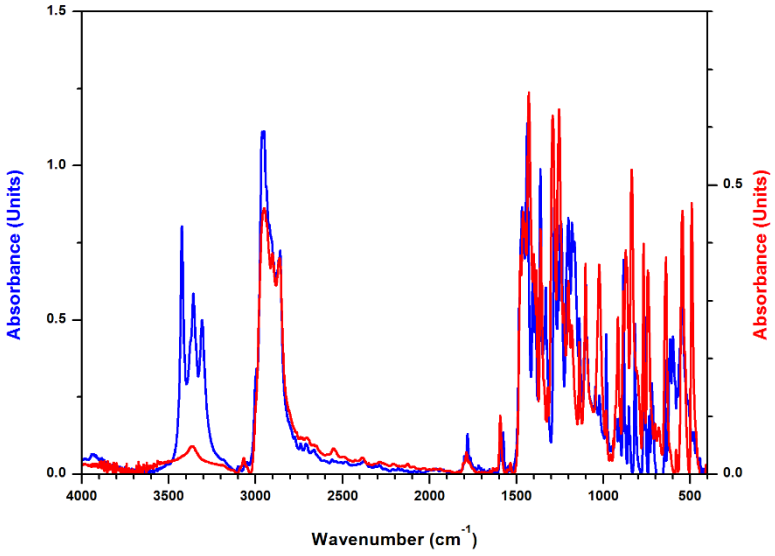


Figure S22 Comparison of the FT-IR spectra of the pro-ligand **L4** (blue curve) and of the iron(III) complex **4** (red curve).

Crystallographic data of the Iron(III) complex 2

The X-ray intensity data for **2** used for collecting frames of data, indexing reflections, and determining lattice parameters. The collected frames were then processed for integration by the SAINT program,[1] and an empirical absorption correction was applied using SADABS[1].The structure was solved by direct methods (SIR 97)[2] and subsequent Fourier syntheses and refined by full-matrix least squares on F^2 (SHELXL)[3], using anisotropic thermal parameters for all non-hydrogen atoms. All hydrogen atoms were added in calculated positions, included in the final stage of refinement with isotropic thermal parameters, U(H) = 1.2[Ueq(C)] (U(H) = 1.5[Ueq(C-Me)]), and allowed to ride on their carrier carbons. In the asymmetric unit of compound **2** one CH_3CN solvent molecule is present. Crystal data and details of the data collection for **2** are reported in Table S1.

CCDC 1564256 contains supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1 Crystal data and structure refinement for complex **2**.

Compound	**2**
Formula	$C_{52}H_{55}ClFeN\ O_2S_2.CH_3CN$
Fw	922.44
T, K	293
λ, Å	0.71073
Crystal symmetry	Monoclinic
Space group	$P2_1/c$
a, Å	17.208(4)
b, Å	10.880(3)
c, Å	27.059(6)
α	90
β	101.257(7)
γ	90
Cell volume, Å^3	4969(2)
Z	4
D_C, Mg m^{-3}	1.233
μ(Mo-K_α), mm^{-1}	0.482
F(000)	1948
Crystal size/ mm	0.44 x 0.37 x 0.31
θ limits, °	1.535 to 26.000
Reflections collected	45659
Unique obs. Reflections [$F_o > 4\sigma(F_o)$]	9749 [R(int) = 0.0309]
Goodness-of-fit-on F^2	1.141
R_1 (F)[a], wR_2 (F^2)[b] [$I > 2\sigma(I)$]	0.0412, 0.1251
Largest diff. peak and hole, e. Å^{-3}	0.750 and -0.796

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$ where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ where $P = (F_o^2 + F_c^2)/3$.

Catalytic Activity

Typical procedure for CO_2/epoxide coupling to cyclic carbonates (referred to entry 1, Table 1)

A 60 mL stainless steel pressure reactor equipped with a magnetic stirring bar was charged, under CO_2 atmosphere, with 39.5 mg of catalyst **1** ($4.15 \cdot 10^{-5}$ mol) and 66.9 mg of TBAB ($2.07 \cdot 10^{-4}$ mol) dissolved in 5.0 mL of **5a** ($4.15 \cdot 10^{-2}$ mol). The reaction mixture was pressurized with CO_2 at 1 bar and stirred at 35 °C for 6 h. The reactor was cooled with ice, the CO_2 released, 0.58 mL of mesitylene ($4.15 \cdot 10^{-3}$ mol) was added as an internal standard and the mixture was analyzed by ^{1}H NMR spectroscopy using $CDCl_3$ as solvent (Figure S23). Conversion = 33.0 %.

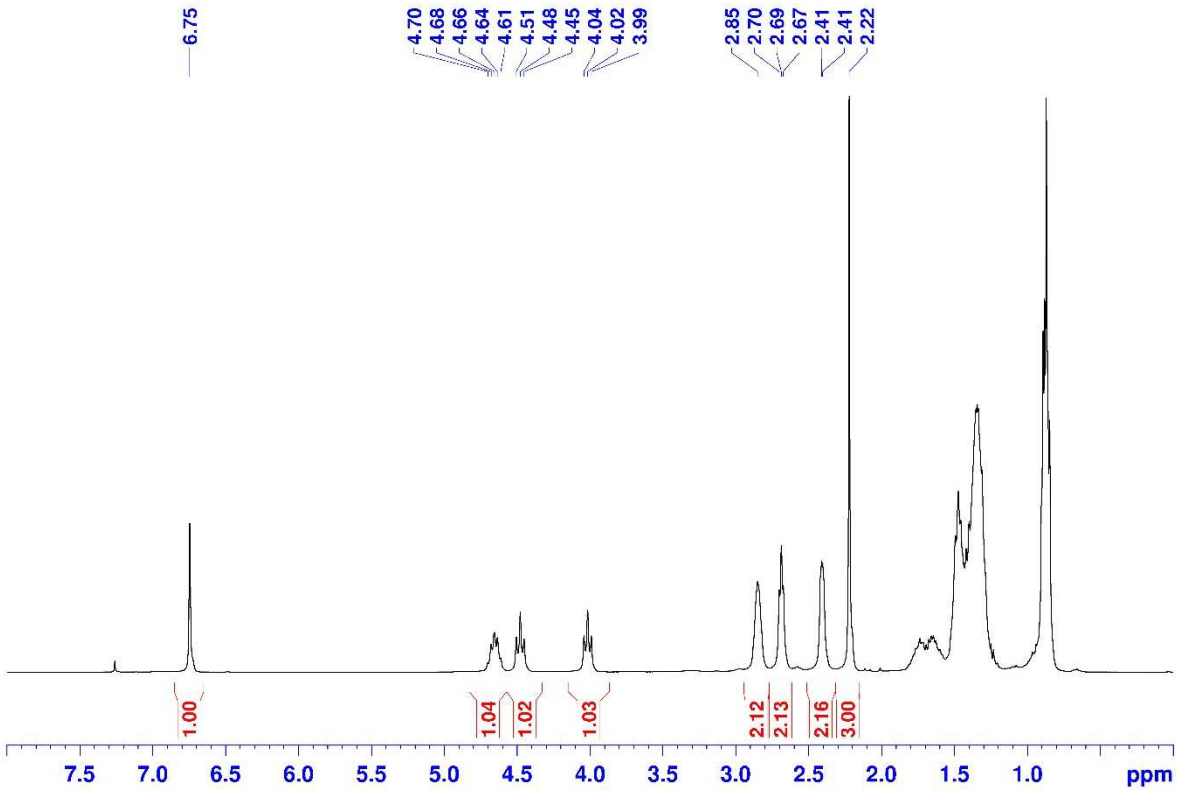
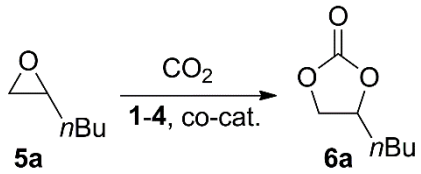


Figure S23 ^{1}H NMR spectra of an aliquot of the reaction mixture for the formation of **6a** from **5a** and CO_2 (entry 1, Table 1), for the determination of the conversion, in the presence of 10 mol% of mesitylene as internal standard ($CDCl_3$, 400 MHz).

Table S2. **5a**/CO_2 coupling promoted by the Iron(III) complexes **1**-**4**[a]



5a **6a**

Entry	Catalyst	Co-catalyst (mol%)	Temperature (°C)	Conversion (%)[b]	TON[c]	TOF (h^{-1})[d]
1	**1**	TBAB (0.1)	35	15.2	152	6.3
2	**2**	TBAB (0.1)	35	16.5	165	6.9
3	**3**	TBAB (0.1)	35	8.2	82	3.4
4	**4**	TBAB (0.1)	35	32.3	323	13.5
5	**4**	TBAB (0.1)	20	18.7	187	7.8
6	**4**	TBAB (0.1)	50	47.4	474	19.8
7	**4**	TBAB (0.1)	70	56.6	566	23.6
8	**4**	DMAP (0.1)	35	2.5	25	1
9	**4**	[PPN]Cl (0.1)	35	31.5	315	13.1
10	**4**	$TABN_3$ (0.1)	35	20.6	206	8.6
11	**4**	TBAC (0.1)	35	29.1	291	12.1
12	**4**	TBAI (0.1)	35	30.8	308	12.8
13	**4**	TBAB (0.2)	35	57.7	577	24
14	**4**	TBAB (0.5)	35	88.9	889	37
15	**4**	TBAB (1.0)	35	93	930	38.8

[a]Reaction conditions: **5a** = 5.0 mL, $4.15 \cdot 10^{-2}$ mol; Catalyst = $4.15 \cdot 10^{-5}$ mol (0.1 mol%); $P(CO_2)$ = 1 bar; reaction time = 24 h, neat. [b]Determined by ^1H NMR using mesitylene as internal standard. The selectivity toward the formation of **6a** was always found to be >99%. [c]Turnover number ($mol_{\mathbf{6a}} \cdot mol_{Catalyst}^{-1}$). [d]Turnover frequency ($mol_{\mathbf{6a}} \cdot mol_{Catalyst}^{-1} \cdot$ reaction $time^{-1}$).

Typical procedure for CO_2/5m co-polymerization to 6m (referred to entry 6, Table 2)

A 60 mL stainless steel pressure reactor equipped with a magnetic stirring bar was charged, under CO_2 atmosphere, with 49.8 mg of catalyst **2** ($5.93 \cdot 10^{-5}$ mol) and 16.5 mg of TBAC ($5.93 \cdot 10^{-5}$ mol) dissolved in 6.0 mL of **5m** ($5.93 \cdot 10^{-2}$ mol). The reaction mixture was pressurized with CO_2 at 10 bar and stirred at 80 °C for 1 h. The reactor was cooled with ice, the CO_2 released, 5 mL of CH_2Cl_2 was added to dissolve the sample and an aliquot was analyzed by ^{1}H NMR spectroscopy using $CDCl_3$ as solvent to determine the selectivity toward the polymer. The reaction mixture was poured into acidified methanol. The polymer was collected, dissolved in CH_2Cl_2, reprecipitated from methanol and dried in vacuum. Polymer composition was determined from ^{1}H NMR of isolated sample (Figure S24). Yield 3.36 g (40.0 %).

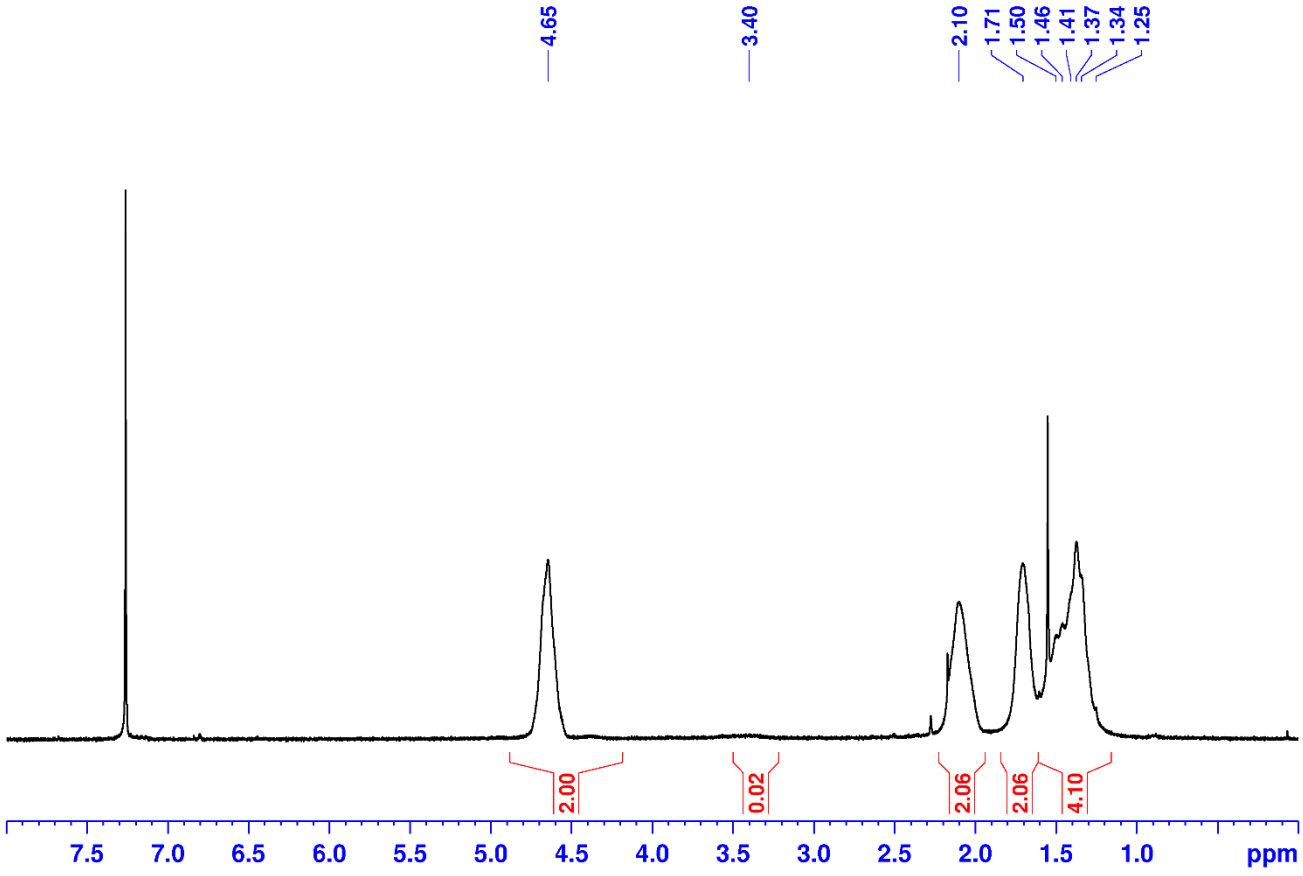
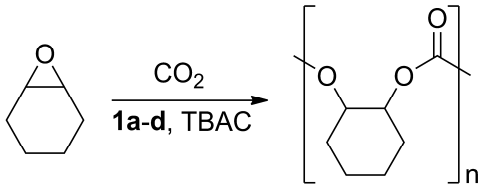


Figure S24 ^{1}H NMR spectra of **6m** isolated from MeOH (99% linkage carbonate) (entry 6, Table 2) ($CDCl_3$, 250 MHz).

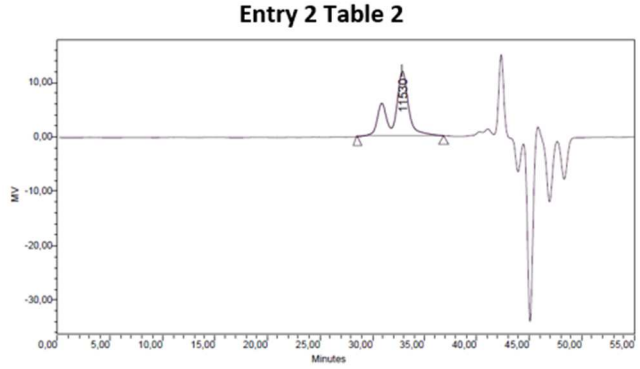
Table S3. **5m**/CO_2 co-polymerization promoted by the Iron(III) complexes **1**-**4**[a]



Entry	Catalyst (mol%)	Co-catalyst (mol%)	Temperature (°C)	P(CO2) (bar)	Time (h)	Conversion[b] (%)	TOF[c] (h^{-1})	Carbonate linkage[d] (%)	M_n(1)[e] (kDa)	PDI(1)[e]	M_n(2)[e] (kDa)	PDI(2)[e]	M_n(1)/M_n(2)[e]
1	**4** (0.2)	TBAB (1.0)	50	10	24	70	15	98	24.3	1.01	11.2	1.04	6/94
2	**1** (0.1)	TBAB (0.1)	80	10	2	22	110	99	21.1	1.01	10.1	1.03	12/88
3	**2** (0.1)	TBAB (0.1)	80	10	2	41	205	99	32.1	1.01	15.8	1.03	11/89
4	**3** (0.1)	TBAB (0.1)	80	10	2	traces	-	n.d.	-	-	-	-	-
5	**4** (0.1)	TBAB (0.1)	80	10	2	20.5	103	99	19.1	1.01	8.9	1.03	15/85
6	**2** (0.1)	-	80	10	1	traces	-	n.d.	-	-	-	-	-
7	**2** (0.1)	-	80	10	6	16	27	7	63.4	1.4	-	-	-
8	**2** (0.1)	DMAP (0.1)	80	10	6	47	78	99	12.2	1.21	-	-	-
9	**2** (0.1)	DMAP (0.1)	80	10	1	4.5	45	n.d.	-	-	-	-	-
11	**2** (0.1)	[PPN]Cl(0.1)	80	10	1	30.3	300	99	17.5	1.01	8.5	1.04	19/81
12	**2** (0.1)	TBAB (0.1)	80	10	1	19.3	190	99	11.8	1.01	5.2	1.03	38/62
13	**2** (0.1)	TBAI (0.1)	80	10	1	21.2	210	98	14.4	1.01	6.2	1.04	23/77
14	**2** (0.1)	$TABN_3$ (0.1)	80	10	1	29.4	290	99	19.6	1.01	9.4	1.03	23/77
15	**2** (0.1)	TBAC (0.05)	80	10	1	14.5	145	98	10.1	1.01	4.5	1.03	42/68
16	**2** (0.1)	TBAC (0.1)	80	10	1	34.0	340	99	23.2	1.01	11.0	1.03	31/69
17	**2** (0.1)	TBAC (0.2)	80	10	1	40.4	400	99	22.3	1.01	10.9	1.02	24/76
18	**2** (0.1)	TBAC (0.5)	80	10	1	26.6	265	99	7.7	1.01	3.4	1.05	9/91
19	**2** (0.1)	TBAC (0.1)	40	10	1	2	20	n.d.	-	-	-	-	-
20	**2** (0.1)	TBAC (0.1)	60	10	1	7.6	75	99	5.5	1.01	4.5	1.04	23/77
21	**2** (0.1)	TBAC (0.1)	100	10	1	42.1	420	99	24.0	1.01	11.1	1.04	23/77
22	**2** (0.1)	TBAC (0.1)	80	1	1	16.9	170	99	13.4	1.01	6.1	1.04	23/77
23	**2** (0.1)	TBAC (0.1)	80	5	1	29.7	300	99	22.5	1.01	10.5	1.04	25/75
24	**2** (0.1)	TBAC (0.1)	80	20	1	16.5	165	98	7.7	1.02	3.6	1.02	63/37

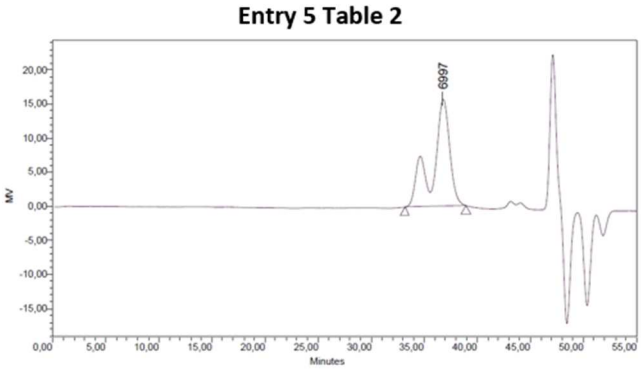
[a]Reaction conditions: **5m** = $5.93 \cdot 10^{-2}$ mol. [b]Gravimetic. [c]Turnover Frequency (yield · 0.01 · $mol_{Catalyst}^{-1}$ · reaction $time^{-1}$). [d]Determined by ^{1}H NMR. [e]Determined by Gel Permeation Chromatography at 30 °C in THF respect to polystyrene standards

Representative GPC traces of poly-(cyclohexene carbonate) 6m



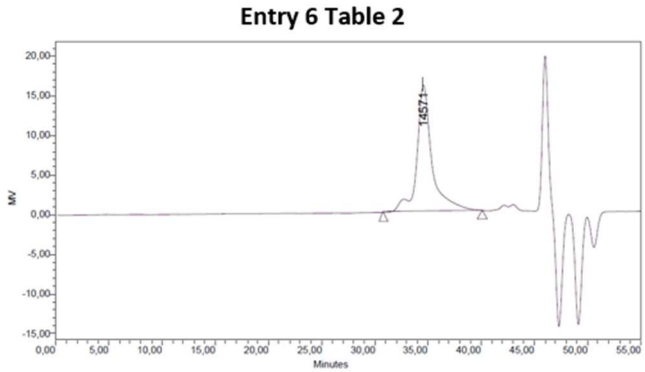
	Distribution Name	Mn (Daltons)	Mw (Daltons)	MP (Daltons)	Mz (Daltons)	Mz+1 (Daltons)	Polydispersity	Mz/Mw	Mz+1/Mw
1		23194	23511	23271	23833	24158	1,013638	1,013690	1,027546
1		11056	11334	11530	11593	11837	1,025084	1,022842	1,044384

Figure S25. GPC trace of sample obtained as in entry 2 table 2.



	Distribution Name	Mn (Daltons)	Mw (Daltons)	MP (Daltons)	Mz (Daltons)	Mz+1 (Daltons)	Polydispersity	Mz/Mw	Mz+1/Mw
1		14308	14489	14347	14671	14853	1,012640	1,012563	1,025125
1		6713	6897	6958	7076	7250	1,027425	1,026003	1,051176

Figure S26 GPC trace of sample obtained as in entry 5 table 2.



