Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Elucidating the Structure of a High-Spin σ-Phenyliron(III) Species in Live $FeCl_3$-PhZnCl Reaction System

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Contents

XANES and EXAFS Data Collection and Analysis

General Information

X-ray absorption measurements were acquired in transmission mode at beamline 17C11 at National Synchrotron Radiation Research Center (NSSRC) in Taiwan. A Fe foil spectrum (edge energy 7112 eV) was acquired simultaneously with each measurement for energy calibration. All solution samples were prepared in a glove box and placed in a sample holder made of PEEK (polyether ether ketone) equipped with a screw top and O-ring fitting to prevent exposure to air and water[1]. The edge energy of the X-Ray absorption near edge structure (XANES) spectrum was determined from the inflection point in the edge, i.e., the maximum in the first derivative of the XANES spectrum. The pre-edge energy was determined from the maximum of the pre-edge peak. Background removal and normalization procedures were carried out using the Athena software package using standard methods.[2] Standard procedures based on Artemis software (Demeter 0.9.20) were used to extract the extended X-ray absorption fine structure (EXAFS) data. The coordination parameters were obtained by the least square fit in R-space of the nearest neighbor, k^2 weighted Fourier transform data. The data fit equally well with both k^1 and k^3 weightings.

Experimental Details

THF solution of $FeCl_3$: In a glovebox, $FeCl_3$ (0.5 mmol, 81.3 mg) was dissolved in 5 mL dry THF, and then the solution was transferred into the XAS solution cell and sealed with the screw top. After the cell was taken out of the glovebox, the XAS spectrum of $FeCl_3$ THF solution was measured at room temperature.

THF solution of $FeCl_3$ + 10 PhZnCl in 25 °C: In a glovebox, $FeCl_3$ (0.5 mmol, 81.3 mg) and PhZnCl (5 mmol, 5 mL) were dissolved in 5 mL dry THF, and then the solution was transferred into the XAS solution cell and sealed with the screw top. After being taken out of the glovebox, the XAS spectrum was measured at room temperature.

THF solution of $FeCl_2$ + 10 PhZnCl in 25 °C: In a glovebox, $FeCl_2$ (0.5 mmol, 63.5 mg) and PhZnCl

(5 mmol, 5 mL) were dissolved in 5 mL dry THF, and then the solution was transferred into the XAS solution cell and sealed with the screw top. After being taken out of the glovebox, the XAS spectrum was measured at room temperature.

THF solution of $FeCl_3$ + 10 PhZnCl in -78 °C: In a glovebox, $FeCl_3$ (0.5 mmol, 81.3 mg) was dissolved in 5 mL dry THF in a vial. After sealed with a septum, the vial was taken out of the glove box and cool to -78 ℃. Finally, PhZnCl (5 mmol, 5 mL) was injected into the cool solution, the mixture was further stirred for 30 mins at -78 ℃. The sample was then transferred to the XAS solution cell and freeze by liquid nitrogen. After sealed with the screw top, the XAS spectrum was measured at -150 ℃.

Table S1 XAS Pre-Edge Energies and Edge Energy and Oxidation States for Iron Complexes

Sample	Conditions	Pre-edge Energy (eV)	Edge Energy (eV)	Oxidation State	Comments
Fe Foil	RT, air	N.A.	7112.0	0	Standard Samples for determination of oxidation states.
FeO	Solid, N_2, RT	7112.4	7117.8	II	
$FeCl_2$	Solid, N_2, RT	7112.6	7120.3	II	
Ferrocene	Solid, air, RT	7112.2	7119.6	II	
$Fe(acac)_2$	Solid, N_2, RT	7112.9	7120.4	II	
$FeBr_2$	Solid, N_2, RT	7112.8	7119.5	II	
$FeBr_3$	Solid, N_2, RT	7113.7	7120.2	III	
Fe_2O_3	Solid, air, RT	7115.0	7123.3	III	
Fe(III) oxolate	Solid, N_2, RT	7114.8	7126.8	III	
$Fe(acac)_3$	Solid, air, RT	7114.1	7127.4	III	
$FeCl_3$	Solid, N_2, RT	7114.1	7122.0	III	
$Fe(NO_3)_3 \cdot xH_2O$	Solid, air, RT	7114.0	7126.9	III	
$FeCl_3$/THF	THF solution, N_2, RT	7114.1	7121.9	III	
$FeCl_3$+10PhZnCl	THF solution, N_2, RT	7112.6	7118.8	II	

$FeCl_3$+10PhZnCl	THF solution, N_2, -78 °C	7114.2	7120.0	III	
$FeCl_2$+10PhZnCl	THF solution, N_2, RT	7112.6	7118.8	II	