Broad Unknown Relative Peak Table

	Distribution Name	Mn (Daltons)	Mw (Daltons)	MP (Daltons)	Mz (Daltons)	Mz+1 (Daltons)	Polydispersity	Mz/Mw	Mz+1/Mw
1		12866	13684	14571	14298	14785	1,063576	1,044883	1,080451
1		27833	27987	27900	28142	28296	1.005538	1.005518	1.011023

Figure S27. GPC trace of sample obtained as in entry 6 table 2.

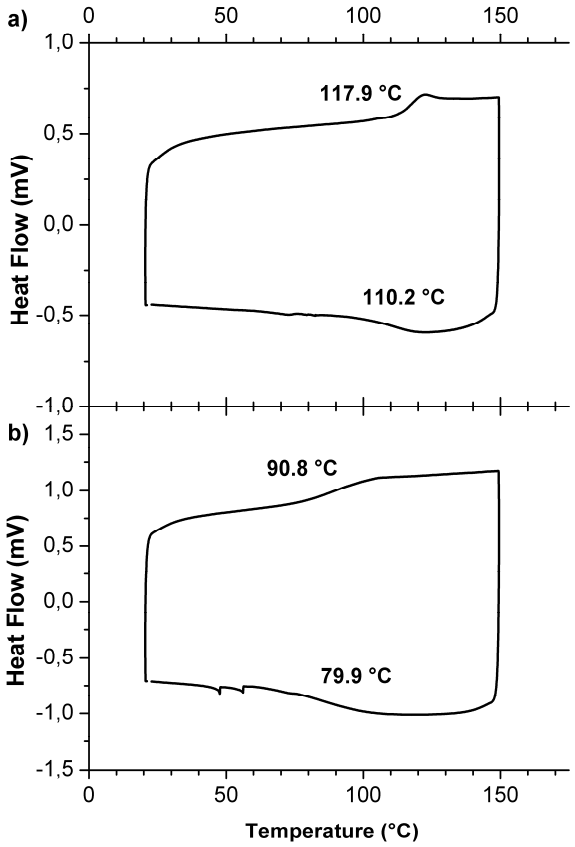


Figure S28. DSC analysis of poly-(cyclohexene carbonate) **6m** a) sample in entry 6 Table 2, b) sample in entry 5 Table 2.

Kinetic experiments for 6b formation promoted by 4/TBAB

General procedure for 5b/CO_2 coupling with in situ ATR-IR

The appropriate amount of complex **4** and TBAB were dissolved in **5b** and methylene chloride. The reaction mixture was put in the preheated autoclave and immediately pressurized with CO_2. The reaction was terminated after the signal of the carbonyl oxygen (1802 cm^{-1}) was constant (Figure S29). Value of initial velocities v_0 were obtained from slope of the initial straight line at low conversion of the epoxide.

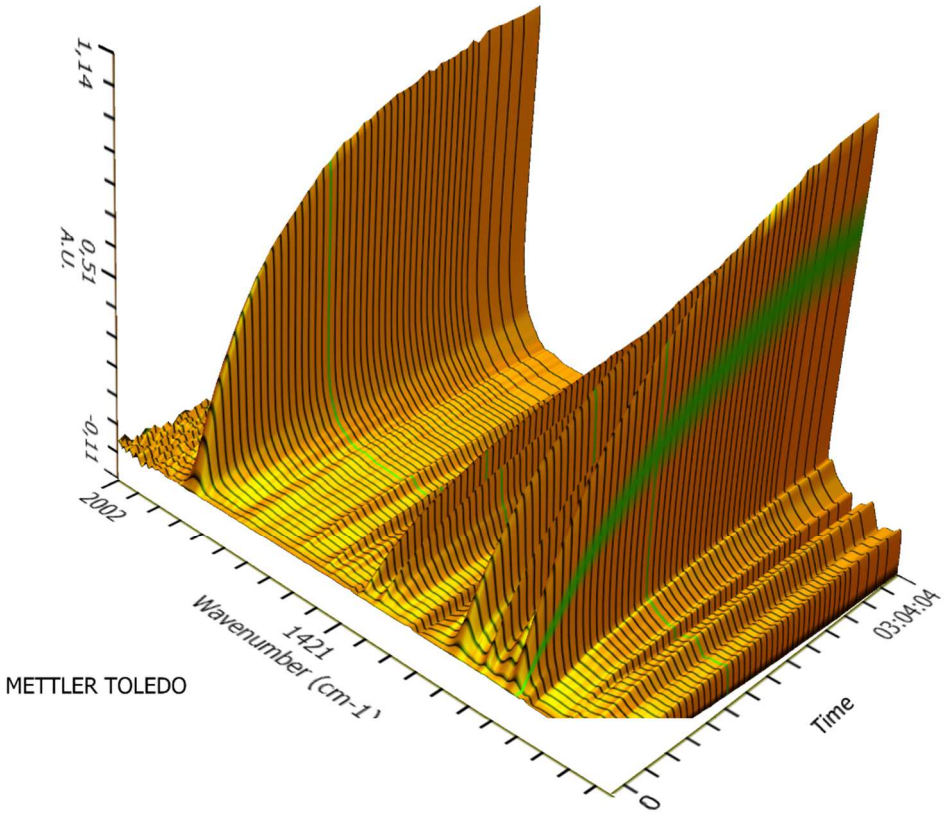


Figure S29 **6b** growth trace for the coupling of **5b** and CO_2 utilizing in situ ATR-FTIR spectroscopy. Carbonate signal of **6b** grows at 1802 cm^{-1}. Reaction conditions: [**5b**] = 4.94 M in methylene chloride; P(CO_2) = 10 bar; **4** = 0.1 mol%; TBAB = 0.1 mol%; T = 50°C.

Reaction order with respect to [4]

Table S4 Summary of the **5b**/CO_2 experiments for reaction order with respect to **4**

Entry	5b/TBAB/4	[4] mM	v_0 l/s·10^4
S1	500/1/1	28.6	5.33
S2	1000/2/1	14.3	5.30
S3	1500/3/1	9.5	3.10
S4	2000/4/1	7.2	1.81
S5	3000/6/1	4.8	0.47

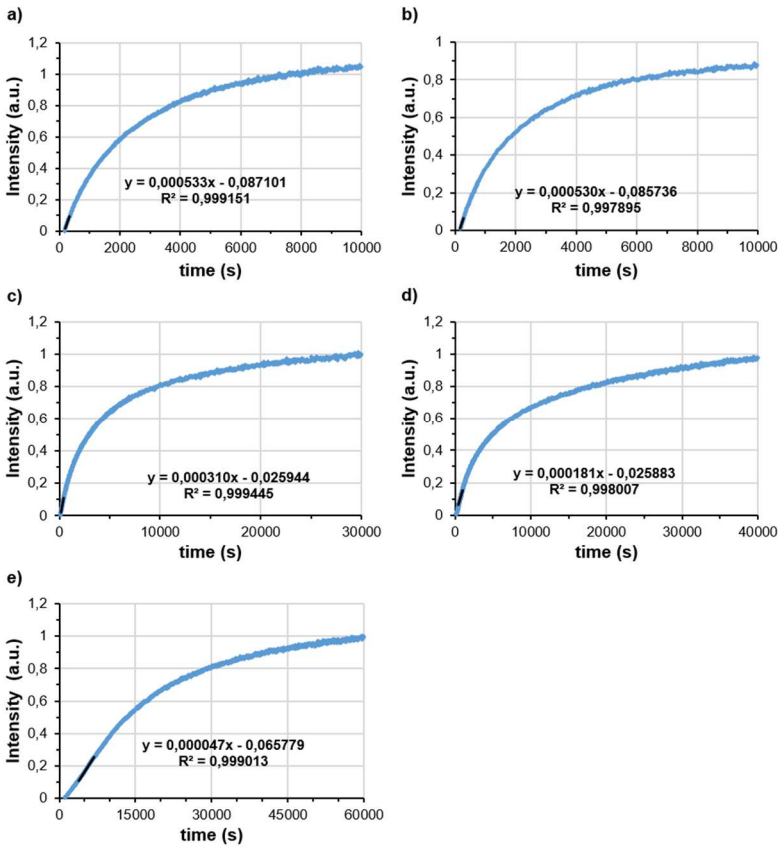


Figure S30 Variation of the intensity of the **6b** C=O stretching band with respect to time for experiments in Table S4. a) [**4**] = 28.6 mM, b) [**4**] = 14.3 mM, c) [**4**] = 9.5 mM, d) [**4**] = 7.2 mM, e) [**4**] = 4.8 mM.

Reaction order with respect to [TBAB]

Table S5 Summary of the **5b**/CO_2 experiments for reaction order with respect to TBAB

Entry	5b/TBAB/4	[TBAB] mM	v_0 l/s·10^4
S1	1000/1/1	14.3	3.12
S2	1000/2/1	28.6	5.30
S3	1000/3/1	42.9	5.28
S4	1000/4/1	57.2	6.19
S5	1000/5/1	71.5	5.26

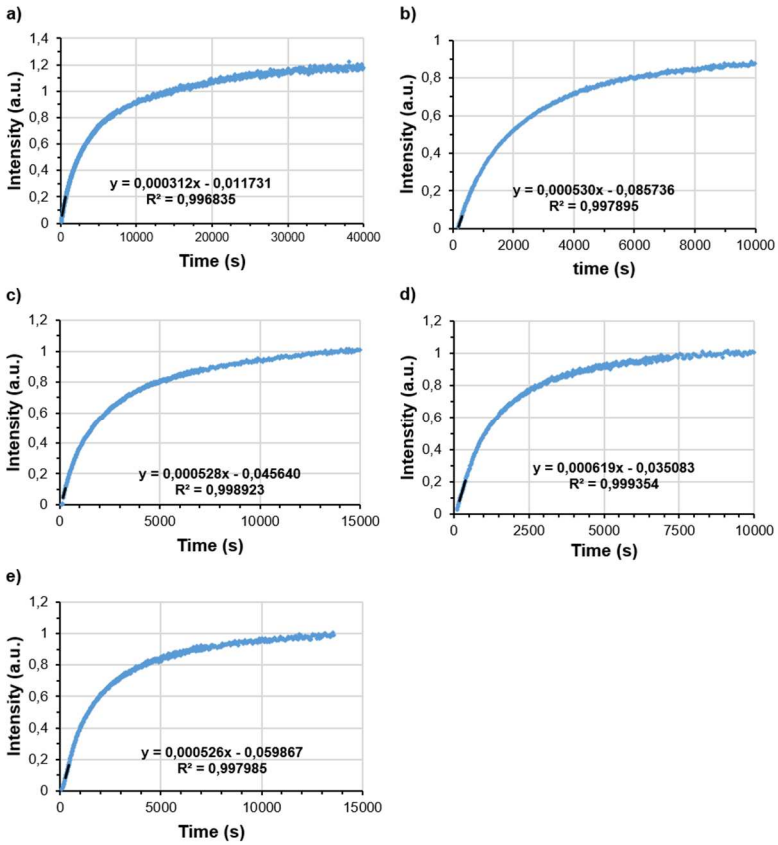


Figure S31 Variation of the intensity of the **6b** C=O stretching band with respect to time for experiments in Table S5. a) [TBAB] = 14.3 mM, b) [TBAB] = 28.6 mM, c) [TBAB] = 42.9 mM, d) [TBAB] = 57.2 mM, e) [TBAB] = 71.5 mM.

Reaction order with respect to [5b]

Table S6 Summary of the **5b**/CO_2 experiments for reaction order with respect to **5b**

Entry	[5b] mol/L	v_0 l/s·10^4
S1	4.29	1.09
S2	5.72	1.45
S3	7.15	1.68
S4	8.57	2.40

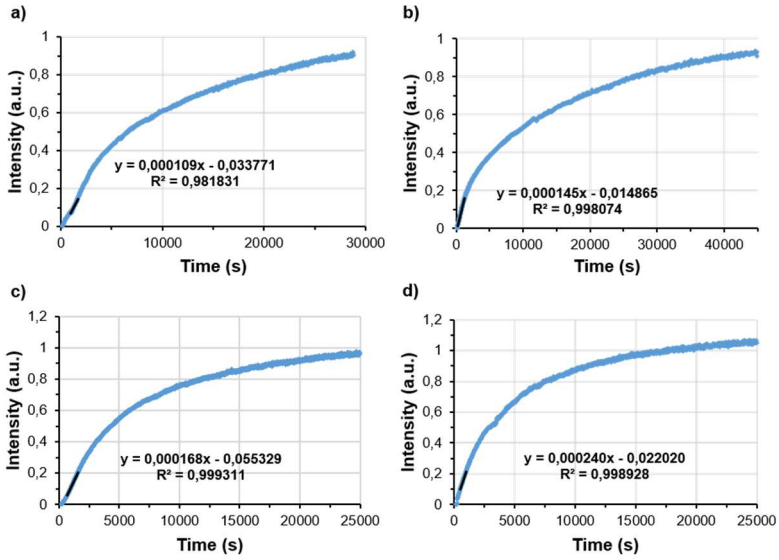


Figure S32 Variation of the intensity of the **6b** C=O stretching band with respect to time for experiments in Table S6. a) [**5b**] = 4.29 M, b) [**5b**] = 5.72 M, c) [**5b**] = 7.15 M, d) [**5b**] = 8.57 M.

Reaction order with respect to P(CO_2)

Table S7 Summary of the **5b**/CO_2 experiments for reaction order with respect to CO_2

Entry	P(CO_2) bar	v_0 l/s·10^4
S1	2	1.39
S2	3.5	1.58
S3	6	1.59
S4	8.5	1.68

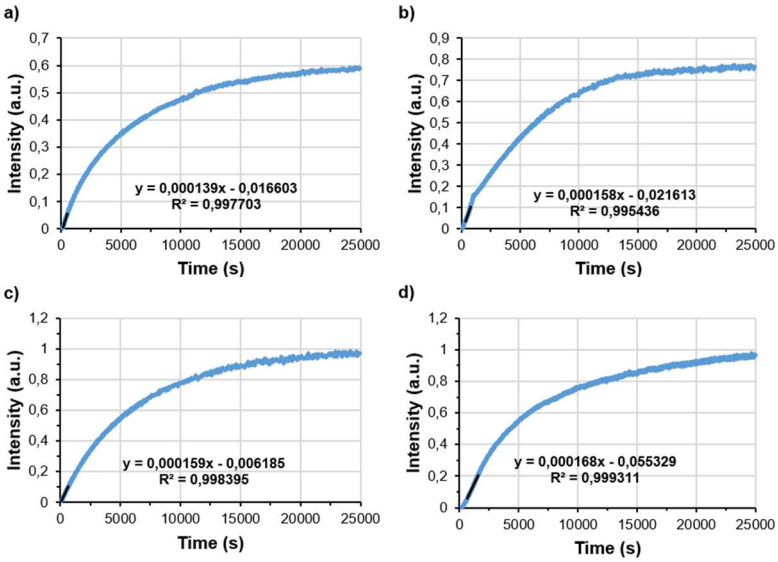


Figure S33 Variation of the intensity of the **6b** C=O stretching band with respect to time for experiments in Table S7. a) P(CO_2) = 2.0 bar, b) P(CO_2) = 3.5 bar, c) P(CO_2) = 6.0 bar, d) P(CO_2) = 8.5 bar.

Eyring plot

Table S8 Summary of the **5b**/CO_2 experiments at different temperatures for the determination of the activation parameters.

Entry	5b/TBAB/4	Temperature °C	v_0 l/s·10^4	k[a]
S1	1666/5/1	30	0.52	0.40
S2	1666/5/1	40	0.74	0.56
S3	1666/5/1	50	1.68	1.28
S4	1666/5/1	70	2.73	2.08

[a]Calculated on the basis of the kinetic equation $v_0 = k \cdot [\mathbf{5b}] \cdot [\mathbf{4}]^2$.

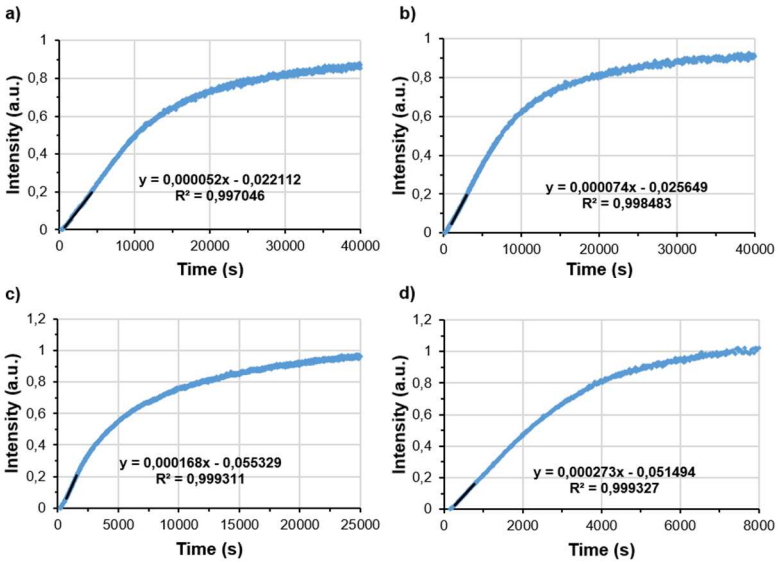


Figure S34 Variation of the intensity of the **5b** C=O stretching band with respect to time for experiments in Table S8. a) T = 30°C, b) T = 40°C, c) T = 50°C, d) T = 70°C.

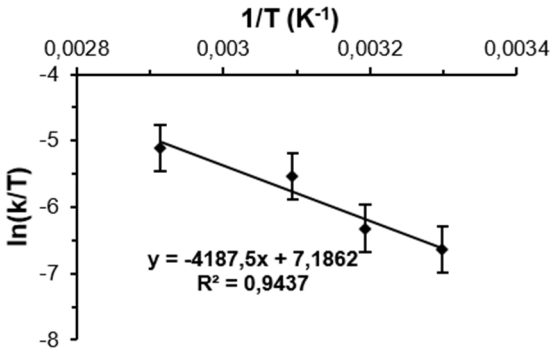


Figure S35 Plot of ln(k/T) versus ln(1/T) in the range from 30 to 70 °C, for the formation of **6b** using **4**/TBAB.

Kinetic experiments for 6m formation promoted by 2/TBAC

General procedure for 5m/CO_2 co-polymerization with in situ ATR-IR

The appropriate amount of complex **2** and TBAC were dissolved in **5m** and toluene. The reaction mixture was put in the preheated autoclave and immediately pressurized with CO_2. The reaction was terminated after the signal of the carbonyl oxygen (1750 cm^{-1}) was constant (Figure S36), with the addition of methanol and methylene chloride. Value of initial velocities v_0 were obtained from slope of the initial straight line at low conversion of the epoxide.

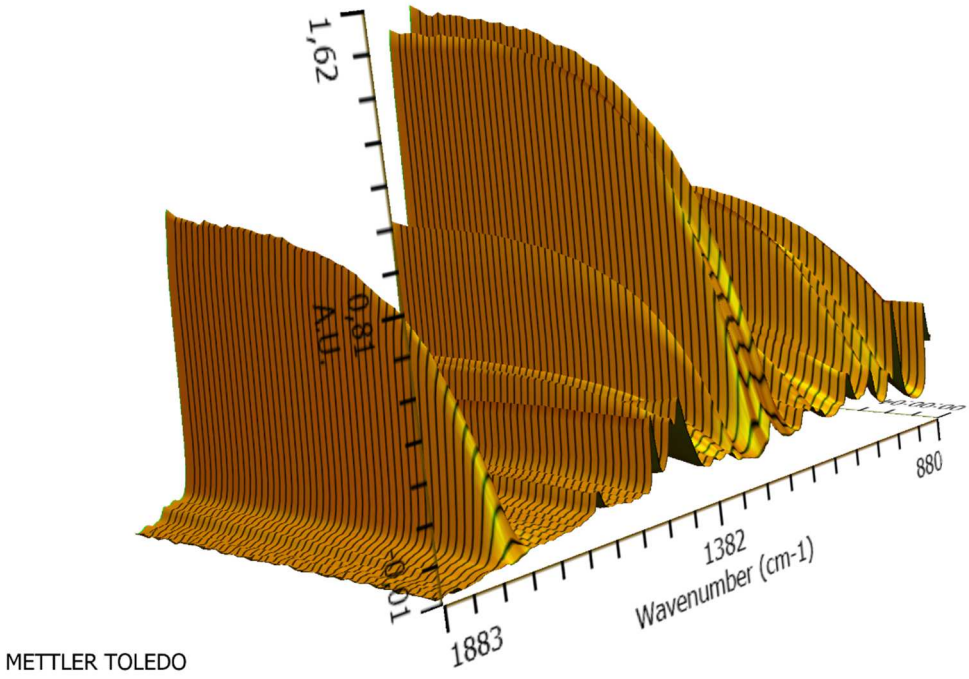


Figure S36 **6m** growth trace for the co-polymerization of **5m** and CO_2 utilizing in situ ATR-FTIR spectroscopy. Carbonate signal of **6m** grows at 1750 cm^{-1}. Reaction conditions: [**5m**] = 4.94 M in toluene; P(CO_2) = 10 bar; **2** = 0.1 mol%; TBAC = 0.1 mol%; T = 70°C.

Reaction order with respect to [2]

Table S9 Summary of the **5m**/CO_2 experiments for reaction order with respect to **2**

Entry	5m/TBAC/2	[2] mM	v_0 l/s·10^4
S1	2500/2.5/1	3.6	0.55
S2	2000/2/1	4.6	0.71
S3	1500/1.5/1	6.1	0.96
S4	1000/1/1	9.1	1.37
S5	500/0.5/1	18.2	2.67

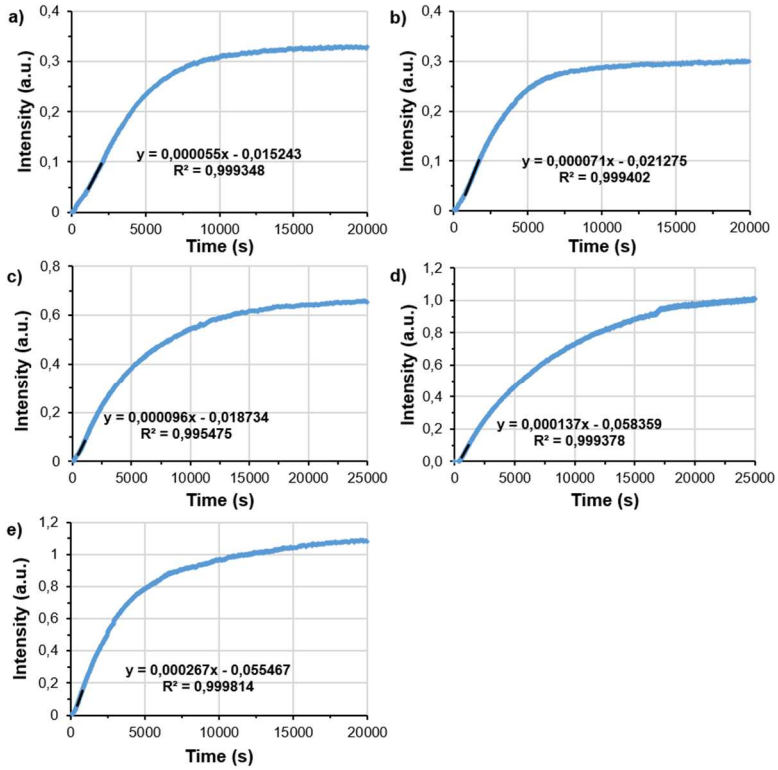


Figure S37 Variation of the intensity of the **6m** C=O stretching band with respect to time for experiments in Table S9. a) [**2**] = 3.6 mM, b) [**2**] = 4.6 mM, c) [**2**] = 6.1 mM, d) [**2**] = 9.1 mM, e) [**2**] = 18.2 mM.

Reaction order with respect to [TBAC]

Table S10 Summary of the **5m**/CO_2 experiments for reaction order with respect to TBAC

Entry	5m/TBAC/2	[TBAC] mM	v_0 l/s·10^4
S1	1000/0.77/1	7.6	0.73
S2	1000/1/1	9.8	1.37
S3	1000/1.5/1	14.8	1.52
S4	1000/2/1	19.8	1.54
S5	1000/2.5/1	24.8	1.56
S6	1000/3/1	29.7	1.57

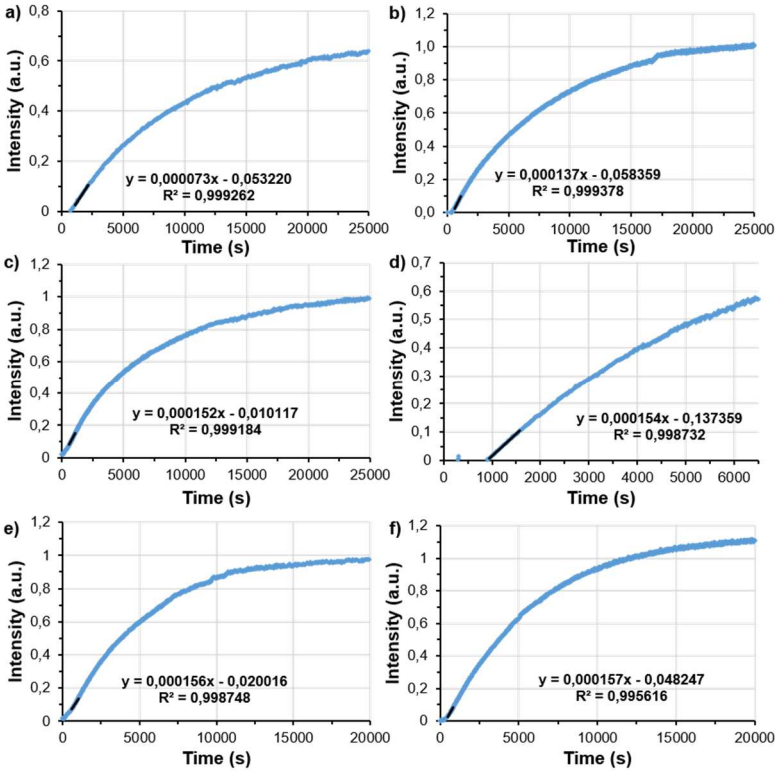


Figure S38 Variation of the intensity of the **6m** C=O stretching band with respect to time for experiments in Table S10. a) [TBAC] = 7.6 mM, b) [TBAC] = 9.8 mM, c) [TBAC] = 14.8 mM, d) [TBAC] = 19.8 mM, e) [TBAC] = 24.8 mM, f) [TBAC] = 29.7 mM.

Reaction order with respect to [5m]

Table S11 Summary of the **5m**/CO_2 experiments for reaction order with respect to **5m**

Entry	5m/TBAC/2	[5m] M	v_0 l/s·10^4
S1	600/1/1	2.97	0.85
S2	800/1/1	3.95	1.11
S3	1000/1/1	4.94	1.37
S4	1200/1/1	5.93	1.65

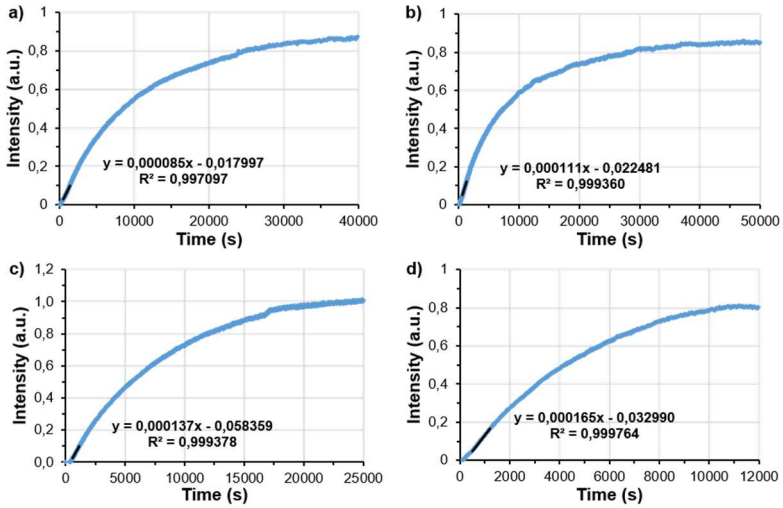


Figure S39 Variation of the intensity of the 6m C=O stretching band with respect to time for experiments in Table S11. a) [**5m**] = 2.97 M, b) [**5m**] = 3.95 M, c) [**5m**] = 4.94 M, d) [**5m**] = 5.93 mM.

Reaction order with respect to P(CO_2)

Table S12 Summary of the **5m**/CO_2 experiments for reaction order with respect to CO_2

Entry	P(CO_2) bar	K l/s·10^4
S1	6	1.33
S2	7.4	1.58
S3	9	1.59

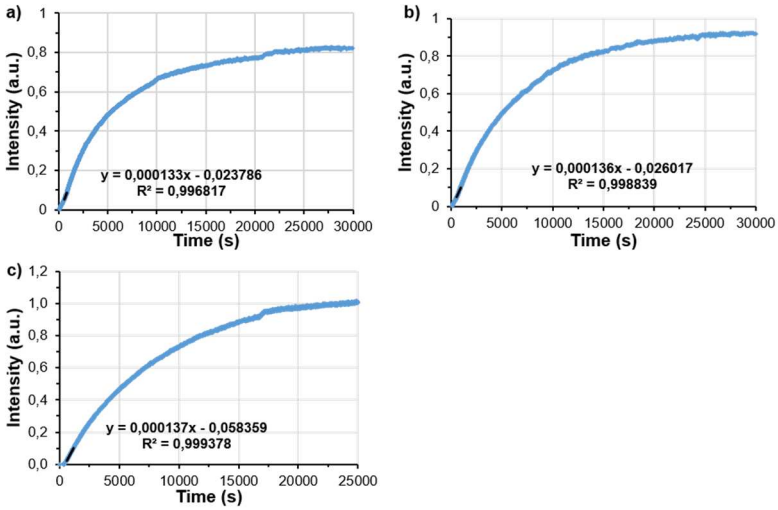


Figure S40 Variation of the intensity of the **5m** C=O stretching band with respect to time for experiments in Table S12. a) P(CO_2) = 6.0 bar, b) P(CO_2) = 7.4 bar, c) P(CO_2) = 9.0 bar.

Eyring plot

Table S13 Summary of the **5m**/CO_2 experiments at different temperatures for the determination of the activation parameters.

Entry	5m/TBAC/2	Temperature °C	v_0 l/s·10^4	k
S1	1000/1/1	60	0.48	0.002
S2	1000/1/1	70	0.85	0.0035
S3	1000/1/1	80	1.37	0.0056
S4	1000/1/1	90	2.33	0.0095

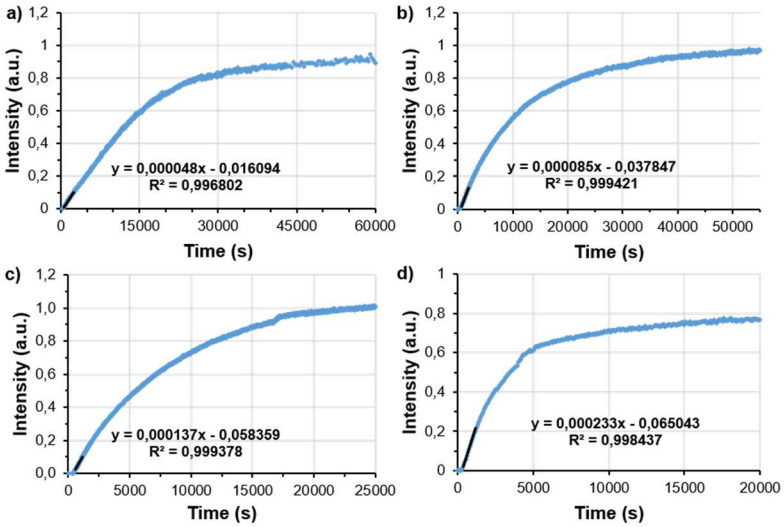


Figure S41 Variation of the intensity of the **6m** C=O stretching band with respect to time for experiments in Table S8. a) T = 30°C, b) T = 40°C, c) T = 50°C, d) T = 70°C.

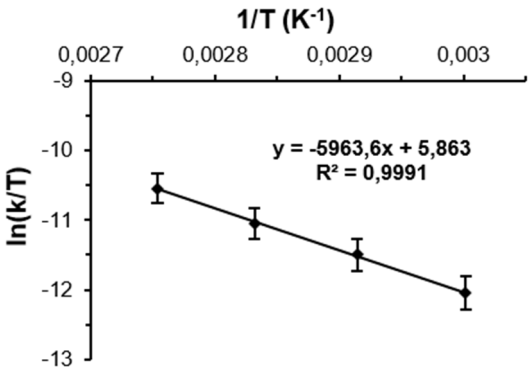
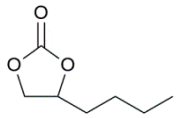


Figure S42 Plot of ln(k/T) versus ln(1/T) in the range from 60 to 90 °C, for the formation of **6m** using **2**/TBAC.

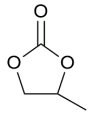
List of ^{1}H MNR data for the Cyclic Organic Carbonate products

6a. 4-butyl-1,3-dioxolan-2-one ($CDCl_3$, 250MHz)



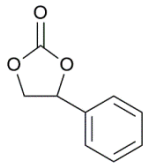
4.72-4.66 (m, 1H, ring *CH*CH_3), 4.52 (t, 1H, *J* = 8.1 Hz, ring C*H*H), 4.07 (dd, 1H, *J* = 8.2 Hz, *J* = 7.3 Hz, ring CH*H*), 1.85-1.77 (m, 1H, CHC*H*$_2$$CH_2$), 1.74-1.67 (m, 1H, CHC*H*$_2$$CH_2$), 1.52-1.33 (m, 4H, CH_2C*H*$_2$$CH_2$ and CH_2C*H*$_2$$CH_3$), 0.92 (t, 3H, ^{3}J = 6.9 Hz, CH_3).

6b. 4-methyl-1,3-dioxolan-2-one ($CDCl_3$, 300MHz)



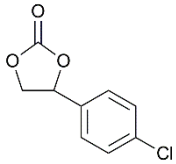
4.91-4.80 (m, 1H, ring *CH*CH_3), 4.55 (t, 1H, *J* = 8.3 Hz, ring C*H*H), 4.02 (t, 1H, *J* = 8.3 Hz, *J* = 7.4 Hz, ring CH*H*), 1.49 (d, 3H, *J* = 6.3 Hz, C*H*$_3$).

6c. 4-phenyl-1,3-dioxolan-2-one ($CDCl_3$, 250MHz)



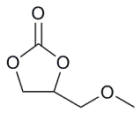
7.44-7.41 (m, 2H, Ar-H), 7.38-7.30 m, 2H, Ar-H), 5.52 (t, 1H, J = 8.0 ring *CH*Ph), 4.64 (t, 1H, *J* = 8.1, ring C*H*H), 4.19 (t, 1H, *J* = 8.0 Hz, ring CH*H*).

6d. 4-(*p*-chloro-phenyl)-1,3-dioxolan-2-one ($CDCl_3$, 250MHz)



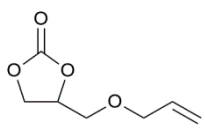
7.41 (t, 2H, Ar-H), 7.30 (t, 2H, Ar-H), 5.65 (m, 1H, ring *CH*Ph), 4.79 (m, 1H, ring C*H*H), 4.29 (m, 1H, ring CH*H*).

6e. 4- methyloxymethyl-1,3-dioxolan-2-one ($CDCl_3$, 300MHz)



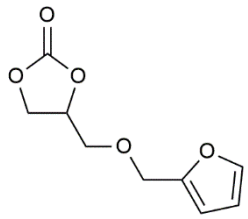
4.84-4.77 (m, 1H, ring *CH*CH_3), 4.49 (dd, *J* = 8.4, *J* = 8.4 Hz, 1H,), 4.38 (dd, 1H, *J* = 8.3 Hz, *J* = 6.1 Hz, ring C*H*H), 3.64 (dd, 1H, *J* = 10.9 Hz, *J* = 3.8 Hz, ring CH*H*), 3.57 (dd, 1H, *J* = 10.9 Hz, *J* = 3.8 Hz, ring CH*H*), 3.42 (s, 3H, C*H*$_3$).

6f. allyloxymethyl-1,3-dioxolan-2-one ($CDCl_3$, 400MHz)



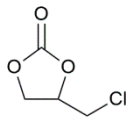
5.84-5.74 (m, 1H, *CH*=CH_2), 5.22 (dd, 1H, (E)-CH=C*H*H, *J* = 17.3 Hz, *J* = 1.4 Hz), 5.15 (dd, 1H, (Z)-CH=CH*H*, *J* = 10.4 Hz, *J* = 1.4 Hz), 4.82-4.75 (m, 1H, ring *CH*CH_2), 4.44 (t, 1H, ring *C*HC*H*$_2$, *J* = 8.3 Hz), 4.31 (dd, 1H, ring *C*HC*H*$_2$, *J* = 8.3 Hz, *J* = 6.1 Hz), 3.99 (d, 1H, ring *C*HC*H*$_2$, *J* = 5.3 Hz), 3.66-3.51 (m, 2H, C*H*$_2$-CH=CH_2).

6g furfuryloxymethyl-1,3-dioxaolan-2-one ($CDCl_3$, 400MHz)



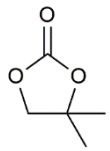
7.43 (m, 1H, O-*CH*=CH, furane ring), 6.36 (m, 2H, *CH*=*CH*, furane ring), 4.79 (m, 1H, ring *CH*CH_2), 4.54 (m, 1H, O-*CH_2*-carbonate), 4.46 (m, 1H, ring *CH*HCH), 4.35 (m, 1H, ring *CH*HCH), 3.67 (m, 2H, O-*CH_2*-furane*)*.

6h.4-chloromethyl-1,3-dioxolan-2-one ($CDCl_3$, 300MHz)



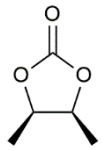
5.02-4.93 (m, 1H, ring *CH*CH_3), 4.60 (dd, 1H, *J* = 8.8 Hz, *J* = 8.1 Hz, ring C*H*H), 4.42 (dd, 1H*, J* = 8.8 Hz, *J* = 5.8 Hz, ring CH*H*), 3.76 (m, 2H, C*H_2*Cl).

6i 4,4'-dimethyl-1,3-dioxolan-2-one ($CDCl_3$, 300MHz)



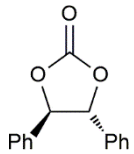
4.15 (s, 2H, ring C*H_2*C(CH_3)$_2$), 1.53 (s, 6H, C*H_3*).

6j *cis*-4,5-dimethyl-1,3-dioxolan-2-one ($CDCl_3$, 300MHz)



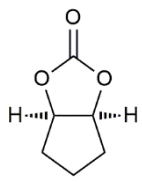
4.83 (m, 2H, ring CH_3C*H*C*H*CH_3), 1.37 (d, 6H, *J* = 6.1 Hz, C*H_3*).

6k *trans*-4,5-diphenyl-1,3-dioxolan-2-one ($CDCl_3$, 300MHz)



7.43-7.18 (m, 10H, Ar-H), 5.44 (s, 2H, ring *CH*Ph).

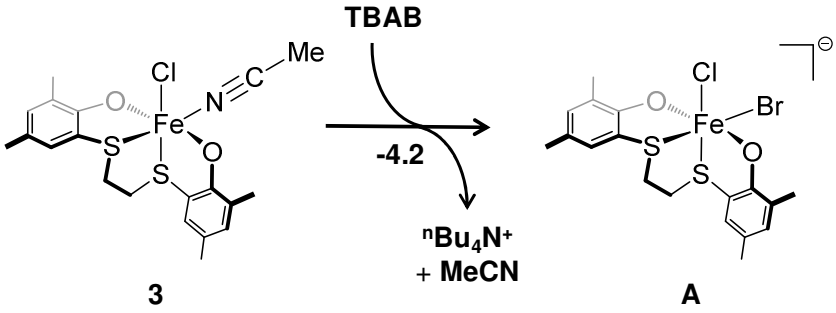
6l (3aR,6aS)-tetrahydro-3aH-cyclopenta[d][1,3]dioxol-2-one ($CDCl_3$, 300MHz)



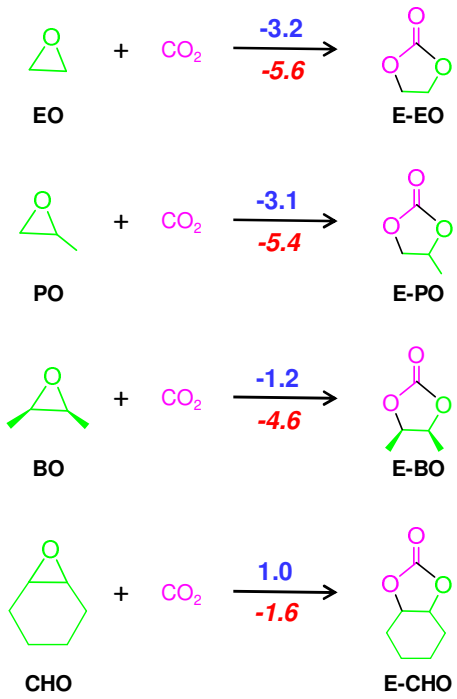
5.11 (s, 2H, ring *CH*CH_2), 2.20-2.14 (m, 2H), 1.85-1.75 (m, 2H), 1.72-1.65 (m, 2H).

Computational Methods

All the geometries were optimized with the generalized gradient approximation (GGA) method with Gaussian 09 program packages,[4] using the UBP86 functional.[5] The electronic configuration of all the non-metal elements (H, C, N, O, S, Cl and Br) were described with the Ahlrichs split-valance polarization basis function SVP[6] while Fe is treated with the small-core, quasi-relativistic Stuttgart-Dresden effective core potential, with the associated triple-ζ valence basis set SDD.[7] Geometries were optimized without any symmetry constraints. Harmonic force constants were computed at the optimized geometries to characterize the stationary points as minima or saddle points. All transition states were optimized using the default Berny algorithm implemented in Gaussian09.[4] For further validation of energetics, single-point calculations were performed on the UBP86/SDD/SVP optimized geometries using meta-hybrid-GGA functional UM06,[8] employing a valence triple-ζ of basis set (TZVP)[9] for non-metals except Br, TZVPD was used for Br and SDD(ECP) for Fe. Solvent effect (i.e. DCM, ε = 8.93; Toluene, ε = 2.37) was evaluated implicitly by a self-consistent reaction field (SCRF) approach for all the intermediates and transitions states, using the PCM continuum solvation model.[10] Unless specified otherwise, the ΔG was used throughout the text. The ΔG value was obtained by augmenting the ΔE_e energy terms at UM06(PCM)/SDD(Fe)/TZVPD(Br)/TZVP(C,H,N,O,Cl,S) with the respective free energy corrections at the UBP86/SDD(Fe)/SVP(C,H,N,O,Cl,S,Br) level in gas phase. Since the thermal correction to the Gibbs energy of each component depends on its concentration in solution, one can incorporate the concentration terms into calculations. In the Gaussian program, the concentration can be specified by adjusting the pressure value based on the ideal gas law $p_i = \frac{n_i}{V}RT$, where p_i is the pressure, R the gas constant, T the absolute temperature, n_i the molar quantity, and V the reaction volume.[11] The experimental concentrations of catalyst and reactants at the reaction temperature are approximated by setting the partial pressures of the substrates and catalyst. For **PO/CO₂** coupling reaction at 35ºC: **PO**: 4.15x10^{-2} mol ≙ 14.3 mol/lit ≙ 361 atm; **CO₂**: 1.0 atm; **TBAB**: 7.15x10^{-2} mol/lit ≙ 1.8 atm and catalyst (**3**): 1.43x10^{-2} mol/lit ≙ 0.36 atm. For **CHO/CO₂** co-polymerization reaction at 80ºC: **CHO**: 5.93x10^{-2} mol ≙ 9.88 mol/lit ≙ 286 atm; and catalyst (**3**): 9.88x10^{-2} mol/lit ≙ 0.3 atm. Natural bond orbital (NBO)[12] analysis were performed using *NBO Version 3.1* program.



Scheme S1 Active catalyst formation from the pre-catalyst **3** in presence of TBAB. For energy convention refer Computational Details.



Scheme S2 Cycloaddition of epoxides with CO_2. Energies are ΔG_{298}(gas) at M06/TZVP//BP86/SVP (blue values) and DLPNO-CCSD(T)/aug-cc-pVTZ//BP86/SVP (italics red values).

Table S14. Cartesian coordinates (Å) of the optimized structures of all intermediates and transition states at UBP86/SDD(Fe)/SVP(C,H,N,O,Cl,S) level of theory. E_L^S represents the absolute electronic energy in Hartree at UM06(PCM)/SDD(Fe)/TZVPD(Br)/TZVP(C,H,N,O,Cl,S) level of theory in DCM solvent. [a]Toluene was used for implicit solvation energy.