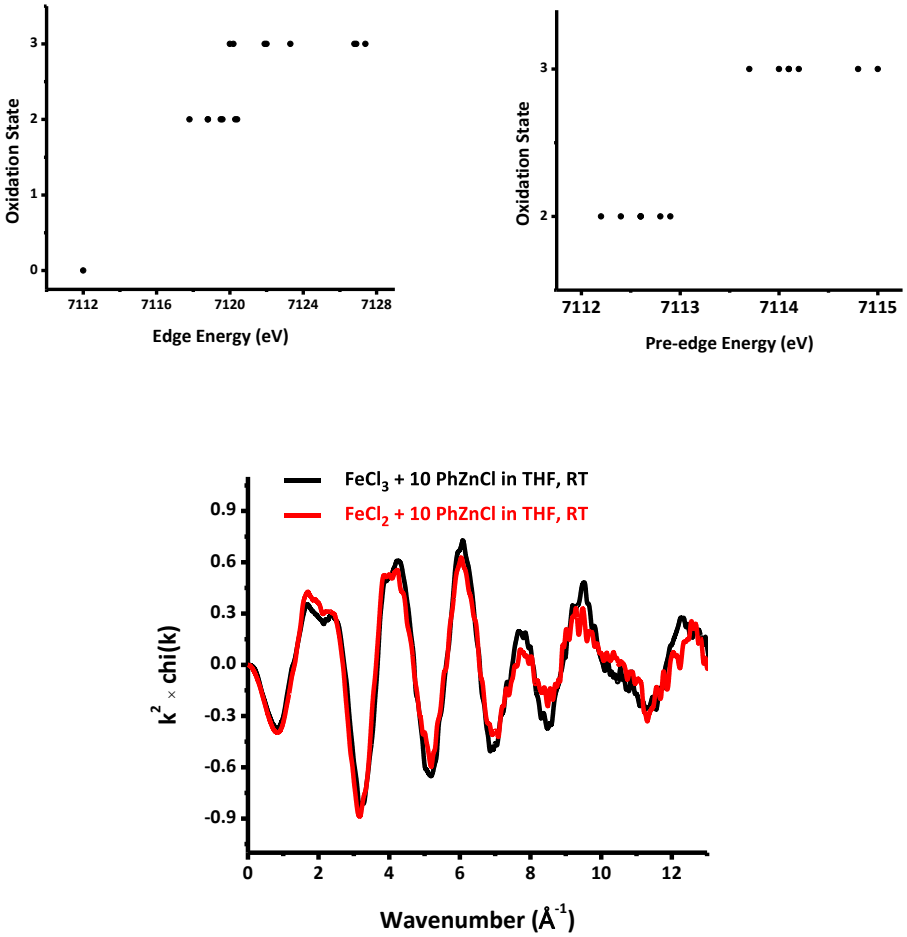


Figure S1A k^2-weighted K-space EXAFS spectra for the reaction of iron(III)/iron(II) salts with PhZnCl

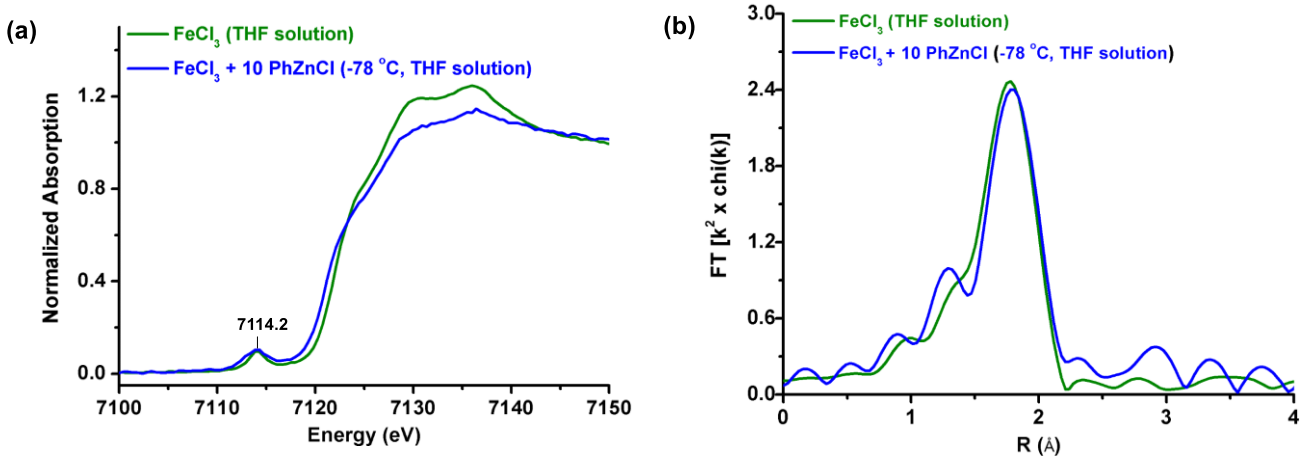


Figure S1B. XANES and EXAFS spectra of various iron species. (a) XANES spectra of the reaction of $FeCl_3$ and phenylzinc chloride at -78 °C and the THF solution of $FeCl_3$. (b) R space EXAFS spectra.

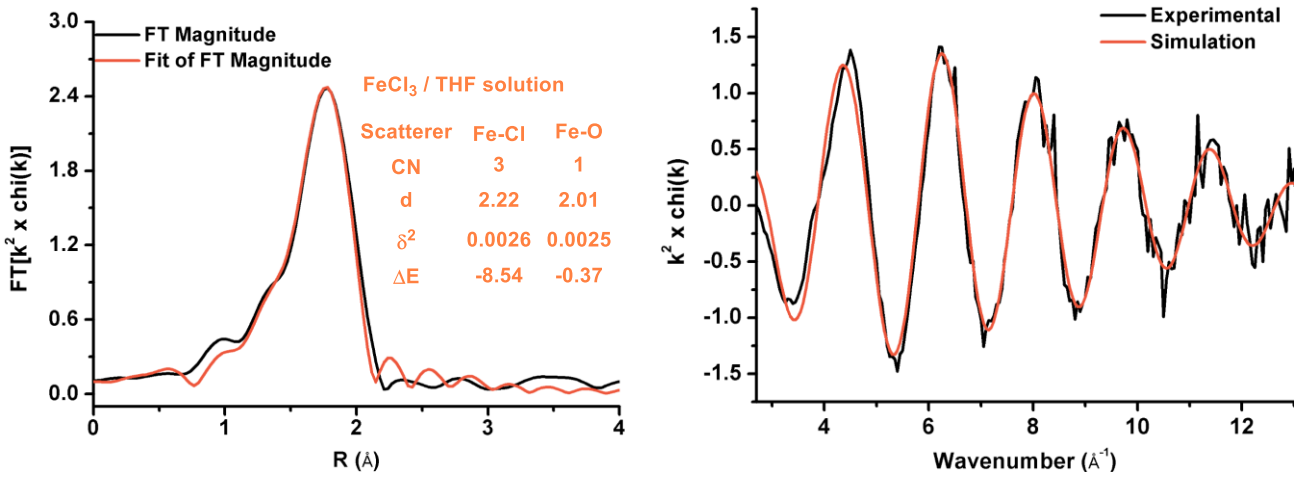


Figure S1C Fitting results of the k^2-weighted R-space (left) and k-space (right) EXAFS spectrum of $FeCl_3$ in THF. FT range: 2.71-13.30 Å-1; fitting range: 0.5-3 Å