PO

10

E_e = -193.048510557

C	-1.054819	0.612187	-0.057791
C	0.154384	-0.043185	0.487592
O	-0.828727	-0.789263	-0.248024
H	-1.892093	0.880807	0.616907
H	-0.967544	1.242396	-0.965700
H	0.161325	-0.264715	1.576145
C	1.517505	0.104188	-0.148100
H	2.100764	0.908666	0.348586
H	2.097576	-0.838284	-0.055476
H	1.427370	0.346091	-1.226475

1c

50

E_e = -2361.43063721

Fe	-0.043339	1.055907	0.496276
S	-1.003362	-1.217539	1.356470
S	0.883563	-0.554639	-1.610258
Cl	-0.678265	2.212757	2.326027
C	-0.147471	-2.452850	0.268074
H	0.861944	-2.561925	0.718940
H	-0.680093	-3.420227	0.389129
C	-0.062245	-2.094267	-1.208729
H	-1.070666	-1.912644	-1.637743
H	0.399350	-2.934676	-1.769940
C	-2.575496	-0.992736	0.530665
C	-2.695045	0.139978	-0.332886
C	-5.000541	-0.558979	-0.754395
H	-5.963358	-0.384511	-1.266808
C	-3.954813	0.342614	-0.993664
C	-4.886949	-1.673029	0.116459
C	-3.654349	-1.870416	0.761552
H	-3.522757	-2.715666	1.457420
C	2.460102	-0.843824	-0.817065
C	3.456998	-1.642848	-1.408744
H	3.253455	-2.124109	-2.379771
C	4.702047	-1.825743	-0.778009
C	2.684784	-0.170710	0.425757
C	3.956799	-0.350922	1.072142
C	4.917703	-1.166686	0.459159
H	5.889760	-1.296602	0.966831
O	-1.697220	0.978583	-0.533515
O	1.770869	0.598318	0.981496
N	0.597180	2.785386	-0.705759
C	0.896689	3.822287	-1.148489
C	1.263915	5.125511	-1.681805
H	0.544541	5.432624	-2.467492
H	2.281614	5.088090	-2.119993
H	1.250507	5.879751	-0.868839
C	5.783084	-2.685529	-1.394182
H	6.711517	-2.103396	-1.581634
H	6.065650	-3.527964	-0.725836
H	5.458491	-3.119202	-2.361225
C	4.202332	0.341817	2.387678
H	4.097365	1.442980	2.285408
H	3.447748	0.039747	3.144807
H	5.212574	0.116071	2.782648
C	-6.062151	-2.598105	0.346116
H	-6.432695	-3.036127	-0.606222
H	-5.794899	-3.437277	1.019368
H	-6.921046	-2.062139	0.806215
C	-4.102187	1.530349	-1.910263
H	-3.930769	2.479851	-1.358977
H	-3.342836	1.507601	-2.721283
H	-5.109977	1.565798	-2.369806

TBAB

54

E_e = -3259.89057770

N	0.419750	-0.332961	-0.349864
Br	-2.853316	0.720073	1.158876
C	0.540605	-0.299094	1.177894
H	1.279887	0.487995	1.415491
H	-0.472110	0.048205	1.514958
C	0.930415	-1.604676	1.870403
H	0.182365	-2.400030	1.667006
H	1.914621	-1.989185	1.516093
C	0.998193	-1.385055	3.395255
H	0.015116	-0.998391	3.742548
H	1.737384	-0.582735	3.619406
C	1.365419	-2.655603	4.170565
H	1.405977	-2.463172	5.262215
H	0.620107	-3.461857	4.002806
H	2.358050	-3.050257	3.863739
C	-0.686435	-1.348596	-0.697602
H	-1.553140	-1.025155	-0.063681
H	-0.315375	-2.333410	-0.352810
C	-1.117562	-1.433040	-2.161748
H	-1.431357	-0.435839	-2.535378
H	-0.294520	-1.786047	-2.824287
C	-2.318208	-2.392752	-2.288729
H	-2.036890	-3.393441	-1.888621
H	-3.134984	-2.018052	-1.633507
C	-2.823745	-2.536522	-3.728653
H	-2.036748	-2.938463	-4.402793
H	-3.692161	-3.224611	-3.782779
H	-3.149349	-1.558327	-4.141914
C	1.707870	-0.767052	-1.025192
H	1.879075	-1.818177	-0.714682
H	1.490901	-0.785179	-2.111846
C	2.960724	0.068413	-0.761980
H	3.172061	0.126599	0.327532
H	2.809690	1.111481	-1.111320
C	4.183762	-0.532577	-1.480649
H	3.972191	-0.601107	-2.571826
H	4.333827	-1.581096	-1.136721
C	5.469414	0.272232	-1.255489
H	6.329907	-0.186454	-1.783885
H	5.366669	1.314141	-1.626114
H	5.730175	0.327493	-0.177307
C	-0.057825	1.052502	-0.850098
H	0.220660	1.095817	-1.922405
H	-1.167084	1.019278	-0.727141
C	0.407210	2.302780	-0.101440
H	1.512838	2.377042	-0.010208
H	-0.026908	2.283984	0.920235
C	-0.137876	3.553597	-0.818443
H	0.235156	3.580140	-1.868405
H	-1.244868	3.463634	-0.879436
C	0.233051	4.858171	-0.103293
H	1.334645	4.990628	-0.035171
H	-0.176794	5.740412	-0.636666
H	-0.171272	4.875931	0.930469

$^{n}Bu_4N^+$

53

E_e = -685.637764039

N	-0.343886	0.038968	-0.181544
C	0.551379	0.857884	-1.118926
H	1.556439	0.400221	-1.066632
H	0.158231	0.669035	-2.139267
C	0.652404	2.360951	-0.852604
H	-0.341698	2.851831	-0.920252
H	1.037345	2.554867	0.172135
C	1.600696	3.026244	-1.872855
H	1.226494	2.829679	-2.902559
H	2.601114	2.541509	-1.814916
C	1.743688	4.536969	-1.653797
H	2.429686	4.982232	-2.401572
H	0.767076	5.056740	-1.746709

H	2.153061	4.766328	-0.647595
C	-1.782690	0.579513	-0.298296
H	-1.993654	0.615678	-1.387038
H	-1.744651	1.623010	0.068226
C	-2.887379	-0.186947	0.432233
H	-2.955598	-1.234886	0.071172
H	-2.684495	-0.235197	1.523746
C	-4.251852	0.501985	0.214349
H	-4.194538	1.553521	0.574699
H	-4.460678	0.564573	-0.877205
C	-5.402232	-0.225554	0.920318
H	-5.244961	-0.268263	2.018516
H	-6.365962	0.291632	0.742096
H	-5.510854	-1.268111	0.554557
C	0.091690	0.181527	1.281428
H	-0.091880	1.242906	1.542654
H	-0.628037	-0.423888	1.865384
C	1.522868	-0.208132	1.649059
H	2.260042	0.327322	1.012492
H	1.687019	-1.294231	1.488851
C	1.809280	0.123500	3.129306
H	1.059932	-0.389805	3.772802
H	1.658389	1.213573	3.296622
C	3.224140	-0.276677	3.563658
H	3.398320	-0.022974	4.628218
H	3.392138	-1.368134	3.449418
H	3.998158	0.247892	2.964984
C	-0.355716	-1.438011	-0.634325
H	-0.721856	-2.012959	0.238809
H	-1.137696	-1.499605	-1.418082
C	0.936132	-2.056167	-1.178857
H	1.782530	-1.926232	-0.473964
H	1.232029	-1.566425	-2.130252
C	0.729941	-3.563087	-1.443691
H	0.462216	-4.070365	-0.489727
H	-0.144597	-3.702940	-2.118344
C	1.966840	-4.230097	-2.057484
H	2.851587	-4.138340	-1.393068
H	1.790101	-5.310515	-2.229217
H	2.231307	-3.775853	-3.035264

MeCN

6

E_e = -132.709068097

C	0.000000	0.000000	-1.183298
H	1.039061	0.000000	-1.571028
H	-0.519530	0.899853	-1.571028
H	-0.519530	-0.899853	-1.571028
C	0.000000	0.000000	0.277879
N	0.000000	0.000000	1.449371

A

45

E_e = -4802.96644424

Br	0.824278	2.990310	-0.987200
Fe	-0.033650	1.151176	0.401266
S	-0.985847	-1.303475	1.349380
S	0.877149	-0.586601	-1.592047
Cl	-0.824469	2.059993	2.342750
C	-0.158351	-2.533569	0.240712
H	0.852126	-2.662225	0.684953
H	-0.697957	-3.501644	0.332955
C	-0.059213	-2.143357	-1.229368
H	-1.066581	-1.958836	-1.660525
H	0.409722	-2.972829	-1.803174
C	-2.573453	-1.093889	0.554207
C	-2.724002	0.047627	-0.299775
C	-5.042097	-0.673089	-0.672701
H	-6.019591	-0.501359	-1.160438
C	-4.010789	0.239654	-0.924003
C	-4.893917	-1.796127	0.182320
C	-3.642747	-1.981465	0.794916
H	-3.483531	-2.831308	1.480788
C	2.431711	-0.881712	-0.760751

C	3.453755	-1.649429	-1.356282
H	3.278237	-2.081553	-2.356508
C	4.678854	-1.863455	-0.701807
C	2.607689	-0.261865	0.520298
C	3.867924	-0.479241	1.189172
C	4.850757	-1.262714	0.572489
H	5.807703	-1.411602	1.106202
O	-1.758002	0.896941	-0.536547
O	1.688459	0.469318	1.095088
C	5.783779	-2.686849	-1.329051
H	6.708067	-2.088359	-1.493628
H	6.076091	-3.550095	-0.689500
H	5.475200	-3.094075	-2.314053
C	4.068149	0.161756	2.538640
H	3.959304	1.265660	2.471608
H	3.286273	-0.166991	3.256942
H	5.066362	-0.076961	2.959953
C	-6.050814	-2.740810	0.430700
H	-6.427556	-3.196854	-0.512561
H	-5.757275	-3.570953	1.105859
H	-6.918051	-2.223704	0.899969
C	-4.183630	1.437821	-1.821896
H	-3.981323	2.378897	-1.266496
H	-3.445859	1.424549	-2.653050
H	-5.206341	1.484357	-2.249526

B

54

E_e = -2421.77423224

Fe	-0.025644	0.952976	0.427642
S	0.873359	-0.825589	-1.532812
S	-0.920556	-1.225934	1.524308
C	0.055927	-2.367445	-0.920217
H	-0.966927	-2.325129	-1.351223
H	0.579924	-3.235336	-1.374350
C	0.008396	-2.535189	0.592034
H	1.025397	-2.514166	1.038251
H	-0.455073	-3.511484	0.848932
C	2.503610	-0.944876	-0.804804
C	2.743496	-0.160049	0.366319
C	5.034473	-1.010215	0.361757
H	6.036372	-1.037344	0.825170
C	4.051952	-0.208140	0.958962
C	4.803878	-1.779738	-0.806625
C	3.520949	-1.726477	-1.384051
H	3.303998	-2.297285	-2.302142
C	-2.485941	-1.157978	0.658606
C	-3.513027	-2.081022	0.939902
H	-3.344894	-2.857653	1.704353
C	-4.740889	-2.014908	0.259572
C	-2.656135	-0.103209	-0.291191
C	-3.909523	-0.037431	-0.990615
C	-4.901992	-0.983983	-0.700786
H	-5.859348	-0.914302	-1.246896
O	1.806655	0.596330	0.905230
O	-1.708776	0.785072	-0.532772
C	-5.859521	-2.993621	0.542156
H	-6.771278	-2.476208	0.912346
H	-6.158160	-3.552019	-0.371700
H	-5.565106	-3.738243	1.308714
C	-4.116202	1.058741	-2.004803
H	-4.100795	2.058162	-1.518232
H	-3.299921	1.067660	-2.757980
H	-5.084431	0.946434	-2.531830
C	5.907694	-2.621412	-1.407026
H	6.244975	-3.414100	-0.703830
H	5.579466	-3.120100	-2.340811
H	6.803041	-2.008848	-1.648834
C	4.314754	0.606537	2.199308
H	4.133923	1.686759	2.013836
H	3.619710	0.323929	3.018411
H	5.355693	0.478034	2.556128
Cl	-0.587280	2.325044	2.155914
O	0.665734	2.490201	-0.990115

C	1.285269	3.734266	-0.574417
C	0.109400	3.754955	-1.475364
H	2.302442	3.884580	-0.977495
H	1.139264	3.967784	0.495770
H	0.316243	3.878912	-2.556172
C	-1.268800	4.152017	-1.018956
H	-1.428836	5.229594	-1.235580
H	-2.039128	3.569933	-1.562118
H	-1.396425	3.973917	0.066806

[AB-C]‡

99

E_e = -7224.72892056

Fe	3.526089	-0.227743	1.171567
S	2.562421	0.649424	-1.311183
S	5.296488	-1.455513	-0.446649
C	3.499311	-0.466835	-2.449936
H	2.931786	-1.421551	-2.424127
H	3.420880	-0.053385	-3.478807
C	4.965356	-0.688926	-2.100590
H	5.519895	0.273544	-2.071238
H	5.440378	-1.332673	-2.872191
C	3.576527	2.121777	-1.293032
C	4.411779	2.310733	-0.145770
C	5.131916	4.429748	-1.143584
H	5.749859	5.343873	-1.081297
C	5.209298	3.508413	-0.091176
C	4.295178	4.248309	-2.274663
C	3.513450	3.080921	-2.324010
H	2.832247	2.907155	-3.173995
C	4.340573	-2.965252	-0.528348
C	4.862483	-4.125645	-1.136510
H	5.874036	-4.089826	-1.575289
C	4.115062	-5.313960	-1.180812
C	3.049367	-2.953106	0.089502
C	2.283707	-4.172429	0.046803
C	2.830135	-5.300207	-0.579723
H	2.226541	-6.225699	-0.596266
O	4.472295	1.443605	0.838646
O	2.555932	-1.883653	0.675177
C	4.656257	-6.571721	-1.826298
H	3.993637	-6.937342	-2.641948
H	5.661510	-6.403143	-2.264028
H	4.748213	-7.405164	-1.094752
C	0.919978	-4.189277	0.687963
H	0.974842	-3.876054	1.751902
H	0.228115	-3.469749	0.199565
H	0.460080	-5.196593	0.638688
C	4.238941	5.289272	-3.372074
H	3.553356	4.982334	-4.188020
H	3.882179	6.271819	-2.990984
H	5.239427	5.468144	-3.824865
C	6.093582	3.718994	1.111055
H	5.493135	3.737764	2.045848
H	6.806995	2.876165	1.234696
H	6.666236	4.665485	1.035002
O	1.889244	0.580967	1.994637
C	1.067719	-0.111998	2.941299
C	0.168136	-0.109896	1.770974
H	1.474583	-1.113315	3.200427
H	-0.406564	0.795960	1.525606
H	0.346853	-0.867767	0.997101
Br	-2.061612	-1.208836	2.399946
Cl	4.661374	-0.989708	2.995863
C	0.717420	0.704281	4.170232
H	0.331115	1.702397	3.882266
H	-0.062523	0.181629	4.761440
H	1.618836	0.837729	4.802214
Fe	-3.671109	0.319247	1.087929
S	-4.834302	1.802056	-0.826352
S	-2.407399	-0.739270	-1.162380
Cl	-5.003756	1.278850	2.650977
C	-4.315883	0.984760	-2.405911
H	-5.029908	0.141510	-2.522712

H	-4.500367	1.704545	-3.232649
C	-2.874609	0.495385	-2.458355
H	-2.159341	1.331374	-2.304317
H	-2.666565	0.050179	-3.455501
C	-3.645513	3.128317	-0.667947
C	-2.536984	2.909906	0.210339
C	-1.822240	5.195003	-0.310988
H	-1.097398	6.015048	-0.159783
C	-1.608858	3.997208	0.384220
C	-2.920495	5.408595	-1.182418
C	-3.835325	4.354749	-1.337746
H	-4.720558	4.478939	-1.984269
C	-3.649627	-2.008613	-1.372856
C	-3.543794	-2.986571	-2.382027
H	-2.678143	-2.957285	-3.064999
C	-4.515772	-3.993346	-2.519009
C	-4.730062	-2.018483	-0.433537
C	-5.723988	-3.051612	-0.569472
C	-5.592931	-3.995559	-1.596023
H	-6.364650	-4.781926	-1.681889
O	-2.354689	1.770546	0.847187
O	-4.842817	-1.133610	0.530001
C	-4.414919	-5.053331	-3.594701
H	-4.317374	-6.073261	-3.160756
H	-5.317179	-5.069796	-4.245454
H	-3.534552	-4.886398	-4.248193
C	-6.866418	-3.071775	0.413232
H	-6.491131	-3.178675	1.453562
H	-7.423950	-2.110813	0.397363
H	-7.572333	-3.900029	0.200477
C	-3.098405	6.730693	-1.897666
H	-2.240539	6.956770	-2.569403
H	-4.017579	6.735931	-2.518671
H	-3.174329	7.580013	-1.183105
C	-0.445850	3.817645	1.325546
H	-0.800287	3.500696	2.329476
H	0.251316	3.023673	0.982497
H	0.134590	4.755538	1.434034

C

55

E_e = -4996.02883559

Fe	-0.092676	-0.070807	1.023728
S	-1.217112	0.014501	-1.560224
S	-0.654135	2.645516	0.757246
C	-1.256104	1.827794	-1.922517
H	-0.216413	2.064190	-2.235599
H	-1.921534	1.993411	-2.798134
C	-1.693542	2.728056	-0.771895
H	-2.714018	2.458363	-0.423943
H	-1.720408	3.784347	-1.118880
C	-2.870527	-0.293859	-0.953933
C	-3.027016	-0.406539	0.467665
C	-5.410328	-0.845764	0.056365
H	-6.415436	-1.064035	0.462371
C	-4.353669	-0.689849	0.961603
C	-5.249757	-0.744510	-1.350098
C	-3.958313	-0.474523	-1.833761
H	-3.778930	-0.404687	-2.920557
C	0.975277	3.016864	0.118578
C	1.393102	4.348904	-0.081910
H	0.687880	5.165489	0.150537
C	2.680177	4.645070	-0.561486
C	1.850799	1.908076	-0.131241
C	3.175457	2.215766	-0.615679
C	3.546221	3.550845	-0.817697
H	4.568047	3.756636	-1.186925
O	-2.039891	-0.259520	1.312774
O	1.497786	0.660816	0.049937
C	3.140888	6.070181	-0.783250
H	4.021350	6.327012	-0.152056
H	3.445222	6.251780	-1.838801
H	2.338348	6.797086	-0.540753
C	4.117395	1.068119	-0.876264

H	4.288107	0.478194	0.050153
H	3.687577	0.351475	-1.609088
H	5.097249	1.422379	-1.257296
C	-6.426606	-0.935874	-2.283322
H	-7.233356	-0.191227	-2.097316
H	-6.121504	-0.833934	-3.345351
H	-6.891774	-1.940708	-2.167843
C	-4.536791	-0.810033	2.453045
H	-3.890383	-1.613641	2.867337
H	-4.215883	0.119558	2.970967
H	-5.592333	-1.023940	2.719582
O	0.341733	-1.877629	0.714795
C	1.614100	-2.456180	0.622382
C	1.478901	-3.499532	-0.500989
H	2.369779	-1.696032	0.300869
H	0.785836	-4.315114	-0.216034
H	1.135574	-3.020258	-1.435593
Br	3.205200	-4.404649	-0.984379
Cl	0.602087	0.407625	3.173389
C	2.043860	-3.050360	1.971190
H	1.320252	-3.829776	2.294156
H	3.055928	-3.502853	1.910741
H	2.044714	-2.245145	2.733100

[Fe]

44

E_e = -2228.70005144

Fe	0.040082	1.360803	0.278541
S	0.954185	-0.016614	-1.618998
S	-0.915464	-1.118324	1.274915
Cl	0.601377	3.440909	-0.283767
C	-0.020925	-1.589383	-1.416470
H	-1.028884	-1.334293	-1.808195
H	0.432187	-2.333437	-2.105677
C	-0.090868	-2.165470	-0.008909
H	0.925942	-2.343040	0.401896
H	-0.615977	-3.143803	-0.040316
C	2.494038	-0.346334	-0.758646
C	2.596093	0.111549	0.591171
C	4.878414	-0.753259	0.599619
H	5.827401	-0.912372	1.141150
C	3.835312	-0.110211	1.279820
C	4.781568	-1.198466	-0.744389
C	3.569322	-0.975681	-1.418344
H	3.451641	-1.289786	-2.468541
C	-2.546833	-0.842394	0.598931
C	-3.579204	-1.792030	0.706030
H	-3.370766	-2.764224	1.181975
C	-4.871503	-1.503769	0.225328
C	-2.783174	0.446508	0.028033
C	-4.100177	0.754284	-0.453333
C	-5.096987	-0.225909	-0.346369
H	-6.107037	0.016288	-0.720171
O	1.589626	0.715663	1.202412
O	-1.821712	1.348995	-0.073190
C	-5.994997	-2.510152	0.328772
H	-6.841156	-2.113076	0.930232
H	-6.407230	-2.764200	-0.671778
H	-5.658224	-3.452842	0.804001
C	-4.356676	2.110201	-1.057602
H	-4.120938	2.919582	-0.334665
H	-3.697876	2.288502	-1.933938
H	-5.411124	2.216841	-1.379363
C	5.952668	-1.877828	-1.419119
H	6.245944	-2.810025	-0.889058
H	5.719153	-2.147912	-2.468401
H	6.850390	-1.222638	-1.433545
C	3.968204	0.373321	2.701123
H	3.829554	1.474060	2.760088
H	3.182458	-0.068007	3.350619
H	4.960481	0.119958	3.123351