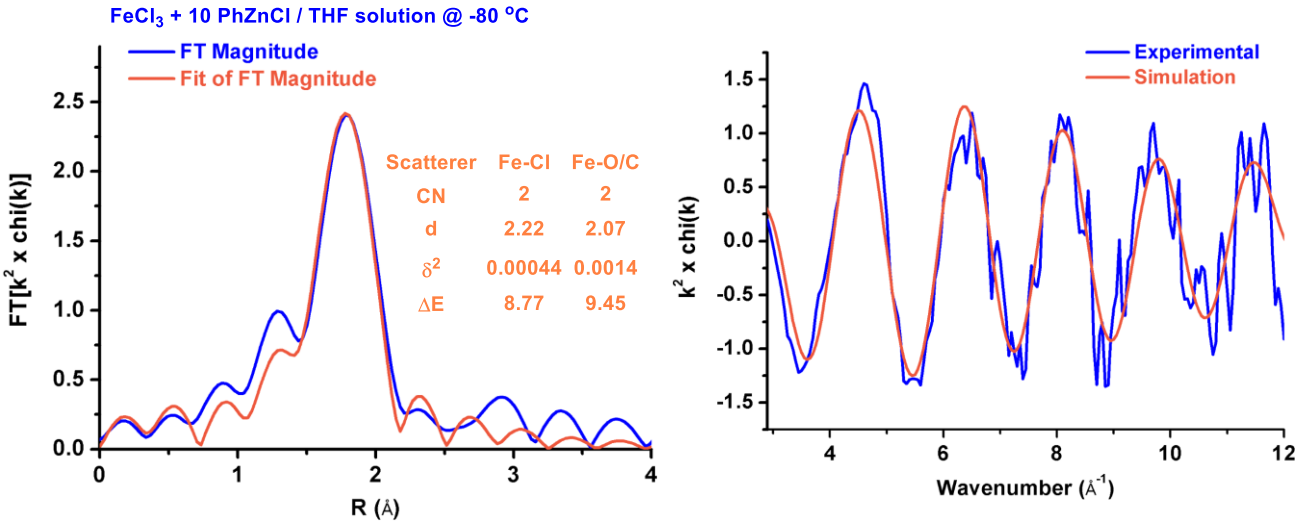


Figure S1D Fitting results of the k^2-weighted R-space (left) and k-space (right) EXAFS spectrum of the reaction of phenylzinc chloride with $FeCl_3$ in THF at -78 °C. FT range: 2.93-12.61 $Å^{-1}$; fitting range: 0.23-3.50 Å.

Operando IR and EPR Experimental Details

General Information

Unless mentioned, amount of product was determined by a Varian GC 2000 gas chromatography instrument with a FID detector.

For the ReactIR experiments, the reaction spectra were recorded using an iC 15 from Mettler-Toledo AutoChem, Inc. Data manipulation was carried out using the iC IR software (Ver. 4.3.27, Mettler-Toledo AutoChem, Inc.).

EPR spectra were recorded on a Bruker ELEXSYS II E 500 EPR spectrometer. The samples were taken out into an EPR tube and frozen by liquid nitrogen, then recorded by EPR spectrometer at indicated temperature and parameters.

Raman spectra were recorded with a Bruker RFS 100/S Fourier Transform spectrometer with an air-cooled NIR Nd:YAG laser with a wavelength of 1064 nm and a power between 50–800 mW. The scattered light intensity was recorded with a high-sensitivity Ge diode (cooled with liquid nitrogen). For each spectrum 400 scans were accumulated (spectral resolution 4 cm^{-1}).

Operando IR Experiments Data Collection and Analysis

Experimental Details

The reaction of $FeCl_3$ (0.3 mmol) and PhZnCl (0.6 mmol), THF (3 mL) at 25 °C

An oven-dried three necked reaction vessel was fitted with a magnetic stirring bar and filled with nitrogen. The laser probe was inserted through an adapter into the middle neck; the other two necks were capped by a rubber plug for injection and a Schlenk line, respectively. The course of the reaction was monitored via the characteristic IR band of biphenyl at ca. 740 cm^{-1}. When biphenyl peak stopped increasing, 2 mL 2M HCl aqueous solution was added to quench the reaction. The amount of product was determined by GC employing naphthalene as internal standard.

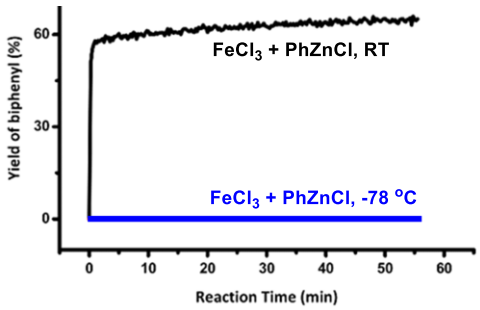


Figure S2. Kinetic plots of the reaction of $FeCl_3$ with phenylzinc chloride (PhZnCl) at 25 °C or -78 °C.

The reaction of $FeCl_3$ and PhZnCl at -78 °C

Following general procedure, liquid nitrogen was poured into the Dewar flask. Keep stirring the ethyl acetate until frozen. During the reaction liquid nitrogen was supplied when necessary to keep ethyl acetate frozen, and the resistance temperature detector (RTD, built-in in the laser probe) showed the system temperature was kept at -78 ± 5 °C. THF (1.6 mL) was injected into the vessel at 25 °C and reactIR spectra collection was started. Then $FeCl_3$ (0.3mmol, 48.8 mg) were added, and then phenylzinc reagent (0.44 M in THF, 1.4 mL) was added into the vessel via a syringe for the reactIR spectra collection. When the IR peak of biphenyl stopped increasing, HCl (2 mL, 2M) aqueous solution was added to quench the reaction. The amount of product was determined by GC employing naphthalene as internal standard.

EPR Experiments Data Collection and Analysis

Experimental Details

The reaction of $FeCl_3$ and PhZnCl at -78 °C

A dried Schlenk tube equipped with a stir bar was loaded with $FeCl_3$ (0.3mmol) in THF (2.3 mL) under the atmosphere of nitrogen. The solution was then stirred at -78 °C. Then, phenylzinc reagent (0.44 M in THF, 2.7 mL) was added into the tube via a syringe. After 30 mins, the solution sample was taken out into a small tube, frozen by liquid nitrogen and then analyzed by EPR. EPR spectra was recorded at 10 K on EPR spectrometer operated at 9.378 GHz. Typical spectrometer parameters are shown as follows, sweepWidth: 3900 G; center field set: 1998 G; time constant: 40 ms; scan time: 40.96 s; modulation amplitude: 2.0 G; modulation frequency: 100 kHz; receiver gain: 60 dB; microwave power: 0.1002 mW.

The reaction of $FeCl_3$ and PhZnCl at 25 °C

A dried Schlenk tube equipped with a stir bar was loaded with $FeCl_3$ (0.3mmol) in THF (2.3 mL) under the atmosphere of nitrogen. The solution was then stirred at -78 °C. Then, phenylzinc reagent (0.44 M in THF, 2.7 mL) was added into the tube via a syringe. After 30 mins, the solution was then stirred at 25 °C for 5 mins. Then, the solution sample was taken out into an EPR tube, frozen by liquid nitrogen and then analyzed by EPR.

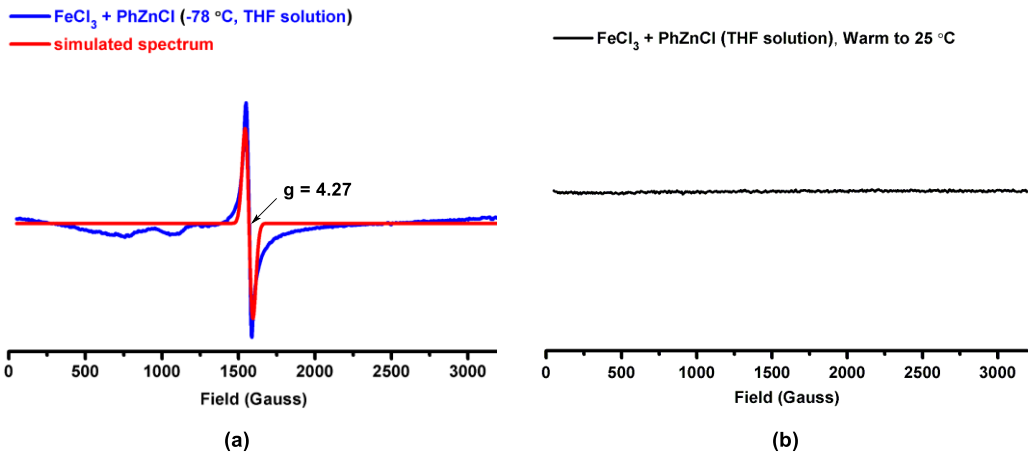


Figure S3. (a) Experimental and simulated EPR spectra of the dark red solution of phenylzinc chloride and $FeCl_3$ at -78 °C, (b) EPR spectrum of the dark red solution of phenylzinc chloride and $FeCl_3$ at 25 °C. (EPR spectra was measured at 10 K)

Raman Experiments Data Collection and Analysis

Experimental Details

The reaction of $FeCl_3$ and PhZnCl at -78 °C

A dried Schlenk tube equipped with a stir bar was loaded with $FeCl_3$ (0.3mmol) in THF (2.3 mL) under the atmosphere of nitrogen. The solution was then stirred at -78 °C (The details of temperature controlled see the IR experiment). Then, phenylzinc reagent (0.44 M in THF, 2.7 mL) was added into the tube via a syringe. After 30 mins, the solution sample was taken out and analyzed by Raman.

The reaction of $FeCl_3$ and PhZnCl at 25 °C

A dried Schlenk tube equipped with a stir bar was loaded with $FeCl_3$ (0.3mmol) in THF (2.3 mL) under the atmosphere of nitrogen. The solution was then stirred at 25 °C. Then, phenylzinc reagent (0.44 M in THF, 2.7 mL) was added into the tube via a syringe. After 30 mins, the solution sample was taken out and analyzed by Raman.

The reaction of $FeCl_2$ and PhZnCl at 25 °C

A dried Schlenk tube equipped with a stir bar was loaded with $FeCl_2$ (0.3mmol) in THF (2.3 mL) under the atmosphere of nitrogen. The solution was then stirred at 25 °C. Then, phenylzinc reagent (0.44 M in THF, 2.7 mL) was added into the tube via a syringe. After 30 mins, the solution sample was taken out and analyzed by Raman.