Fe-CO_2

47

E_e = -2417.27954528

C	-0.628915	3.410481	-1.545148
O	-1.531355	3.951907	-2.055906
O	0.308888	2.894618	-1.046249
S	-0.792105	-1.210149	1.478031
S	0.992770	-0.540424	-1.562392
C	0.168987	-2.417864	0.443090
H	1.184492	-2.412433	0.893672
H	-0.276016	-3.419218	0.625582
C	0.213969	-2.138122	-1.052480
H	-0.809340	-2.087095	-1.481567
H	0.753875	-2.962437	-1.565346
O	1.856011	0.839257	0.910066
O	-1.624888	0.866832	-0.503194
C	2.833248	0.152082	0.347127
C	4.146230	0.174366	0.928854
C	2.623377	-0.627434	-0.833235
C	5.163320	-0.571738	0.317054
C	3.674565	-1.349569	-1.427118
C	4.961942	-1.343542	-0.855324
H	6.169736	-0.549488	0.770132
H	3.484198	-1.916785	-2.353079
C	-2.573661	-0.024999	-0.260601
C	-2.375720	-1.112370	0.644739
C	-3.846910	0.071358	-0.916444
C	-3.394173	-2.046218	0.924946
C	-4.831081	-0.884332	-0.628231
C	-4.641746	-1.951954	0.286414
H	-3.203379	-2.851132	1.653809
H	-5.806580	-0.790938	-1.137083
Fe	-0.004025	1.020424	0.560359
Cl	-0.672432	2.328761	2.252111
C	4.376046	0.995493	2.170806
H	4.120492	2.061944	1.995181
H	3.715866	0.661153	2.999205
H	5.428982	0.932810	2.508901
C	6.102390	-2.122566	-1.470580
H	6.967520	-1.464327	-1.700963
H	6.476384	-2.909692	-0.779921
H	5.797023	-2.620489	-2.412295
C	-4.081514	1.204819	-1.881973
H	-3.959568	2.188874	-1.381842
H	-3.340813	1.189040	-2.710023
H	-5.097648	1.158232	-2.320867
C	-5.753459	-2.939552	0.564833
H	-6.658715	-2.432119	0.963064
H	-6.067115	-3.475305	-0.357446
H	-5.444673	-3.702349	1.307313

[C-D]‡

102

E_e = -7413.31748404

Fe	2.517768	-0.000284	0.134673
S	3.873416	0.610943	-2.259501
S	5.028957	0.559632	1.073133
C	5.639685	0.502164	-1.719573
H	5.842685	-0.588845	-1.666859
H	6.276476	0.927565	-2.525616
C	5.964820	1.184700	-0.396145
H	5.721557	2.268060	-0.437369
H	7.050929	1.086130	-0.180582
C	3.551035	2.363321	-2.113127
C	2.750201	2.772969	-1.001175
C	2.955775	5.070374	-1.825976
H	2.717284	6.143075	-1.709203
C	2.458386	4.176488	-0.868822
C	3.738317	4.662396	-2.936458
C	4.018782	3.290826	-3.065495
H	4.606929	2.925043	-3.924383
C	5.504122	-1.166228	1.076221
C	6.706604	-1.581085	1.683530
H	7.345453	-0.822632	2.167342
C	7.092372	-2.931945	1.681127
C	4.608471	-2.099016	0.460532

C	5.007384	-3.484074	0.454361
C	6.218819	-3.855106	1.053326
H	6.497761	-4.924616	1.038117
O	2.277375	1.924094	-0.115917
O	3.472582	-1.735056	-0.094289
C	8.378368	-3.395715	2.331421
H	8.188524	-4.111862	3.161973
H	9.045675	-3.917280	1.609322
H	8.948531	-2.543467	2.754943
C	4.099437	-4.496088	-0.197418
H	3.110443	-4.539973	0.307618
H	3.885854	-4.227335	-1.254257
H	4.544119	-5.511824	-0.175213
C	4.226748	5.672824	-3.952149
H	4.842311	6.470822	-3.480407
H	4.846799	5.193008	-4.736956
H	3.381460	6.184548	-4.463904
C	1.618249	4.620599	0.301021
H	0.621116	4.131283	0.282186
H	2.081243	4.312719	1.262958
H	1.475687	5.720184	0.305068
O	0.882061	-0.479207	-0.829203
C	0.301496	-1.735225	-1.161976
C	0.304261	-2.590856	0.113626
H	-0.174849	-2.053575	0.950846
H	1.326135	-2.906149	0.392908
C	-0.275205	1.052093	-1.560419
O	0.175044	1.237751	-2.637130
O	-1.031372	1.234594	-0.638719
S	-5.667092	0.564780	0.172895
S	-2.643805	-0.571461	1.646686
C	-5.495850	-0.428650	1.730970
H	-5.445421	0.336673	2.534801
H	-6.440022	-1.000010	1.861330
C	-4.302349	-1.372321	1.793784
H	-4.321391	-2.109830	0.963590
H	-4.327354	-1.940083	2.748710
O	-3.085194	2.334779	1.250877
O	-3.330436	-0.337202	-1.450370
C	-2.902899	2.015797	2.516022
C	-2.910315	3.044802	3.519181
C	-2.697750	0.664706	2.937689
C	-2.704791	2.685179	4.858081
C	-2.473505	0.345343	4.289142
C	-2.480658	1.349152	5.275924
H	-2.706581	3.486154	5.618821
H	-2.273415	-0.702554	4.566919
C	-4.446276	-0.963045	-1.762978
C	-5.684072	-0.694773	-1.097884
C	-4.456151	-1.957553	-2.803066
C	-6.880231	-1.352307	-1.451896
C	-5.660571	-2.599502	-3.119087
C	-6.889489	-2.323844	-2.465807
H	-7.813338	-1.091096	-0.924666
H	-5.647173	-3.355414	-3.924785
Br	-0.756887	-4.276386	-0.098416
H	-0.766464	-1.553110	-1.434978
Fe	-3.196723	1.276006	-0.349153
Cl	-3.862875	2.846275	-1.834077
Cl	1.995502	-0.215743	2.365760
C	-3.163945	-2.271072	-3.511233
H	-2.671968	-1.342519	-3.868612
H	-2.440644	-2.758120	-2.821155
H	-3.328117	-2.947624	-4.373984
C	-8.157986	-3.047462	-2.863617
H	-8.411801	-2.877340	-3.933344
H	-8.065096	-4.148116	-2.729965
H	-9.024822	-2.710595	-2.259102
C	-3.131112	4.470465	3.083825
H	-2.341927	4.792658	2.371532
H	-4.090914	4.577031	2.534538
H	-3.134013	5.163547	3.948949
C	-2.214966	1.028480	6.730293
H	-1.233589	1.433872	7.062501

H	-2.987373	1.469836	7.397063
H	-2.196298	-0.065449	6.909588
C	1.021524	-2.382372	-2.351524
H	2.086048	-2.555833	-2.095013
H	0.549628	-3.350861	-2.618776
H	0.974611	-1.707306	-3.228969

D

102

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Fe	-2.480463	0.198435	-0.927460
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S	-4.770525	1.319542	-1.840426
C	-5.360906	1.356970	0.965368
H	-5.842224	0.358989	0.885690
H	-5.870766	1.915835	1.779881
C	-5.486302	2.134803	-0.338655
H	-4.955291	3.108889	-0.275921
H	-6.557909	2.342709	-0.548418
C	-2.865731	2.601007	1.457350
C	-2.018154	2.867239	0.334923
C	-1.595428	5.076180	1.302283
H	-1.091364	6.057087	1.237064
C	-1.377058	4.154741	0.269739
C	-2.418768	4.805180	2.425335
C	-3.044297	3.547549	2.486220
H	-3.680705	3.286901	3.348766
C	-5.642101	-0.242172	-1.862973
C	-6.915302	-0.361989	-2.456947
H	-7.378737	0.530288	-2.911304
C	-7.587947	-1.595187	-2.478128
C	-4.970068	-1.366696	-1.285242
C	-5.659581	-2.631670	-1.308908
C	-6.930199	-2.708233	-1.893223
H	-7.437547	-3.690134	-1.903760
O	-1.813393	1.989379	-0.620776
O	-3.778721	-1.278483	-0.743075
C	-8.956099	-1.745639	-3.108524
H	-8.950722	-2.488504	-3.936916
H	-9.716305	-2.094823	-2.374351
H	-9.317228	-0.784383	-3.528310
C	-4.968639	-3.830520	-0.711494
H	-4.009118	-4.033355	-1.234542
H	-4.697857	-3.655019	0.351756
H	-5.603317	-4.737912	-0.772012
C	-2.593710	5.832481	3.522998
H	-2.983389	6.797049	3.128603
H	-3.300354	5.479269	4.301575
H	-1.629738	6.062411	4.028820
C	-0.483447	4.448455	-0.906050
H	0.400869	3.775594	-0.908515
H	-1.010591	4.257229	-1.864538
H	-0.122867	5.496205	-0.890217
O	0.436381	-2.250034	0.970192
C	-0.588902	-3.211364	1.331907
C	-1.044735	-2.819696	2.743388
H	-1.471188	-1.800425	2.743827
H	-0.215935	-2.893285	3.473092
C	0.063005	-1.058530	0.415162
O	-1.172678	-0.873405	0.200424
O	1.000643	-0.245256	0.184966
S	5.726772	-0.187486	0.407709
S	3.291648	1.109399	-1.809887
C	6.035029	0.953169	-1.018373
H	5.975974	1.969844	-0.573783
H	7.079336	0.790568	-1.362702
C	5.076632	0.814284	-2.194611
H	5.102093	-0.213415	-2.615430
H	5.375408	1.517396	-3.002181
O	3.067163	1.618263	1.118379
O	3.399442	-1.815591	-0.523703
C	3.217642	2.715889	0.414667
C	3.251931	3.992386	1.080841
C	3.358029	2.707366	-1.010077

C	3.419785	5.156213	0.319147
C	3.506157	3.901693	-1.743292
C	3.551104	5.147934	-1.093304
H	3.444114	6.125582	0.849201
H	3.581129	3.848317	-2.842588
C	4.556967	-2.389299	-0.752551
C	5.803502	-1.788500	-0.386169
C	4.607281	-3.671708	-1.406770
C	7.034655	-2.436252	-0.615363
C	5.849944	-4.277974	-1.630308
C	7.083188	-3.691567	-1.244942
H	7.966296	-1.943060	-0.289492
H	5.864001	-5.265023	-2.127318
Br	-2.497633	-3.991674	3.421698
H	-1.444147	-3.101657	0.633128
Fe	3.005389	-0.262224	0.606950
Cl	-1.828728	-0.137514	-3.073384
Cl	3.259963	-1.161974	2.684072
C	3.101767	4.016448	2.580215
H	2.125812	3.582079	2.885406
H	3.875028	3.385837	3.068845
H	3.173261	5.048438	2.979480
C	3.713445	6.440431	-1.864106
H	2.846442	7.121367	-1.714994
H	4.618416	7.002978	-1.543294
H	3.804586	6.254591	-2.953689
C	3.306033	-4.308885	-1.820984
H	2.630488	-4.426142	-0.947346
H	2.753984	-3.663150	-2.537705
H	3.467907	-5.301276	-2.288418
C	8.393874	-4.406652	-1.495055
H	8.446413	-5.376611	-0.951900
H	8.541184	-4.638482	-2.573389
H	9.258954	-3.795769	-1.164696
C	0.048826	-4.590793	1.226129
H	0.946574	-4.657266	1.874644
H	-0.676048	-5.370830	1.532448
H	0.359285	-4.785247	0.180570

E

111

E_e = -5870.27651134

O	0.097270	-3.046631	0.222720
C	-0.096104	-4.452295	-0.036079
C	0.475456	-4.884030	-1.387044
H	0.024980	-4.308655	-2.215432
H	0.338651	-5.970066	-1.546584
C	-0.530528	-2.105297	-0.592344
O	-1.245727	-2.432840	-1.539100
O	-0.198362	-0.906491	-0.218909
S	-2.920775	2.669405	0.967909
S	-3.235538	0.081516	-1.409450
C	-4.447175	2.258066	0.001610
H	-5.004299	1.554463	0.656153
H	-5.048890	3.187766	-0.088097
C	-4.205436	1.658933	-1.376535
H	-3.623303	2.352564	-2.019872
H	-5.179002	1.469779	-1.877862
O	-2.557632	-0.489039	1.441933
O	-0.636455	1.954924	-0.838105
C	-3.675625	-1.069015	1.051817
C	-4.425081	-1.872807	1.979047
C	-4.182012	-0.935248	-0.278852
C	-5.595206	-2.506595	1.537918
C	-5.353081	-1.600326	-0.689028
C	-6.085411	-2.394913	0.212297
H	-6.157081	-3.123855	2.261441
H	-5.691454	-1.494890	-1.733234
C	-0.995473	3.220565	-0.923871
C	-2.063565	3.774302	-0.147695
C	-0.313477	4.112284	-1.825268
C	-2.414875	5.136307	-0.227063
C	-0.701377	5.457863	-1.890988
C	-1.745402	6.005893	-1.105046

H	-3.227521	5.516698	0.414247
H	-0.161166	6.120257	-2.591026
Br	2.441684	-4.594878	-1.512554
H	0.505169	-4.931427	0.766126
Fe	-1.296494	0.620863	0.467947
Cl	0.019650	1.358388	2.256378
C	-3.916751	-2.001337	3.392700
H	-2.895317	-2.438004	3.413255
H	-3.823414	-1.005084	3.875444
H	-4.586355	-2.633622	4.009384
C	-7.349635	-3.111769	-0.209015
H	-7.577019	-2.940419	-1.280482
H	-7.269945	-4.210153	-0.055543
H	-8.230700	-2.771926	0.378685
C	0.805066	3.568349	-2.676557
H	1.649948	3.212170	-2.046757
H	0.470123	2.688198	-3.265389
H	1.194777	4.336248	-3.374454
C	-2.112515	7.470071	-1.210995
H	-1.251261	8.129469	-0.965951
H	-2.437788	7.740223	-2.239712
H	-2.939247	7.732683	-0.520618
C	-1.559237	-4.896133	0.115467
H	-2.187307	-4.483062	-0.695235
H	-1.627495	-6.003809	0.111948
H	-1.953940	-4.529173	1.083931
N	3.752991	-0.020785	0.167870
C	5.195658	-0.173229	0.631393
H	5.196532	0.037552	1.716537
H	5.433130	-1.250605	0.511496
C	6.254913	0.684349	-0.068973
H	6.396145	0.358773	-1.121535
H	5.937463	1.748616	-0.109218
C	7.608103	0.589153	0.662158
H	7.905498	-0.480608	0.746884
H	7.486062	0.952008	1.707632
C	8.722533	1.379946	-0.033244
H	9.679868	1.297196	0.520307
H	8.900508	1.010071	-1.065268
H	8.470312	2.459169	-0.105190
C	3.692963	-0.384358	-1.327289
H	3.960803	-1.460150	-1.371363
H	4.505977	0.188361	-1.813852
C	2.372575	-0.136495	-2.052169
H	1.508979	-0.523385	-1.473858
H	2.189635	0.951696	-2.167192
C	2.391977	-0.799106	-3.444367
H	3.240677	-0.395186	-4.045011
H	2.592103	-1.887777	-3.323180
C	1.073803	-0.607377	-4.205168
H	0.857050	0.468075	-4.376893
H	1.108055	-1.105357	-5.196130
H	0.220728	-1.031209	-3.635676
C	3.222845	1.411639	0.353233
H	3.560649	1.974630	-0.540405
H	2.117221	1.335317	0.309442
C	3.635151	2.166849	1.619216
H	4.740261	2.277845	1.682478
H	3.309567	1.621129	2.526162
C	2.987248	3.565673	1.631367
H	1.883826	3.438725	1.595934
H	3.274925	4.117581	0.707299
C	3.375628	4.386074	2.866443
H	2.898640	5.387128	2.846350
H	3.048525	3.882822	3.800699
H	4.474778	4.539494	2.933644
C	2.885195	-1.057110	0.916121
H	1.865296	-0.977912	0.487406
H	3.301997	-2.039809	0.611905
C	2.796575	-0.956006	2.438608
H	2.190229	-0.067424	2.712223
H	3.797111	-0.858769	2.916545
C	2.094389	-2.206024	3.006215
H	1.134859	-2.351898	2.465962

H	2.711026	-3.107814	2.786256
C	1.838038	-2.099294	4.513791
H	1.174798	-1.239035	4.741949
H	1.345943	-3.014235	4.903404
H	2.781970	-1.959642	5.084654

[E-F]‡

111

E_e = -5870.24168837

O	0.347400	-2.320486	-0.821150
C	1.463850	-3.191291	-1.171130
C	2.247274	-2.516158	-2.286496
H	2.565496	-1.477955	-2.182915
H	2.477692	-3.029094	-3.225843
C	-0.124179	-1.645676	-1.912162
O	0.519454	-1.817983	-2.998624
O	-1.124992	-0.893551	-1.763749
S	-3.558286	1.590692	1.397714
S	-4.360504	-0.857454	-1.039883
C	-5.199840	0.763287	1.162257
H	-5.163692	-0.116798	1.839154
H	-5.981493	1.454179	1.544507
C	-5.530361	0.350670	-0.265461
H	-5.518283	1.223972	-0.951808
H	-6.547961	-0.093964	-0.300711
O	-2.260473	-1.365702	1.011029
O	-2.370727	1.642990	-1.334135
C	-3.237785	-2.249019	1.045550
C	-3.204033	-3.320817	2.003523
C	-4.353338	-2.191064	0.152012
C	-4.243855	-4.260465	2.011425
C	-5.372121	-3.163460	0.178845
C	-5.340642	-4.213735	1.113831
H	-4.199473	-5.078712	2.752009
H	-6.198563	-3.094932	-0.548007
C	-3.007259	2.754064	-1.029879
C	-3.651323	2.945491	0.232673
C	-3.073916	3.829582	-1.982702
C	-4.299403	4.153408	0.558291
C	-3.739921	5.010886	-1.629492
C	-4.360419	5.208356	-0.369258
H	-4.759990	4.264730	1.554105
H	-3.777927	5.827449	-2.372427
Br	4.576610	-3.026743	-1.500075
H	2.074644	-3.229015	-0.250470
Fe	-1.956950	0.125690	-0.189971
Cl	-0.084300	1.050406	0.886737
C	-2.041527	-3.393431	2.959429
H	-1.083029	-3.493003	2.406703
H	-1.952157	-2.458526	3.552667
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C	-6.424512	-5.268197	1.160288
H	-6.911898	-5.312451	2.158678
H	-7.216116	-5.072581	0.409303
H	-6.017280	-6.283302	0.959528
C	-2.417669	3.639671	-3.325957
H	-1.331770	3.434161	-3.212422
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H	-2.545676	4.531760	-3.970968
C	-5.052363	6.513887	-0.043223
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H	-5.498660	6.496349	0.971497
H	-4.347629	7.373286	-0.083171
C	0.974913	-4.589335	-1.537733
H	0.368012	-4.564252	-2.465375
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H	0.358539	-5.008007	-0.718316
N	4.022630	0.812692	0.391357
C	5.440346	0.498171	0.863153
H	5.387920	0.424275	1.965391
H	5.654477	-0.518109	0.470245
C	6.547220	1.474913	0.454586
H	6.733946	1.422304	-0.638816
H	6.256126	2.525109	0.676332

C	7.860333	1.149201	1.193025
H	8.128138	0.084817	1.008344
H	7.694856	1.233589	2.290976
C	9.024618	2.054504	0.773976
H	9.951621	1.798471	1.326160
H	9.244589	1.956796	-0.310173
H	8.801152	3.124178	0.973739
C	4.043517	0.848108	-1.147029
H	4.377202	-0.168867	-1.453574
H	4.842179	1.565368	-1.418146
C	2.750161	1.242796	-1.862487
H	1.910541	0.568155	-1.595850
H	2.417663	2.259435	-1.565091
C	2.966997	1.213032	-3.389816
H	3.755001	1.953010	-3.661026
H	3.374698	0.220046	-3.685430
C	1.682415	1.492060	-4.178904
H	1.241340	2.473278	-3.903618
H	1.881954	1.506571	-5.269996
H	0.921847	0.708648	-3.983009
C	3.492479	2.154952	0.907816
H	3.867280	2.924641	0.202589
H	2.389990	2.098275	0.787443
C	3.847990	2.567742	2.339233
H	4.943234	2.725429	2.447832
H	3.566382	1.779881	3.064797
C	3.112404	3.871162	2.709714
H	2.016646	3.705045	2.616068
H	3.364512	4.662286	1.967379
C	3.446103	4.364866	4.122368
H	2.897642	5.298770	4.360815
H	3.169773	3.611542	4.890267
H	4.531013	4.575612	4.237057
C	3.113776	-0.361222	0.807932
H	2.128900	-0.163622	0.341374
H	3.576572	-1.251038	0.326626
C	2.890485	-0.597647	2.301864
H	2.257021	0.211746	2.721723
H	3.846438	-0.614489	2.870866
C	2.162493	-1.938152	2.522569
H	1.214962	-1.929475	1.941494
H	2.785223	-2.763068	2.108907
C	1.860996	-2.206334	4.001624
H	1.203107	-1.419525	4.427231
H	1.344461	-3.178559	4.135550
H	2.790006	-2.235347	4.611402

F

57

E_e = -2610.36390545

Fe	-0.027023	0.435022	0.400948
S	1.261227	-1.036452	-1.576035
S	-0.408202	-1.914626	1.460910
C	0.780389	-2.735125	-1.019081
H	-0.229149	-2.894307	-1.454782
H	1.473414	-3.457994	-1.500124
C	0.774877	-2.961790	0.486407
H	1.767028	-2.740849	0.934909
H	0.531141	-4.022924	0.707170
C	2.865848	-0.830261	-0.813417
C	2.908673	-0.050058	0.384603
C	5.327416	-0.394591	0.418783
H	6.302484	-0.223275	0.907972
C	4.185304	0.163427	1.009450
C	5.290062	-1.158657	-0.775294
C	4.037717	-1.359672	-1.385903
H	3.966126	-1.933081	-2.324993
C	-1.961699	-2.170973	0.609511
C	-2.775126	-3.286863	0.891733
H	-2.441786	-4.020691	1.644391
C	-4.000844	-3.463964	0.227438
C	-2.354557	-1.167450	-0.329819
C	-3.606102	-1.349224	-1.012478
C	-4.383050	-2.477824	-0.718202

H	-5.344330	-2.598451	-1.248634
O	1.821858	0.468876	0.920098
O	-1.612442	-0.105950	-0.577166
C	-4.894758	-4.651180	0.511599
H	-5.877469	-4.334480	0.924675
H	-5.109275	-5.234078	-0.410513
H	-4.433201	-5.342468	1.245104
C	-4.032970	-0.309379	-2.016857
H	-4.068502	0.698859	-1.552773
H	-3.299974	-0.230973	-2.848855
H	-5.028080	-0.542902	-2.444982
C	6.561162	-1.721398	-1.371167
H	7.082537	-2.397124	-0.658683
H	6.358800	-2.299077	-2.295286
H	7.281846	-0.915525	-1.630733
C	4.242572	0.981927	2.273217
H	3.838603	2.002659	2.103247
H	3.606658	0.536821	3.067910
H	5.279495	1.068216	2.653961
O	-1.772590	3.299805	-0.957426
C	-2.235723	4.636862	-0.603318
C	-0.924792	5.458330	-0.698084
H	-0.825981	6.015807	-1.653373
H	-0.784571	6.155256	0.151309
C	-0.437139	3.237118	-0.834236
O	0.226810	2.214774	-0.900759
O	0.109601	4.456009	-0.641045
H	-2.960214	4.934010	-1.388614
Cl	-0.935885	1.600380	2.138488
C	-2.889081	4.611100	0.770739
H	-2.172027	4.261170	1.541221
H	-3.250772	5.626557	1.035734
H	-3.753501	3.918819	0.774439

[D-F]‡

102

E_e = -7413.29911515

Fe	4.549675	0.698235	-0.837640
S	4.961559	-1.006339	1.355894
S	5.829228	2.381670	0.734745
C	5.539564	0.228453	2.606773
H	4.601711	0.679530	2.995611
H	6.021403	-0.324472	3.441911
C	6.489942	1.298768	2.087633
H	7.407513	0.847400	1.652956
H	6.799820	1.963925	2.922314
C	6.501533	-1.629762	0.693158
C	6.897323	-1.131928	-0.588827
C	8.844945	-2.608271	-0.459915
H	9.772802	-2.994873	-0.918442
C	8.110006	-1.647023	-1.166540
C	8.448942	-3.111046	0.805654
C	7.259064	-2.609790	1.363995
H	6.902488	-2.988339	2.336595
C	4.318500	3.018129	1.451536
C	4.340129	4.146288	2.297346
H	5.304172	4.636381	2.514206
C	3.151269	4.644435	2.853808
C	3.099470	2.358392	1.098460
C	1.881071	2.861528	1.676203
C	1.944681	3.974987	2.525493
H	0.997625	4.349270	2.953317
O	6.195000	-0.233271	-1.245581
O	3.075218	1.318650	0.285273
C	3.142812	5.858185	3.757865
H	2.567589	6.699093	3.311045
H	2.671174	5.637609	4.740679
H	4.170394	6.226630	3.954345
C	0.577626	2.181046	1.349186
H	0.338463	2.235412	0.265393
H	0.617755	1.099519	1.601886
H	-0.265538	2.634233	1.906995
C	9.274779	-4.163696	1.512744
H	8.836460	-4.432593	2.495148

H	9.349327	-5.098192	0.913983
H	10.316419	-3.817763	1.693324
C	8.535010	-1.129573	-2.516612
H	7.754330	-1.329848	-3.281282
H	8.658516	-0.025632	-2.500858
H	9.486497	-1.591727	-2.848237
O	-1.212717	-1.009062	-1.555971
C	0.063032	-1.212410	-2.207838
C	1.042519	-0.099119	-1.835212
H	1.174410	0.193420	-0.785989
H	1.378940	0.628341	-2.582787
C	-1.588947	0.308269	-1.498345
O	-0.719987	1.175590	-1.779244
O	-2.789927	0.538744	-1.150939
S	-6.640517	-1.834270	0.119986
S	-4.947436	1.071282	1.290187
C	-7.260789	-0.615642	1.369832
H	-7.831974	0.124083	0.768776
H	-7.980505	-1.145032	2.031369
C	-6.197193	0.071668	2.217494
H	-5.591530	-0.672315	2.777940
H	-6.689162	0.736710	2.960318
O	-5.662211	0.754778	-1.593468
O	-3.676911	-1.747967	0.491060
C	-6.172078	1.832918	-1.047070
C	-6.968048	2.728212	-1.847467
C	-5.977885	2.172292	0.330554
C	-7.506772	3.878664	-1.257608
C	-6.523805	3.348474	0.883190
C	-7.305076	4.219981	0.104510
H	-8.111465	4.553434	-1.890530
H	-6.323011	3.582650	1.942397
C	-4.252524	-2.725783	1.149177
C	-5.667025	-2.946856	1.126383
C	-3.453056	-3.626241	1.940060
C	-6.260217	-4.017583	1.826355
C	-4.080214	-4.669455	2.632730
C	-5.480780	-4.895817	2.598027
H	-7.351751	-4.161804	1.755910
H	-3.446704	-5.351950	3.228152
Br	3.064155	-1.244624	-1.878114
H	0.421040	-2.166836	-1.772345
Fe	-4.435383	-0.604725	-0.910611
Cl	4.494031	2.230293	-2.499192
Cl	-4.507360	-2.048897	-2.665240
C	-7.178001	2.384295	-3.299667
H	-6.205811	2.312862	-3.832991
H	-7.649697	1.384221	-3.409597
H	-7.811506	3.138102	-3.809791
C	-7.895900	5.488511	0.681629
H	-7.669264	5.586322	1.763048
H	-7.498756	6.396873	0.176120
H	-9.002337	5.520008	0.567692
C	-1.963298	-3.401717	1.979528
H	-1.543641	-3.362785	0.952370
H	-1.718361	-2.417661	2.435584
H	-1.445209	-4.195464	2.554874
C	-6.098235	-6.053407	3.353375
H	-5.712840	-7.034228	2.995556
H	-5.876751	-6.004148	4.442828
H	-7.201503	-6.070183	3.238672
C	-0.130156	-1.361610	-3.716913
H	-0.490487	-0.408313	-4.154536
H	0.830838	-1.632188	-4.200534
H	-0.878659	-2.150607	-3.925702

CHO

17

E_e = -309.731743603[a]

C	1.283065	-0.809145	0.440160
C	0.130431	-1.517694	-0.293747
C	-1.101870	-0.637809	-0.409265
C	-0.993434	0.840313	-0.295202
C	0.345007	1.524215	-0.036920

C	1.554384	0.575402	-0.171344
H	-1.937018	-1.058179	-1.008271
H	0.447355	-1.801154	-1.324055
H	-0.143889	-2.465993	0.219792
H	1.019516	-0.699060	1.514786
H	2.197213	-1.438243	0.397138
H	-1.765780	1.457837	-0.798145
H	0.454451	2.386305	-0.729734
H	0.304448	1.955730	0.988416
H	1.800569	0.445422	-1.250406
H	2.449379	1.040051	0.294591
O	-1.516467	0.040700	0.786724

TBAC

54

E_e = -1145.99812579[a]

N	0.038284	-0.145675	0.293632
Cl	2.316996	0.331605	-2.341169
C	-0.530513	-0.765157	-0.989421
H	-1.432833	-0.179836	-1.246025
H	0.269405	-0.552745	-1.751625
C	-0.877269	-2.253064	-0.938990
H	0.020918	-2.862830	-0.704369
H	-1.633830	-2.480788	-0.152757
C	-1.425631	-2.710013	-2.305485
H	-0.670826	-2.476954	-3.088118
H	-2.325522	-2.106126	-2.562598
C	-1.777828	-4.201615	-2.345736
H	-2.169956	-4.496348	-3.340694
H	-0.888229	-4.833818	-2.138797
H	-2.552391	-4.460399	-1.591849
C	1.370193	-0.865957	0.587291
H	1.928034	-0.773952	-0.384381
H	1.109018	-1.924049	0.784280
C	2.218435	-0.311980	1.731716
H	2.408665	0.772182	1.587704
H	1.720679	-0.426540	2.722048
C	3.579632	-1.035735	1.762272
H	3.415178	-2.132454	1.866786
H	4.072167	-0.891750	0.775704
C	4.498067	-0.542859	2.886304
H	4.043702	-0.701775	3.888198
H	5.471444	-1.074914	2.873747
H	4.711875	0.542606	2.786304
C	-0.885785	-0.315742	1.483709
H	-0.953839	-1.407672	1.669327
H	-0.351779	0.124121	2.349539
C	-2.286297	0.287506	1.376560
H	-2.818380	-0.114510	0.487276
H	-2.221426	1.386969	1.235766
C	-3.116636	-0.011957	2.639014
H	-2.580638	0.379156	3.533404
H	-3.180508	-1.114193	2.784746
C	-4.528614	0.583909	2.585428
H	-5.100545	0.351160	3.506810
H	-4.498507	1.689225	2.481069
H	-5.105327	0.184724	1.724223
C	0.380028	1.342412	0.030684
H	0.432508	1.818249	1.030805
H	1.382110	1.298716	-0.466143
C	-0.510362	2.139980	-0.922805
H	-1.584501	2.138815	-0.634548
H	-0.418115	1.699302	-1.937195
C	0.004227	3.590547	-1.000738
H	-0.005039	4.052254	0.013625
H	1.067997	3.560001	-1.323874
C	-0.805538	4.458766	-1.971062
H	-1.873472	4.524829	-1.669557
H	-0.407163	5.493320	-2.016157
H	-0.774451	4.044221	-3.000665

Ecno

118

E_e = -3873.06567541[a]

Fe	-1.544813	0.078445	0.411596
S	-3.764959	-0.434162	-1.127652
S	-3.029346	2.255735	0.989544
C	-4.682231	1.174250	-1.066837
H	-4.186229	1.806550	-1.833953
H	-5.724241	0.988041	-1.405406
C	-4.697697	1.864865	0.289267
H	-5.173147	1.223032	1.061272
H	-5.273725	2.813343	0.231637
C	-4.581830	-1.344496	0.178527
C	-3.857298	-1.500457	1.398805
C	-5.754294	-2.783907	2.255599
H	-6.218114	-3.352714	3.081071
C	-4.477965	-2.241119	2.461227
C	-6.468343	-2.641650	1.039877
C	-5.852873	-1.918055	0.000723
H	-6.364331	-1.804410	-0.969583
C	-2.306459	3.232987	-0.325220
C	-2.631318	4.595747	-0.478386
H	-3.323434	5.064093	0.241535
C	-2.091217	5.355076	-1.531047
C	-1.389205	2.573485	-1.205395
C	-0.852926	3.345836	-2.296522
C	-1.210705	4.695448	-2.425385
H	-0.785275	5.267660	-3.269466
O	-2.654783	-0.987639	1.570570
O	-1.038777	1.314195	-1.052632
C	-2.432246	6.818164	-1.714487
H	-1.529092	7.464204	-1.650802
H	-2.892544	7.012483	-2.708091
H	-3.146198	7.169096	-0.942216
C	0.060428	2.664115	-3.284314
H	0.940629	2.205036	-2.785433
H	-0.462900	1.828188	-3.797906
H	0.423912	3.372088	-4.056060
C	-7.833905	-3.269459	0.865237
H	-8.546679	-2.929232	1.647921
H	-8.273640	-3.019086	-0.121181
H	-7.787030	-4.378437	0.936863
C	-3.724960	-2.410799	3.755904
H	-2.763884	-2.942502	3.587532
H	-3.451885	-1.426835	4.193393
H	-4.318381	-2.979826	4.499328
O	-0.070871	-3.043336	-1.989830
C	1.275087	-2.572292	-2.131772
C	1.253451	-1.281827	-2.982120
H	0.615232	-0.522260	-2.491746
C	-0.965218	-2.382862	-1.126078
O	-0.449692	-1.367956	-0.493030
O	-2.099810	-2.834856	-1.078483
H	1.693002	-2.334556	-1.130118
Cl	-0.132421	0.908456	2.118531
C	2.073865	-3.698612	-2.805673
H	3.148049	-3.410546	-2.802104
H	1.974840	-4.615206	-2.187052
C	0.855859	-1.535840	-4.434304
C	1.605859	-3.956369	-4.249619
C	1.660317	-2.669767	-5.092910
H	-0.221773	-1.813647	-4.399862
H	0.922902	-0.592294	-5.014621
H	2.228056	-4.751408	-4.713849
H	0.563016	-4.340013	-4.222057
H	2.717835	-2.342337	-5.211131
H	1.272281	-2.857557	-6.116753
Cl	2.959767	-0.508924	-2.920996
N	4.083031	0.023762	1.119243
C	2.759978	-0.747296	1.244103
H	2.056005	-0.104398	1.808826
H	2.351084	-0.801066	0.215799
C	2.848841	-2.143954	1.866935
H	3.317319	-2.864655	1.160471
H	3.490523	-2.140279	2.777408
C	1.446649	-2.663122	2.245824
H	0.781480	-2.595488	1.358519

H	0.992201	-1.974964	2.990702
C	1.472030	-4.095760	2.787869
H	0.450839	-4.435825	3.053850
H	1.873724	-4.811479	2.038480
H	2.101785	-4.181001	3.700497
C	5.044913	-0.828683	0.283156
H	4.522322	-0.995218	-0.681796
H	5.109884	-1.803413	0.803252
C	6.455674	-0.284210	0.044666
H	6.427109	0.684713	-0.498052
H	6.979036	-0.095300	1.007215
C	7.282301	-1.286231	-0.786319
H	7.320808	-2.263121	-0.253455
H	6.754525	-1.485355	-1.745456
C	8.707141	-0.796595	-1.070671
H	9.274034	-0.623628	-0.131194
H	9.273557	-1.537730	-1.670275
H	8.702978	0.158053	-1.638250
C	4.713937	0.307655	2.485685
H	5.325689	-0.582799	2.736727
H	5.419233	1.147936	2.323328
C	3.770034	0.622888	3.650596
H	3.168061	-0.272059	3.910813
H	3.040184	1.409264	3.378179
C	4.572045	1.069639	4.888088
H	5.158921	1.982543	4.636365
H	5.324167	0.289392	5.146850
C	3.679834	1.349440	6.103673
H	4.279977	1.679755	6.975863
H	2.936669	2.144321	5.884274
H	3.114001	0.443985	6.408076
C	3.823421	1.322517	0.334584
H	4.826097	1.728458	0.095957
H	3.361979	0.987765	-0.617524
C	2.970330	2.405451	0.990199
H	3.493765	2.831200	1.874229
H	1.993921	1.998522	1.335745
C	2.694638	3.544273	-0.011967
H	3.656844	3.932504	-0.420664
H	2.132371	3.132134	-0.878093
C	1.890382	4.689342	0.614433
H	2.431519	5.147343	1.470472
H	1.691511	5.489377	-0.126727
H	0.910059	4.326283	0.985373

[E$_{CHO}$-F$_{CHO}$]‡

118

E_e = -3873.03205736[a]

O	0.456600	-2.197327	-0.471354
C	1.541368	-3.147660	-0.674426
C	2.308961	-2.778063	-1.949866
H	2.622007	-1.738150	-2.066751
C	-0.059318	-1.721431	-1.641858
O	0.510344	-2.120130	-2.704482
O	-1.024536	-0.909718	-1.579053
S	-3.482998	1.872294	1.297715
S	-4.243822	-0.827374	-0.867515
C	-5.114562	1.006419	1.147048
H	-5.072639	0.204862	1.915074
H	-5.905421	1.725734	1.449746
C	-5.433961	0.438733	-0.229121
H	-5.430960	1.233839	-1.004841
H	-6.445345	-0.021179	-0.219263
O	-2.144985	-1.089919	1.232260
O	-2.282588	1.651757	-1.421197
C	-3.111947	-1.976316	1.356622
C	-3.070805	-2.939513	2.423776
C	-4.223956	-2.027949	0.458014
C	-4.098482	-3.886894	2.527186
C	-5.230548	-3.005324	0.584317
C	-5.190741	-3.950414	1.625155
H	-4.047976	-4.620723	3.351183
H	-6.054239	-3.024510	-0.148647
C	-2.934292	2.780313	-1.237352

C	-3.587116	3.095039	-0.004284
C	-3.010271	3.748941	-2.298134
C	-4.252257	4.321833	0.189943
C	-3.693264	4.951823	-2.073728
C	-4.322499	5.272489	-0.843561
H	-4.718706	4.531245	1.167070
H	-3.737955	5.685188	-2.898590
H	2.198128	-2.966720	0.192232
Fe	-1.850732	0.270747	-0.120254
Cl	-0.007817	1.340644	0.859042
C	-1.914785	-2.892868	3.389181
H	-0.950265	-3.034929	2.856665
H	-1.844244	-1.899266	3.880916
H	-2.007155	-3.671976	4.171942
C	-6.261354	-5.008326	1.778628
H	-7.052712	-4.901942	1.009619
H	-5.840855	-6.033585	1.685303
H	-6.751746	-4.954996	2.775105
C	-2.344828	3.427989	-3.611618
H	-1.256447	3.252872	-3.473377
H	-2.745450	2.486335	-4.044104
H	-2.483056	4.244738	-4.347908
C	-5.032384	6.595937	-0.658834
H	-5.847478	6.732923	-1.402745
H	-5.483557	6.678907	0.350492
H	-4.338256	7.455549	-0.785748
C	1.046311	-4.611176	-0.629494
N	4.103744	0.892150	0.376765
C	5.517901	0.549637	0.841269
H	5.500780	0.604702	1.945944
H	5.656752	-0.515569	0.558294
C	6.661895	1.405864	0.289676
H	6.803243	1.219395	-0.795889
H	6.440699	2.490440	0.398504
C	7.981428	1.085206	1.018554
H	8.179730	-0.007687	0.948390
H	7.863425	1.302180	2.104408
C	9.179268	1.864184	0.462555
H	10.110675	1.615042	1.010591
H	9.351289	1.632450	-0.609878
H	9.025815	2.961308	0.545803
C	4.074937	0.734093	-1.153895
H	4.358945	-0.327820	-1.333764
H	4.889885	1.380424	-1.533965
C	2.773628	1.090682	-1.874273
H	1.927819	0.463649	-1.524606
H	2.468740	2.138400	-1.669267
C	2.950914	0.912519	-3.396224
H	3.751292	1.600752	-3.753877
H	3.325636	-0.114622	-3.607461
C	1.655756	1.154371	-4.180082
H	1.252919	2.172058	-3.993110
H	1.826435	1.054713	-5.271680
H	0.874420	0.422467	-3.890018
C	3.666418	2.315095	0.735680
H	4.055985	2.969549	-0.070885
H	2.559097	2.308247	0.654805
C	4.095380	2.880512	2.093102
H	5.201534	2.973653	2.153036
H	3.787447	2.211556	2.920203
C	3.461907	4.268749	2.312537
H	2.354736	4.172087	2.266504
H	3.743099	4.941289	1.470416
C	3.873400	4.909695	3.643221
H	3.398259	5.903157	3.774361
H	3.571196	4.279692	4.506528
H	4.973335	5.054274	3.704990
C	3.149434	-0.167514	0.962158
H	2.165576	0.011786	0.486972
H	3.562924	-1.132812	0.595063
C	2.948252	-0.188748	2.477264
H	2.364601	0.700438	2.796425
H	3.914490	-0.178380	3.029255
C	2.160831	-1.448952	2.886250

H	1.204753	-1.471485	2.319704
H	2.735443	-2.352054	2.580405
C	1.873968	-1.500959	4.391373
H	1.261800	-0.632590	4.714483
H	1.314662	-2.419666	4.661982
H	2.811523	-1.492908	4.988698
C	2.609893	-3.742471	-3.075667
C	2.265982	-5.204222	-2.747356
C	0.928297	-5.304869	-1.996690
Cl	4.528844	-2.890229	-0.894557
H	0.648195	-6.368716	-1.841663
H	0.116916	-4.844528	-2.601766
H	2.243898	-5.794816	-3.687168
H	3.073780	-5.636436	-2.115234
H	2.004594	-3.399206	-3.942018
H	3.673629	-3.631615	-3.361236
H	1.772807	-5.183295	-0.011935
H	0.084787	-4.619985	-0.075564

F$_{\mathbf{CHO}}$

64

E_e = -2727.03724154[a]

O	-2.657485	-1.916039	0.917168
C	-3.962410	-2.560033	0.902058
C	-3.918460	-3.410696	-0.406261
H	-3.760190	-4.487954	-0.187738
C	-2.016771	-2.131153	-0.240805
O	-2.710481	-2.937026	-1.067698
O	-0.930896	-1.659919	-0.539975
S	2.563798	1.080062	1.201895
S	0.391306	1.268588	-1.628716
C	2.387108	2.493907	0.015095
H	1.618062	3.147425	0.479382
H	3.350639	3.047020	0.022779
C	2.016158	2.127236	-1.414761
H	2.755244	1.425106	-1.855683
H	2.004968	3.044500	-2.041636
O	-0.745895	0.895902	1.094859
O	1.919303	-1.292238	-0.477597
C	-1.172569	1.995555	0.507560
C	-2.105685	2.851686	1.189065
C	-0.742343	2.378477	-0.802341
C	-2.561612	4.009050	0.542926
C	-1.234682	3.542660	-1.423744
C	-2.147997	4.383601	-0.760877
H	-3.277804	4.656948	1.078739
H	-0.898617	3.788733	-2.444738
C	3.215837	-1.074831	-0.373690
C	3.746280	0.019073	0.377594
C	4.150001	-1.948397	-1.028558
C	5.133905	0.229556	0.508308
C	5.522245	-1.699664	-0.891157
C	6.049021	-0.624281	-0.130328
H	5.495858	1.070780	1.122530
H	6.226321	-2.384648	-1.396116
H	-4.009180	-3.195779	1.808864
Fe	0.531453	-0.460831	0.588967
Cl	0.641534	-1.662876	2.496228
C	-2.545188	2.471280	2.579661
H	-2.976192	1.447916	2.595965
H	-1.679688	2.436861	3.275725
H	-3.292845	3.184367	2.980269
C	-2.681777	5.641413	-1.410035
H	-2.261541	5.786504	-2.425464
H	-3.789222	5.615464	-1.505956
H	-2.435751	6.546353	-0.812663
C	3.610471	-3.108967	-1.824736
H	3.009338	-3.785337	-1.179976
H	2.920721	-2.761682	-2.623550
H	4.426790	-3.696363	-2.290248
C	7.543601	-0.422781	-0.005825
H	8.023816	-0.277770	-0.998235
H	7.784707	0.463376	0.615251
H	8.037702	-1.302227	0.462015

C	-5.071755	-1.505255	0.904700
C	-5.135829	-3.209732	-1.303570
C	-5.409511	-1.727234	-1.640963
C	-5.159841	-0.766620	-0.440763
H	-5.954960	0.004590	-0.388738
H	-4.215080	-0.201886	-0.591039
H	-4.771626	-1.423886	-2.496027
H	-6.456720	-1.640970	-1.998190
H	-5.013589	-3.811148	-2.228084
H	-5.999504	-3.655698	-0.762662
H	-6.030032	-2.018545	1.140992
H	-4.882721	-0.798493	1.738975