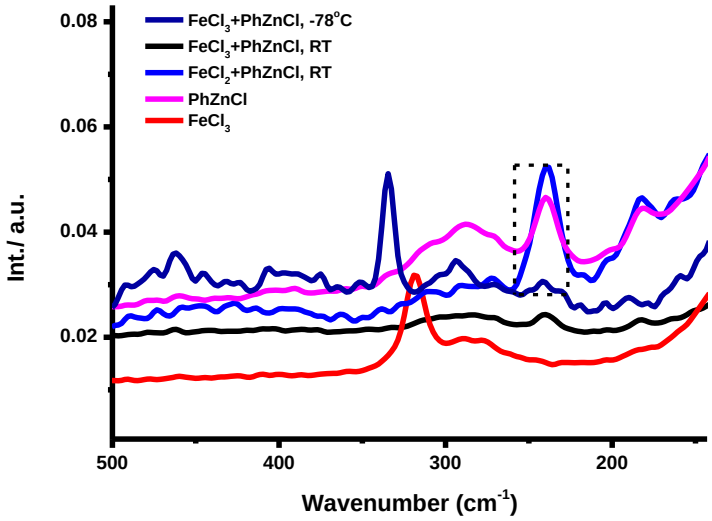


Figure S4 Raman spectra of freeze-trapped experiment

General Computational Calculation Details

Computational methods

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. DFT method B3LYP[3] with a standard 6–311G(d) basis set was used for geometry optimizations. Harmonic vibrational frequency calculations were performed for all of the stationary points to confirm if the points were local minima or a transition structure and to

derive the thermochemical corrections for the enthalpies and free energies. In this study, the stability of wavefunction has been tested for singlet, triplet, quintet, and sextet state intermediates. All the test results confirmed that the wavefunction is stable under the perturbations considered. The solvation effects were considered by single point calculations on the gas-phase stationary points with an SMD continuum solvation model.[4] The M06[5] functional with the 6–311+G(d, p) basis set (def2-TZVP basis set for Fe) was employed to calculate the solvation single point energies in a acetonitrile solvent to provide more accurate energy information. The Gibbs free energy of each stationary point calculated by M06 is provided for discussion of the energy. The Mulliken atomic spin density of certain atoms was also calculated using the same method. The optimized structures were displayed using CYLview.

Additionally, the MECP location program developed by Harvey and co-workers was used in this study to gain the structures of MECPs at the B3LYP/6–311G(d) level of theory. The solvation single point energies of the MECPs, which were calculated at M06/6–311+G(d,p) in THF, have also been summarized. It is also noteworthy that all the iron complexes considered in this study are high spin state. The corresponding low spin state structures were determined to be energetically unfavorable.

Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

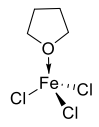
Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	$E_{(elec\text{-}B3LYP)}$[a]	$G_{(corr\text{-}B3LYP)}$[b]	$H_{(corr\text{-}B3LYP)}$[c]	$E_{(solv,\ M06)}$[d]	IF[e]
1-sextet	-2877.036364	0.078801	0.135981	-2876.765622	-

1-quartet	-2876.994591	0.081575	0.134980	-2876.702093	-
2	-5580.851173	0.266944	0.363148	-5580.191559	-
3-ts	-5580.842721	0.268501	0.362108	-5580.180556	-67.96
4	-5580.85143	0.263443	0.362814	-5580.184083	-
5	-2648.447227	0.16031	0.228069	-2648.023341	-
6	-5352.272502	0.345536	0.455289	-5351.446513	-
7	-5352.258334	0.347745	0.455079	-5351.448237	-
8-ts	-5352.244054	0.351143	0.454267	-5351.430702	-68.13
9	-5352.25624	0.346436	0.45481	-5351.437982	-
10	-2419.848388	0.243135	0.32001	-2419.276418	-
11	-2647.699548	0.130755	0.196893	-2647.292972	-
$Ph(THF)_2ZnCl$	-2936.33124	0.273066	0.350645	-2935.780597	-
THF	-232.497862	0.089904	0.121086	-232.3483128	-
$Zn(THF)_2Cl_2$	-3164.917541	0.190082	0.257911	-3164.525441	-
$[Zn(THF)_3Cl]^+$	-2936.959814	0.302697	0.379616	-2936.484671	
A1	-2416.784277	0.078369	0.132659	-2416.531249	-
A2	-231.6105603	0.059004	0.092375	-231.4353578	-
A3	-2649.31575	0.187081	0.257868	-2648.916046	
A4-MECP	-462.8601927	-	-	-	-
A5	-463.4003522	0.146284	0.190773	-463.0540906	-
B1-ts	-464.1081948	0.160938	0.211398	-463.7822732	-1135.05
B2	-231.8469749	0.074943	0.10889	-231.6973621	-
B3-MECP	-463.3907513	-	-	-	-
C1-ts	-2880.047305	0.240655	0.320723	-2879.456702	-269.15
C2	-2880.192382	0.245942	0.32572	-2879.598734	-
D1	-5064.371744	0.238538	0.333089	-5063.681747	-
D2-ts	-5064.318852	0.233154	0.329789	-5063.632343	-298.68
D3	-5064.474518	0.236952	0.334646	-5063.779587	-
D4	-4833.598644	0.176681	0.267136	-4833.05176	-