G$_{\mathbf{CHO}}$

135

E_e = -4182.80472215[a]

Fe	1.359256	0.102128	-0.091334
S	4.351404	1.184242	-0.032789
S	1.737683	2.241334	-1.948752
C	4.495001	2.554991	-1.255123
H	4.314599	3.471603	-0.654887
H	5.535825	2.600963	-1.642965
C	3.515173	2.469847	-2.418907
H	3.726569	1.586172	-3.058104
H	3.599596	3.374965	-3.059007
C	4.788846	-0.224238	-1.050820
C	3.762625	-1.133374	-1.463888
C	5.481467	-2.396855	-2.672975
H	5.747871	-3.249553	-3.322389
C	4.137071	-2.234561	-2.313615
C	6.506321	-1.519922	-2.239612
C	6.132415	-0.438088	-1.422754
H	6.899762	0.264626	-1.056695
C	1.536331	3.459833	-0.650517
C	1.610281	4.841759	-0.919693
H	1.777972	5.175470	-1.957657
C	1.479448	5.794065	0.107106
C	1.279666	2.975788	0.671675
C	1.157053	3.946788	1.726486
C	1.257195	5.311586	1.420898
H	1.159857	6.038997	2.246597
O	2.499098	-1.013554	-1.109052
O	1.140989	1.696243	0.954355
C	1.573434	7.279135	-0.169858
H	1.731332	7.482681	-1.248322
H	0.650597	7.816711	0.140236
H	2.415180	7.749034	0.384967
C	0.942855	3.453632	3.135510
H	0.076077	2.762401	3.194308
H	1.818801	2.866857	3.488319
H	0.784599	4.294020	3.840760
C	7.946967	-1.752320	-2.638754
H	8.069444	-1.770128	-3.743887
H	8.613281	-0.960625	-2.240517
H	8.325008	-2.728218	-2.262134
C	3.058759	-3.168600	-2.797431
H	2.532026	-3.661383	-1.953385
H	2.272237	-2.613110	-3.351670
H	3.472669	-3.953979	-3.461157
O	-1.554522	-2.476389	1.420512
C	-0.806835	-3.654125	1.045268
C	-0.917337	-3.827949	-0.485858
H	-0.544670	-2.915308	-0.991900
C	-0.936029	-1.219263	1.398036
O	0.308882	-1.216200	1.080476
O	-1.671802	-0.272888	1.707673
H	0.260586	-3.508360	1.305814
Cl	-0.575502	0.005597	-1.566280
C	-1.408949	-4.842884	1.807788
H	-0.754626	-5.722987	1.628304
H	-1.371416	-4.622267	2.895465
C	5.118489	-0.422721	3.722232
C	3.730525	0.201423	3.957599
C	2.645463	-0.454446	3.125618

C	2.842654	-1.814210	2.556770
C	4.139345	-2.584982	2.765114
C	5.059773	-1.955652	3.831765
H	1.607125	-0.115494	3.301373
H	3.439405	0.097820	5.028574
H	3.744560	1.291688	3.739563
H	5.487620	-0.130021	2.715139
H	5.840945	-0.009794	4.458081
H	1.932333	-2.393195	2.321219
H	3.893711	-3.633629	3.038440
H	4.659485	-2.637005	1.783245
H	4.684858	-2.226629	4.845933
H	6.078194	-2.392242	3.752500
O	2.950634	-0.626743	1.724505
C	-2.338688	-4.182118	-0.932272
C	-2.847025	-5.160843	1.358138
C	-2.925292	-5.379371	-0.164026
H	-2.955368	-3.275144	-0.738983
H	-2.353120	-4.355063	-2.028641
H	-3.224884	-6.055828	1.898015
H	-3.508152	-4.313508	1.646311
H	-2.355098	-6.294078	-0.439532
H	-3.976358	-5.555091	-0.480805
Cl	0.248575	-5.163943	-0.997486
N	-4.506479	0.690892	-0.475260
C	-3.474688	1.760244	-0.067114
H	-2.484704	1.261062	-0.142233
H	-3.535910	2.532674	-0.858840
C	-3.634862	2.404433	1.307623
H	-4.677699	2.753393	1.482621
H	-3.380371	1.663287	2.092594
C	-2.683157	3.608152	1.441218
H	-2.894284	4.341846	0.630096
H	-1.639475	3.264094	1.277665
C	-2.794070	4.302578	2.802979
H	-2.087342	5.154110	2.874237
H	-3.817813	4.698544	2.980451
H	-2.558182	3.603352	3.632654
C	-4.000847	0.049235	-1.776586
H	-4.723092	-0.754643	-2.020504
H	-3.028281	-0.416849	-1.509729
C	-3.794798	0.974921	-2.974087
H	-4.722136	1.538649	-3.224839
H	-3.000216	1.715882	-2.748111
C	-3.346609	0.157431	-4.202050
H	-2.417561	-0.390270	-3.932561
H	-4.115211	-0.614107	-4.437483
C	-3.090855	1.030415	-5.435815
H	-2.292224	1.776135	-5.238921
H	-2.765763	0.416516	-6.300519
H	-4.002751	1.586504	-5.743954
C	-5.863032	1.342694	-0.673476
H	-6.170135	1.728642	0.316913
H	-5.692620	2.224091	-1.323564
C	-6.959263	0.451883	-1.262133
H	-7.024415	-0.507144	-0.703599
H	-6.719575	0.186787	-2.314217
C	-8.329502	1.154263	-1.223270
H	-8.255397	2.134284	-1.746874
H	-8.587711	1.395604	-0.167397
C	-9.451027	0.318703	-1.851852
H	-10.423636	0.849451	-1.805022
H	-9.242556	0.097141	-2.920004
H	-9.575200	-0.653253	-1.328846
C	-4.541851	-0.450950	0.561170
H	-4.828565	-1.360330	-0.003809
H	-3.486104	-0.567968	0.902056
C	-5.460902	-0.299101	1.775617
H	-6.533155	-0.260750	1.479999
H	-5.247753	0.639826	2.324488
C	-5.243243	-1.488285	2.733258
H	-5.454293	-2.438654	2.192600
H	-4.166643	-1.529556	3.005063
C	-6.112234	-1.408784	3.993405

H	-7.195699	-1.396650	3.745791
H	-5.932649	-2.276709	4.660264
H	-5.894853	-0.489949	4.578696

[G$_{CHO}$-H$_{CHO}$]‡

135

E_e = -4182.77958867[a]

Fe	-2.620261	0.118263	0.050366
S	-4.825964	-0.469117	-1.480728
S	-4.255523	2.055002	0.903323
C	-5.904512	1.003582	-1.183119
H	-5.526785	1.767261	-1.895944
H	-6.939092	0.737075	-1.488091
C	-5.906834	1.534251	0.243826
H	-6.256078	0.761896	0.961982
H	-6.592866	2.404743	0.321874
C	-5.451653	-1.653466	-0.294127
C	-4.680406	-1.844510	0.895008
C	-6.326928	-3.521390	1.576844
H	-6.673414	-4.260005	2.321348
C	-5.151672	-2.808996	1.851529
C	-7.084727	-3.343043	0.391540
C	-6.620355	-2.399907	-0.542778
H	-7.169067	-2.240667	-1.485980
C	-3.701993	3.220073	-0.338547
C	-4.164127	4.551385	-0.346469
H	-4.875627	4.876614	0.430837
C	-3.728511	5.459540	-1.327138
C	-2.750885	2.748585	-1.297422
C	-2.311675	3.673723	-2.307125
C	-2.805755	4.985462	-2.293620
H	-2.453466	5.681047	-3.076030
O	-3.571313	-1.173261	1.131557
O	-2.281590	1.516142	-1.280358
C	-4.212754	6.892840	-1.355021
H	-3.374213	7.612138	-1.227794
H	-4.702465	7.142784	-2.321475
H	-4.946068	7.090857	-0.547486
C	-1.332991	3.194316	-3.349017
H	-0.387351	2.843785	-2.882235
H	-1.736267	2.322576	-3.907598
H	-1.089184	3.994602	-4.075810
C	-8.338502	-4.153210	0.145326
H	-9.093443	-3.994584	0.946137
H	-8.813468	-3.886364	-0.820126
H	-8.123590	-5.243916	0.121977
C	-4.355385	-3.017181	3.114307
H	-3.324152	-3.359779	2.882164
H	-4.236960	-2.064788	3.673756
H	-4.834995	-3.763718	3.778237
O	4.106031	-1.883910	-2.687038
C	5.406851	-1.634016	-2.135442
C	5.672171	-0.115885	-2.255166
H	4.853409	0.429891	-1.748964
C	2.991610	-1.747754	-1.829715
O	1.908800	-1.988345	-2.423454
O	3.201936	-1.419729	-0.630258
H	5.408067	-1.913045	-1.061429
Cl	-1.099851	0.815416	1.701306
C	6.428020	-2.462993	-2.926498
H	7.410324	-2.368137	-2.413918
H	6.130282	-3.531134	-2.870478
C	-1.646575	-3.184681	-3.334137
C	-1.283245	-1.698632	-3.501791
C	-0.801046	-1.065551	-2.204471
C	-0.024425	-1.900310	-1.272003
C	-0.155675	-3.401879	-1.273608
C	-0.501223	-3.964639	-2.665175
H	-0.469387	-0.014842	-2.321362
H	-0.452523	-1.588498	-4.233867
H	-2.144580	-1.113233	-3.888929
H	-2.571307	-3.271500	-2.722141
H	-1.881176	-3.624901	-4.326808
H	0.538979	-1.395518	-0.477790

H	0.794975	-3.830903	-0.897167
H	-0.942811	-3.670211	-0.534507
H	0.409331	-3.895661	-3.297520
H	-0.761845	-5.040934	-2.576186
O	-1.671442	-1.254735	-1.074578
C	5.846549	0.341531	-3.704311
C	6.551983	-1.999736	-4.389149
C	6.881244	-0.498155	-4.473144
H	4.846909	0.222738	-4.179822
H	6.094505	1.423326	-3.732815
H	7.329498	-2.596206	-4.913169
H	5.590083	-2.198672	-4.910496
H	7.890909	-0.309769	-4.044139
H	6.920321	-0.164650	-5.532316
Cl	7.175270	0.315537	-1.256703
N	2.783389	0.363189	2.289373
C	2.347930	1.195853	3.486243
H	2.902821	2.150728	3.412259
H	1.276197	1.418766	3.301726
C	2.535185	0.614058	4.888391
H	1.865321	-0.256742	5.041948
H	3.575812	0.250704	5.037198
C	2.216897	1.677367	5.957919
H	1.188379	2.067758	5.789118
H	2.897128	2.549003	5.824295
C	2.337064	1.143373	7.390205
H	2.106100	1.932289	8.134737
H	1.635833	0.300916	7.568992
H	3.362959	0.773562	7.602323
C	1.992599	-0.967068	2.191126
H	2.096822	-1.251965	1.121777
H	0.936867	-0.687608	2.386359
C	2.436293	-2.161380	3.041515
H	3.438271	-2.517839	2.721072
H	2.511946	-1.917742	4.121214
C	1.431851	-3.318392	2.863405
H	0.421441	-2.981919	3.185355
H	1.339969	-3.554296	1.780332
C	1.832151	-4.581055	3.635592
H	1.901940	-4.386736	4.727506
H	1.091706	-5.393932	3.489262
H	2.819748	-4.965634	3.302623
C	4.269041	0.019212	2.284660
H	4.437381	-0.605999	3.182510
H	4.399142	-0.625383	1.390483
C	5.284443	1.163516	2.273334
H	5.042415	1.928659	3.043997
H	5.280282	1.676787	1.290069
C	6.703979	0.621845	2.531305
H	6.936286	-0.150125	1.765457
H	6.728784	0.105187	3.518086
C	7.776523	1.716239	2.488579
H	8.783559	1.299980	2.695784
H	7.814859	2.197236	1.488900
H	7.581613	2.511417	3.240054
C	2.372301	1.126536	1.004100
H	2.861488	0.563913	0.182732
H	1.277869	0.957204	0.924613
C	2.622107	2.634743	0.923948
H	3.681591	2.902441	1.113562
H	2.010710	3.175972	1.677280
C	2.220121	3.146183	-0.474658
H	2.829293	2.622796	-1.245137
H	1.163505	2.861411	-0.673722
C	2.385047	4.663104	-0.624514
H	3.437537	4.978216	-0.457480
H	2.092431	5.000660	-1.639629
H	1.751317	5.212853	0.103344

Нсно

135

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S	3.920689	-0.055734	1.897097
C	5.413771	-1.676097	0.066960
H	5.160462	-2.591069	0.643627
H	6.403255	-1.839054	-0.411661
C	5.473843	-0.449900	0.969695
H	5.685679	0.468339	0.381329
H	6.293137	-0.574605	1.710047
C	4.508451	-0.059020	-2.075748
C	3.677380	1.054682	-1.726371
C	5.054055	2.400049	-3.254239
H	5.273667	3.382878	-3.709106
C	3.998811	2.319994	-2.335287
C	5.848436	1.286237	-3.625114
C	5.553138	0.055053	-3.015303
H	6.142211	-0.842240	-3.269495
C	3.651293	-1.560305	2.825282
C	4.279524	-1.772574	4.068779
H	4.960127	-0.998540	4.461393
C	4.044775	-2.945592	4.806551
C	2.734519	-2.510627	2.273094
C	2.491538	-3.711057	3.029618
C	3.145042	-3.892750	4.256061
H	2.940833	-4.820297	4.820574
O	2.672126	0.956903	-0.883995
O	2.125303	-2.321122	1.120769
C	4.708328	-3.191984	6.144203
H	5.401732	-2.369167	6.412270
H	3.962086	-3.278893	6.964601
H	5.294272	-4.137261	6.146332
C	1.531465	-4.733438	2.477063
H	0.537188	-4.279514	2.279429
H	1.883108	-5.133300	1.501287
H	1.400415	-5.584907	3.174789
C	6.958538	1.426179	-4.644315
H	7.674680	2.230341	-4.367320
H	7.536402	0.485389	-4.747302
H	6.564131	1.684192	-5.652247
C	3.184442	3.529270	-1.951070
H	2.113765	3.389427	-2.215172
H	3.212026	3.692570	-0.851462
H	3.552947	4.445464	-2.455014
O	-4.607719	-2.465548	-1.688245
C	-5.815472	-1.834339	-1.180845
C	-5.759954	-1.903957	0.361460
H	-4.825331	-1.426939	0.713167
C	-3.508647	-1.673340	-1.794759
O	-3.473410	-0.484766	-1.504052
O	-2.518838	-2.423284	-2.279783
H	-5.810996	-0.770903	-1.494232
Cl	0.420133	0.386030	1.508062
C	-7.009445	-2.596416	-1.763765
H	-7.924243	-2.025377	-1.494977
H	-6.932289	-2.584366	-2.871206
O	0.811301	-1.292617	-1.304128
C	-5.905318	-3.329997	0.896321
C	-7.108225	-4.035995	-1.225799
C	-7.126680	-4.060959	0.313210
H	-4.974583	-3.868486	0.606685
H	-5.930727	-3.310543	2.005507
H	-8.017524	-4.526935	-1.633079
H	-6.238908	-4.622030	-1.597121
H	-8.053292	-3.570646	0.686080
H	-7.149798	-5.107054	0.685390
Cl	-7.090951	-0.815949	1.026197
N	-1.569696	3.379436	0.398697
C	-0.575245	3.704310	1.517629
H	-1.182021	3.959327	2.406244
H	-0.054053	2.741265	1.717975
C	0.435549	4.818239	1.241596
H	1.085363	4.555845	0.380764
H	-0.069981	5.777662	0.987780
C	1.332930	5.037041	2.476705
H	1.828844	4.075705	2.734546
H	0.698310	5.299087	3.353691

C	2.391083	6.125205	2.260316
H	3.020181	6.258221	3.163913
H	3.067803	5.867671	1.418550
H	1.926934	7.107724	2.027801
C	-0.761540	2.940066	-0.839875
H	-0.086759	2.136766	-0.473242
H	-0.140806	3.814175	-1.115897
C	-1.565514	2.468901	-2.052505
H	-2.175817	1.574082	-1.806253
H	-2.266847	3.258942	-2.403466
C	-0.610673	2.116900	-3.211584
H	0.047549	2.988706	-3.428615
H	0.067967	1.298766	-2.884707
C	-1.355515	1.712944	-4.489495
H	-1.995842	2.538752	-4.868408
H	-0.646027	1.441366	-5.297434
H	-2.015043	0.837647	-4.313171
C	-2.407431	4.590562	0.014179
H	-1.703771	5.308868	-0.453728
H	-3.090689	4.244446	-0.784911
C	-3.208906	5.288593	1.113208
H	-2.545835	5.610072	1.945320
H	-3.954840	4.593462	1.551109
C	-3.943090	6.522094	0.552711
H	-4.603521	6.206443	-0.286324
H	-3.200604	7.221386	0.105614
C	-4.773011	7.257979	1.611455
H	-5.290696	8.137109	1.176816
H	-5.549474	6.596385	2.050386
H	-4.136874	7.623624	2.445266
C	-2.447304	2.177265	0.820733
H	-3.325451	2.191562	0.146320
H	-1.835965	1.283898	0.582009
C	-2.874865	2.070872	2.286749
H	-3.395501	2.984175	2.645709
H	-1.980443	1.923347	2.926688
C	-3.804849	0.856610	2.474401
H	-4.704724	0.962782	1.828559
H	-3.271420	-0.052346	2.118610
C	-4.241593	0.660212	3.930878
H	-4.777474	1.553079	4.319308
H	-4.929836	-0.203999	4.025046
H	-3.371327	0.475672	4.595423
C	0.667672	-4.105492	-2.492648
C	0.040431	-3.619132	-1.175884
C	-0.316254	-2.115763	-1.216533
C	-1.202518	-1.790147	-2.450290
C	-0.601413	-2.308992	-3.756872
C	-0.246972	-3.805363	-3.693348
H	-0.907825	-1.862531	-0.298798
H	-0.893323	-4.190576	-0.969607
H	0.725360	-3.776840	-0.318985
H	1.647431	-3.598554	-2.635518
H	0.881687	-5.194900	-2.433961
H	-1.360335	-0.695396	-2.485851
H	-1.294445	-2.090180	-4.598017
H	0.321626	-1.714201	-3.928651
H	-1.184808	-4.399067	-3.606580
H	0.236093	-4.116617	-4.644884

E_{PO}

111

E_e = -3756.38042392[a]

Fe	-1.452813	-0.104146	0.283576
S	-3.643779	-0.052614	-1.379661
S	-2.870663	1.855069	1.450870
C	-4.474865	1.526057	-0.884771
H	-3.908609	2.318014	-1.419768
H	-5.507592	1.515074	-1.295435
C	-4.521077	1.797187	0.612071
H	-5.074779	0.998008	1.149450
H	-5.034483	2.761934	0.812386
C	-4.542582	-1.243032	-0.390137
C	-3.861300	-1.774325	0.746707

C	-5.843167	-3.137968	1.183407
H	-6.357869	-3.888722	1.809144
C	-4.547584	-2.747367	1.549759
C	-6.515512	-2.620132	0.048498
C	-5.835889	-1.670207	-0.737780
H	-6.314007	-1.260571	-1.643071
C	-2.055738	3.154263	0.527132
C	-2.317322	4.510445	0.806137
H	-3.006485	4.762770	1.629542
C	-1.717684	5.533727	0.051362
C	-1.143369	2.756400	-0.502507
C	-0.555860	3.804455	-1.297741
C	-0.850256	5.142912	-0.999180
H	-0.384262	5.927791	-1.621718
O	-2.640662	-1.398237	1.071453
O	-0.845610	1.495366	-0.739081
C	-1.986761	6.995743	0.335321
H	-1.056970	7.541580	0.608567
H	-2.411954	7.516464	-0.550623
H	-2.703406	7.122120	1.171853
C	0.336052	3.427019	-2.453625
H	1.200938	2.809355	-2.130584
H	-0.214263	2.807581	-3.194676
H	0.725360	4.324802	-2.974574
C	-7.907123	-3.093943	-0.309384
H	-8.625462	-2.926524	0.522832
H	-8.299678	-2.567375	-1.202497
H	-7.924192	-4.183705	-0.530788
C	-3.840383	-3.315234	2.753662
H	-2.905212	-3.835456	2.454338
H	-3.526442	-2.509639	3.451196
H	-4.484194	-4.031706	3.302014
O	-0.195178	-2.321270	-3.035620
C	1.145207	-1.826603	-3.115027
C	1.084718	-0.325481	-3.434112
H	0.499780	0.216999	-2.666869
C	-0.998812	-2.019170	-1.921395
O	-0.422699	-1.265836	-1.025604
O	-2.127061	-2.487659	-1.929436
H	1.646050	-1.948942	-2.128058
Cl	-0.037234	0.088368	2.160402
C	1.856893	-2.657052	-4.180895
H	2.896376	-2.302060	-4.329223
H	1.877753	-3.724607	-3.884583
Cl	2.759739	0.433185	-3.420027
N	4.072359	-0.497424	0.591845
C	2.746789	-1.270762	0.675737
H	2.179876	-0.853321	1.529762
H	2.167255	-0.981415	-0.224152
C	2.852743	-2.794583	0.777206
H	3.191604	-3.234240	-0.187018
H	3.606094	-3.097350	1.539434
C	1.484222	-3.405281	1.142146
H	0.721469	-3.032022	0.425694
H	1.161421	-3.014433	2.131409
C	1.501077	-4.937264	1.154877
H	0.503651	-5.340830	1.422350
H	1.768159	-5.352340	0.159217
H	2.232671	-5.337981	1.890317
C	4.841146	-1.010433	-0.631407
H	4.170885	-0.823423	-1.495963
H	4.925006	-2.105559	-0.495404
C	6.228642	-0.422758	-0.901353
H	6.176931	0.675487	-1.060727
H	6.910467	-0.589215	-0.039179
C	6.843225	-1.071344	-2.158326
H	6.903216	-2.173372	-2.011328
H	6.155234	-0.917129	-3.018878
C	8.232439	-0.519512	-2.499636
H	8.953988	-0.689845	-1.672399
H	8.644918	-1.005247	-3.407168
H	8.198646	0.573588	-2.693214
C	4.930061	-0.689795	1.846297
H	5.521216	-1.613241	1.678809