D5	-5066.120915	0.283719	0.392542	-5065.466522	-
E1	-4832.721888	0.154192	0.237451	-4832.202067	-
E2-ts	-5064.318648	0.232206	0.329871	-5063.632266	-277.27
Benzene	-232.2979217	0.072685	0.10549	-232.1203204	-

[a]The electronic energy calculated by B3LYP in gas phase. [b]The thermal correction to Gibbs free energy calculated by B3LYP in gas phase. [c]The thermal correction to enthalpy calculated by B3LYP in gas phase. [d]The electronic energy calculated by M06 in acetonitrile solvent. [e]The B3LYP calculated imaginary frequencies for the transition states.



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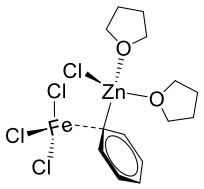

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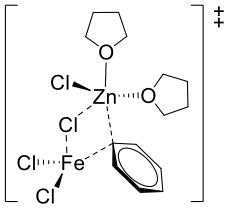

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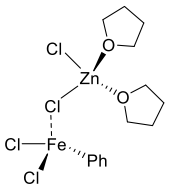

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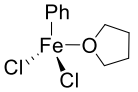

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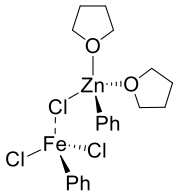

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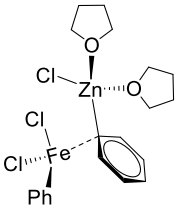

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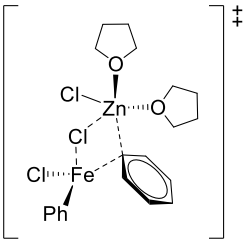

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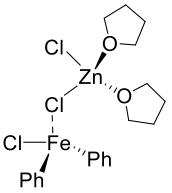

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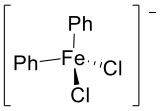

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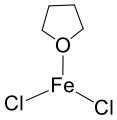
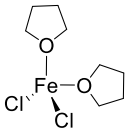


A1

A2



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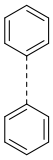
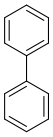
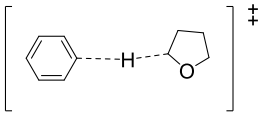


A4-MECP

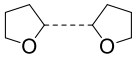


A5



B1-ts

B2



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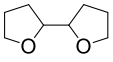

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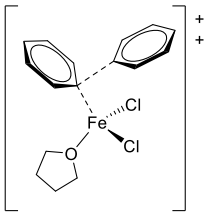
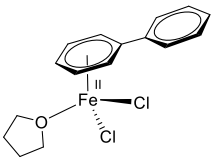


C1-ts



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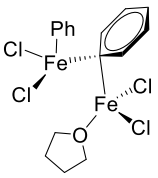
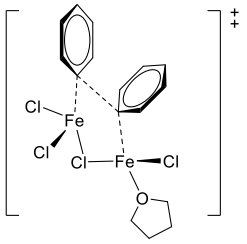


D1



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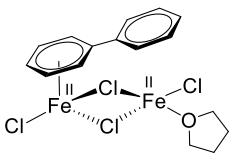

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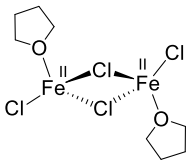

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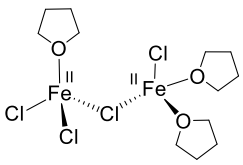

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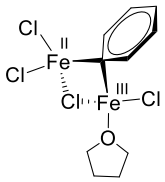
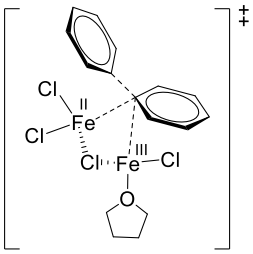
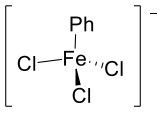


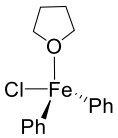
E1



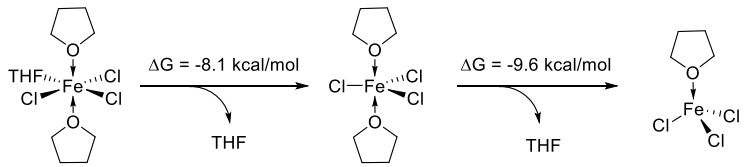
E2-ts



11



12



Scheme S1. Free energy profile for the dissociation of THF.