H	5.647649	0.155503	1.855212
C	4.207877	-0.791021	3.194246
H	3.602687	-1.720164	3.236621
H	3.495506	0.044544	3.336036
C	5.224595	-0.799855	4.351853
H	5.813580	0.145433	4.332128
H	5.963639	-1.618708	4.193823
C	4.560413	-0.964312	5.724321
H	5.313360	-0.958319	6.538523
H	3.839799	-0.144201	5.925736
H	4.000420	-1.920668	5.791742
C	3.759496	0.988812	0.342732
H	4.730611	1.455198	0.085449
H	3.135634	0.995320	-0.574194
C	3.082891	1.781275	1.457805
H	3.768939	1.894262	2.325720
H	2.157748	1.272350	1.808513
C	2.691737	3.184223	0.952370
H	3.580711	3.692824	0.511481
H	1.952503	3.075006	0.129371
C	2.087330	4.053305	2.061082
H	2.809604	4.220578	2.889340
H	1.784705	5.045336	1.669734
H	1.183201	3.572677	2.488089
H	1.316577	-2.581690	-5.147154
H	0.675220	-0.141737	-4.446609

[E_{PO}-F_{PO}]‡

111

E_e = -3756.34992886[a]

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H	2.493109	-1.396875	-2.360547
C	-0.185632	-1.560409	-2.145196
O	0.476754	-1.589032	-3.234531
O	-1.174053	-0.815410	-1.905950
S	-3.229295	1.582929	1.573023
S	-4.346908	-0.603828	-0.988582
C	-4.934310	0.880958	1.384959
H	-4.915015	-0.052265	1.987279
H	-5.642334	1.585266	1.871909
C	-5.380689	0.608027	-0.044879
H	-5.352817	1.532258	-0.660451
H	-6.426294	0.232288	-0.045057
O	-2.182291	-1.412814	0.893475
O	-2.202764	1.768092	-1.216182
C	-3.211829	-2.235039	0.908215
C	-3.198905	-3.387056	1.768695
C	-4.365738	-2.032218	0.087480
C	-4.296403	-4.258505	1.757724
C	-5.443746	-2.939018	0.091582
C	-5.433242	-4.066535	0.932140
H	-4.266994	-5.139832	2.422881
H	-6.300380	-2.756917	-0.578548
C	-2.742765	2.890996	-0.792960
C	-3.298278	3.026244	0.518052
C	-2.790246	4.038331	-1.659334
C	-3.842665	4.244592	0.970161
C	-3.352496	5.229244	-1.180503
C	-3.884696	5.368988	0.127011
H	-4.236341	4.308787	1.998312
H	-3.377128	6.101081	-1.858369
H	1.969858	-3.383407	-0.702016
Fe	-1.835585	0.140522	-0.215862
Cl	0.170124	0.835850	0.787647
C	-1.994127	-3.614977	2.644450
H	-1.075799	-3.722059	2.028528
H	-1.812097	-2.744068	3.309613
H	-2.111813	-4.522424	3.269737
C	-6.580792	-5.052253	0.953091
H	-7.393671	-4.746116	0.264293
H	-6.252052	-6.070436	0.650056
H	-7.020648	-5.149204	1.969720

C	-2.226828	3.909429	-3.051081
H	-1.155003	3.619176	-3.020684
H	-2.737899	3.101108	-3.616641
H	-2.324012	4.856372	-3.618667
C	-4.466051	6.687270	0.589316
H	-5.306789	7.016293	-0.059897
H	-4.850999	6.621363	1.626942
H	-3.708542	7.501174	0.565369
C	0.878700	-4.554810	-2.169409
N	4.336829	0.325045	0.233437
C	5.716204	-0.259001	0.533479
H	5.726221	-0.482936	1.616772
H	5.735660	-1.227104	-0.010926
C	6.933808	0.592125	0.160375
H	7.032693	0.673253	-0.942729
H	6.832895	1.630400	0.546329
C	8.225841	-0.031209	0.723988
H	8.304178	-1.084876	0.374361
H	8.153842	-0.085292	1.833938
C	9.488711	0.740923	0.324349
H	10.398847	0.270699	0.749091
H	9.613190	0.771685	-0.778789
H	9.455545	1.791040	0.685324
C	4.257420	0.553847	-1.287435
H	4.406379	-0.456474	-1.731921
H	5.139588	1.173126	-1.541309
C	2.996170	1.226654	-1.832833
H	2.077008	0.667778	-1.558243
H	2.862860	2.241596	-1.401883
C	3.085210	1.346914	-3.368172
H	3.968870	1.970824	-3.636527
H	3.282212	0.343032	-3.806428
C	1.813664	1.933454	-3.992330
H	1.582753	2.937245	-3.576950
H	1.922553	2.040424	-5.091016
H	0.940804	1.276141	-3.801559
C	4.061970	1.650922	0.947404
H	4.503330	2.442229	0.307450
H	2.959735	1.775148	0.915130
C	4.576349	1.821053	2.380271
H	5.686289	1.771023	2.410824
H	4.203657	1.012480	3.038762
C	4.121513	3.179478	2.949914
H	3.010203	3.227384	2.932069
H	4.470766	3.997535	2.279600
C	4.628369	3.429703	4.375280
H	4.281172	4.410800	4.758344
H	4.263938	2.650193	5.077417
H	5.738470	3.426827	4.420935
C	3.288377	-0.748142	0.589197
H	2.319139	-0.366615	0.211428
H	3.594455	-1.633380	-0.011502
C	3.110744	-1.112598	2.063209
H	2.627010	-0.274682	2.608465
H	4.082280	-1.325194	2.562498
C	2.206796	-2.354016	2.195284
H	1.244672	-2.152739	1.676209
H	2.684520	-3.208474	1.665290
C	1.939296	-2.733668	3.656294
H	1.420693	-1.913814	4.196804
H	1.295604	-3.634084	3.724976
H	2.881833	-2.954295	4.202955
Cl	4.320530	-3.059761	-1.933263
H	1.757547	-5.186208	-2.411259
H	0.255518	-5.082980	-1.421474
H	2.398708	-2.783030	-3.614970
H	0.281198	-4.403363	-3.091201

G_{PO}

121

E_e = -3949.43074666[a]

Fe	1.521989	-0.106619	0.230483
S	4.454277	0.995311	0.388155
S	2.072108	1.592112	-1.969606

C	4.725199	2.124383	-1.040911
H	4.470920	3.128644	-0.641104
H	5.803784	2.130526	-1.310296
C	3.887600	1.801407	-2.271640
H	4.186176	0.827094	-2.714090
H	4.029352	2.581827	-3.050673
C	5.002464	-0.568738	-0.292999
C	4.027977	-1.566464	-0.616768
C	5.866728	-3.008507	-1.356344
H	6.202495	-3.970009	-1.783711
C	4.491734	-2.809977	-1.174972
C	6.837689	-2.035527	-1.013274
C	6.377970	-0.820321	-0.475312
H	7.101732	-0.041459	-0.181690
C	1.680112	3.045905	-0.997383
C	1.717442	4.337145	-1.562212
H	1.979837	4.446165	-2.628036
C	1.430751	5.479669	-0.794003
C	1.303697	2.846595	0.368972
C	1.017808	4.013855	1.160305
C	1.088375	5.282364	0.567129
H	0.866165	6.164166	1.194540
O	2.733190	-1.403275	-0.430022
O	1.201060	1.654140	0.920363
C	1.478312	6.870247	-1.389592
H	1.785419	6.846213	-2.454738
H	0.488433	7.375142	-1.339276
H	2.196463	7.525380	-0.849431
C	0.667226	3.823982	2.614683
H	-0.155896	3.088839	2.736143
H	1.528859	3.406657	3.180194
H	0.374488	4.780813	3.091503
C	8.312382	-2.308299	-1.212536
H	8.548819	-2.529213	-2.276541
H	8.932882	-1.442720	-0.904183
H	8.650078	-3.188905	-0.623167
C	3.473247	-3.852556	-1.556452
H	2.852074	-4.159429	-0.688943
H	2.755003	-3.453418	-2.304170
H	3.958134	-4.755041	-1.979407
O	-1.549422	-2.420819	1.801988
C	-0.793174	-3.634117	1.594370
C	-0.840211	-3.941684	0.091672
H	-0.411704	-3.100402	-0.488747
C	-0.909724	-1.175479	1.726330
O	0.356891	-1.208210	1.520206
O	-1.654763	-0.200138	1.893302
H	0.265599	-3.454514	1.874925
Cl	-0.302127	-0.468862	-1.354690
C	-1.413446	-4.714898	2.474165
H	-0.893439	-5.680312	2.315750
H	-1.334289	-4.436278	3.544099
C	3.365675	0.860897	4.407484
C	2.417673	0.005744	3.602648
C	2.659680	-1.430977	3.344260
H	1.365023	0.344369	3.557033
H	3.028815	0.918881	5.464439
H	3.397930	1.893550	4.003489
H	1.797495	-2.089919	3.147200
O	2.898524	-0.449103	2.315876
Cl	0.117628	-5.433226	-0.322376
N	-4.376428	0.086416	-0.590432
C	-3.407957	1.273204	-0.428531
H	-2.401367	0.820684	-0.303781
H	-3.431460	1.797241	-1.404351
C	-3.682442	2.263727	0.700559
H	-4.747055	2.589766	0.716784
H	-3.454473	1.784472	1.674565
C	-2.788392	3.508498	0.542309
H	-2.980635	3.980159	-0.448358
H	-1.722938	3.193146	0.527668
C	-3.009562	4.540078	1.653861
H	-2.343693	5.416652	1.520879
H	-4.057644	4.910928	1.667587

H	-2.795137	4.107363	2.653673
C	-3.749835	-0.862192	-1.624587
H	-4.422761	-1.740663	-1.677194
H	-2.785625	-1.180798	-1.175609
C	-3.488556	-0.296087	-3.019089
H	-4.414888	0.124397	-3.472070
H	-2.737451	0.518661	-2.962929
C	-2.925310	-1.396276	-3.940220
H	-1.995096	-1.792553	-3.478268
H	-3.644442	-2.245915	-3.991521
C	-2.619628	-0.888292	-5.353849
H	-1.863233	-0.076026	-5.331235
H	-2.215268	-1.700461	-5.991889
H	-3.528491	-0.489861	-5.854760
C	-5.728157	0.596218	-1.055229
H	-6.120947	1.227710	-0.235644
H	-5.527929	1.271059	-1.911430
C	-6.755782	-0.466078	-1.450703
H	-6.863086	-1.228872	-0.649000
H	-6.419968	-1.010573	-2.359318
C	-8.131037	0.169562	-1.729436
H	-8.019054	0.962978	-2.502779
H	-8.486326	0.690885	-0.812015
C	-9.183320	-0.848101	-2.185429
H	-10.161238	-0.359716	-2.372568
H	-8.877922	-1.354906	-3.125294
H	-9.344732	-1.636467	-1.419831
C	-4.465441	-0.728509	0.716025
H	-4.689948	-1.768609	0.407342
H	-3.434585	-0.710222	1.142235
C	-5.473316	-0.284143	1.778267
H	-6.520939	-0.350224	1.408450
H	-5.304962	0.770736	2.073956
C	-5.323453	-1.175471	3.028057
H	-5.495408	-2.238247	2.744035
H	-4.268776	-1.124302	3.374402
C	-6.276883	-0.782879	4.162386
H	-7.340908	-0.855133	3.849325
H	-6.144247	-1.441972	5.044657
H	-6.099537	0.261010	4.498458
H	3.576367	-1.911145	3.735772
H	4.394841	0.449666	4.384741
H	-2.488324	-4.850914	2.230087
H	-1.882296	-4.130863	-0.237868

[G$_{CHO}$-H$_{CHO}$]‡

121

E_e = -3949.40275356[a]

Fe	-2.363289	-0.031246	0.011922
S	-4.616075	0.104722	-1.548787
S	-4.000799	1.106339	1.778499
C	-5.703403	1.191764	-0.519426
H	-5.363097	2.222465	-0.755740
H	-6.744367	1.084096	-0.892499
C	-5.662301	0.925359	0.978858
H	-5.965499	-0.117646	1.212193
H	-6.364468	1.608323	1.503115
C	-5.153334	-1.537801	-1.085837
C	-4.318386	-2.255253	-0.172764
C	-5.885778	-4.124648	-0.361182
H	-6.175453	-5.150211	-0.071083
C	-4.716057	-3.587636	0.193186
C	-6.707128	-3.418972	-1.276941
C	-6.314336	-2.116841	-1.634939
H	-6.913903	-1.537925	-2.357011
C	-3.531782	2.770721	1.315886
C	-4.009747	3.888207	2.029149
H	-4.687420	3.729354	2.884509
C	-3.629187	5.191120	1.663716
C	-2.623155	2.909486	0.220384
C	-2.237831	4.241681	-0.159251
C	-2.744867	5.330261	0.564144
H	-2.433491	6.345413	0.259897
O	-3.216687	-1.737249	0.331078

O	-2.144063	1.868052	-0.433089
C	-4.129807	6.405819	2.414358
H	-4.667766	7.110724	1.743545
H	-4.825832	6.122751	3.229499
H	-3.293890	6.978082	2.873021
C	-1.301225	4.419638	-1.327456
H	-0.359508	3.849673	-1.179935
H	-1.749321	4.027868	-2.266429
H	-1.047553	5.486751	-1.485261
C	-7.951417	-4.058995	-1.852208
H	-8.479664	-3.373611	-2.545085
H	-7.711244	-4.985996	-2.417267
H	-8.669679	-4.349389	-1.054605
C	-3.850584	-4.355776	1.158909
H	-2.824568	-4.487971	0.753370
H	-3.727565	-3.801357	2.113668
H	-4.275868	-5.355217	1.378829
O	3.984597	0.625400	-3.915987
C	5.358532	0.362181	-3.598059
C	5.850321	1.526298	-2.725384
H	5.189025	1.634870	-1.846549
C	3.009397	0.242479	-2.974770
O	1.841959	0.497917	-3.371564
O	3.394734	-0.285437	-1.894433
H	5.424311	-0.569157	-2.994406
Cl	-0.740259	-0.191267	1.695039
C	6.118603	0.214656	-4.912324
H	7.198706	0.058930	-4.717730
H	5.730001	-0.650809	-5.485031
C	-1.383716	-0.197992	-4.175447
C	-0.989478	0.256534	-2.788745
C	0.216289	-0.268193	-2.147636
H	-1.200917	1.325023	-2.583968
H	-0.771197	0.347164	-4.922555
H	-2.455722	0.011137	-4.367862
H	0.647038	0.252211	-1.286810
O	-1.430820	-0.596893	-1.705806
Cl	7.532458	1.242781	-2.074426
N	3.190315	-0.883899	1.465576
C	2.931502	-1.067746	2.953302
H	3.514350	-0.277122	3.463670
H	1.856513	-0.825910	3.087449
C	3.257061	-2.418941	3.592486
H	2.567775	-3.203929	3.219729
H	4.287945	-2.746978	3.334302
C	3.126602	-2.333552	5.125923
H	2.107199	-1.970043	5.385883
H	3.830582	-1.562144	5.512810
C	3.390788	-3.671667	5.826410
H	3.294140	-3.575956	6.927105
H	2.672645	-4.451441	5.495317
H	4.413661	-4.048427	5.612070
C	2.324259	-1.834991	0.599672
H	2.324583	-1.343958	-0.396600
H	1.304879	-1.769868	1.032838
C	2.773331	-3.286733	0.408825
H	3.737995	-3.329092	-0.140001
H	2.925802	-3.819963	1.369511
C	1.714292	-4.046261	-0.416659
H	0.735417	-4.005224	0.110141
H	1.558485	-3.515232	-1.381375
C	2.101454	-5.504911	-0.687262
H	2.231549	-6.074588	0.257970
H	1.322851	-6.023207	-1.283465
H	3.055753	-5.574996	-1.251694
C	4.646704	-1.089709	1.060791
H	4.881125	-2.145512	1.296599
H	4.642085	-0.976938	-0.043780
C	5.710628	-0.187392	1.687956
H	5.616024	-0.156202	2.796347
H	5.599680	0.855115	1.325242
C	7.120819	-0.685848	1.315356
H	7.203088	-0.736759	0.207509
H	7.254863	-1.726267	1.690227

C	8.236011	0.213548	1.860579
H	9.237042	-0.188771	1.603177
H	8.170030	1.234655	1.430098
H	8.186318	0.306803	2.966855
C	2.687275	0.527265	1.063836
H	3.074740	0.670324	0.034022
H	1.584314	0.416268	1.001069
C	2.984193	1.715691	1.982328
H	4.066485	1.830003	2.197128
H	2.471364	1.595559	2.960523
C	2.463819	3.011107	1.325586
H	2.972022	3.156050	0.346228
H	1.382617	2.890097	1.094692
C	2.668885	4.249702	2.205723
H	3.743759	4.416610	2.433295
H	2.287318	5.163888	1.707023
H	2.133505	4.151689	3.173995
H	-1.206755	-1.285240	-4.301098
H	0.593559	-1.257889	-2.426327
H	5.997328	1.123698	-5.537654
H	5.880939	2.476035	-3.295483

HPO

121

E_e = -3949.45992369[a]

Fe	1.826070	-0.593114	-0.310801
S	4.114075	-0.738714	-1.684186
S	3.585404	-0.247609	1.786096
C	5.352204	-1.006557	-0.332138
H	5.235479	-2.078291	-0.064936
H	6.364110	-0.874437	-0.771875
C	5.199146	-0.110002	0.889625
H	5.270175	0.962317	0.608223
H	6.014162	-0.326702	1.613153
C	4.225015	1.025871	-1.954893
C	3.202970	1.837404	-1.363090
C	4.369107	3.779800	-2.316244
H	4.428247	4.875757	-2.444513
C	3.316651	3.261183	-1.549114
C	5.355159	2.968848	-2.931530
C	5.259843	1.580575	-2.734510
H	6.002226	0.906101	-3.193544
C	3.554939	-1.982938	2.219288
C	4.184524	-2.451275	3.389925
H	4.710163	-1.729619	4.037535
C	4.144902	-3.812402	3.738225
C	2.830702	-2.861856	1.351953
C	2.787221	-4.255610	1.709914
C	3.437722	-4.685868	2.874290
H	3.388383	-5.759639	3.129796
O	2.205377	1.333804	-0.667895
O	2.221429	-2.441047	0.262651
C	4.815564	-4.334053	4.990593
H	5.333647	-3.523578	5.542245
H	4.082945	-4.796463	5.688248
H	5.570928	-5.116777	4.758642
C	2.034441	-5.208821	0.816861
H	0.981728	-4.881225	0.682170
H	2.476158	-5.242342	-0.202770
H	2.035890	-6.237708	1.229448
C	6.453195	3.580597	-3.774542
H	7.008961	4.368857	-3.221298
H	7.189587	2.817157	-4.097659
H	6.049742	4.060858	-4.693589
C	2.291811	4.155085	-0.897938
H	1.275816	3.963077	-1.307522
H	2.228064	3.953721	0.193515
H	2.531127	5.226913	-1.049816
O	-4.320756	-3.046514	-2.729131
C	-5.614357	-2.884050	-2.088735
C	-5.489077	-3.473745	-0.676823
H	-4.648860	-2.997025	-0.138643
C	-3.413633	-2.058429	-2.520267
O	-3.611164	-1.053039	-1.851020

O	-2.303390	-2.384185	-3.187539
H	-5.824571	-1.797811	-1.994543
Cl	0.098047	-0.284702	1.342208
C	-6.645063	-3.574616	-2.970613
H	-7.643013	-3.517422	-2.493136
H	-6.697216	-3.086658	-3.963858
O	0.780976	-0.971887	-1.831634
Cl	-6.981807	-3.150199	0.302241
N	-2.396920	2.478054	0.835600
C	-1.526469	2.681708	2.080328
H	-2.194194	2.547940	2.951358
H	-0.809097	1.830564	2.062885
C	-0.788471	4.016126	2.196841
H	-0.090138	4.159900	1.345737
H	-1.495487	4.876346	2.186163
C	0.026671	4.055369	3.505441
H	0.736142	3.199235	3.511955
H	-0.655535	3.892900	4.370694
C	0.794845	5.368777	3.693643
H	1.372722	5.363198	4.640251
H	1.514955	5.538445	2.865525
H	0.109883	6.243266	3.725178
C	-1.470831	2.532566	-0.397510
H	-0.679017	1.779542	-0.195847
H	-1.004180	3.536167	-0.378055
C	-2.123952	2.289488	-1.758500
H	-2.605148	1.288198	-1.795683
H	-2.918014	3.041436	-1.965084
C	-1.061419	2.383199	-2.873314
H	-0.534381	3.361125	-2.798216
H	-0.284259	1.606691	-2.699158
C	-1.658712	2.236570	-4.277747
H	-2.396871	3.038586	-4.495869
H	-0.868943	2.287903	-5.054698
H	-2.181763	1.264483	-4.397722
C	-3.447815	3.568741	0.692401
H	-2.888634	4.505279	0.491735
H	-4.012029	3.327226	-0.228752
C	-4.420862	3.780226	1.852842
H	-3.872386	3.959941	2.802597
H	-5.039887	2.872369	2.009940
C	-5.351308	4.977445	1.576632
H	-5.890233	4.810693	0.616654
H	-4.737101	5.893480	1.422746
C	-6.365769	5.218865	2.700851
H	-7.017984	6.086656	2.474363
H	-7.023349	4.336568	2.850555
H	-5.859575	5.424614	3.667778
C	-3.030870	1.066814	0.867790
H	-3.875447	1.097056	0.152604
H	-2.250882	0.394811	0.457612
C	-3.468809	0.502178	2.221609
H	-4.150392	1.188496	2.768116
H	-2.577149	0.338113	2.861223
C	-4.173588	-0.853350	2.021647
H	-5.058385	-0.725258	1.359385
H	-3.478732	-1.532749	1.480830
C	-4.609678	-1.502711	3.340188
H	-5.298901	-0.843137	3.910545
H	-5.144779	-2.455350	3.151740
H	-3.739336	-1.723408	3.993331
C	0.547024	-3.305460	-2.508423
C	-0.131956	-2.014429	-2.032613
C	-1.162712	-1.490281	-3.054334
H	-0.689321	-2.229516	-1.082574
H	-0.205011	-4.100605	-2.696773
H	1.258594	-3.651976	-1.734962
H	-1.518254	-0.492586	-2.739603
H	1.108059	-3.117352	-3.448453
H	-0.713241	-1.428552	-4.065959
H	-6.383434	-4.642611	-3.118483
H	-5.339496	-4.571058	-0.706969

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