As shown in Scheme S1, the optimal structure of $FeCl_3$ in THF solution was studied, and computational results showed that the sextet Fe(III) complex coordinated by three Cl and one THF is favored over other structures.

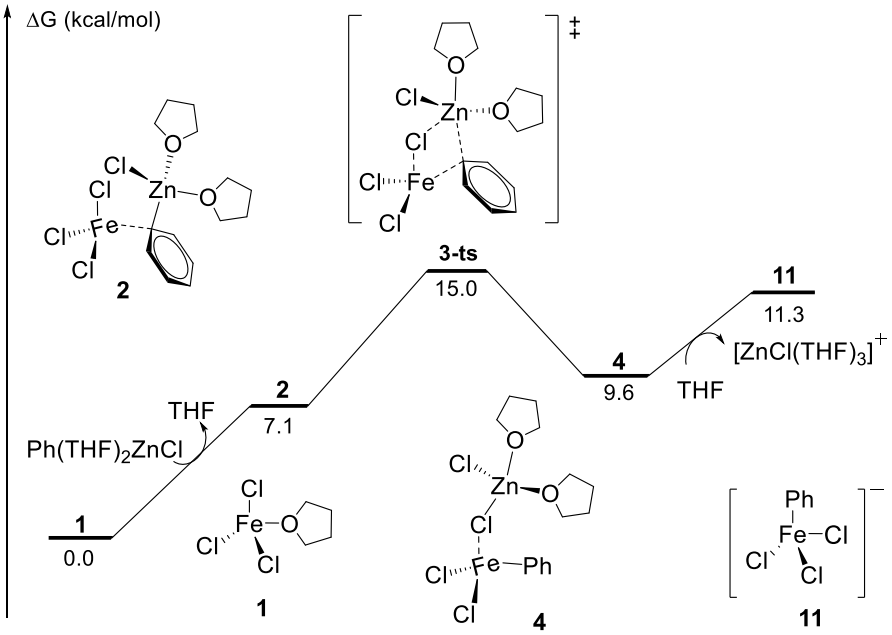


Figure S5. Free energy profile for the formation of **11** by a transmetallation process.

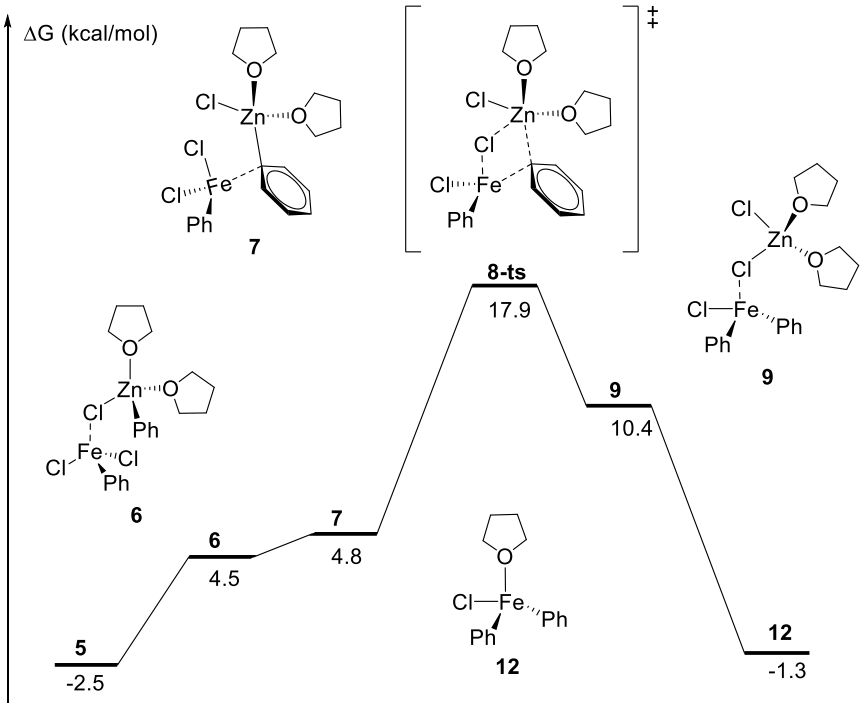


Figure S6. Free energy profile for the formation of **12** by a second transmetallation process.

As shown in Figure S4, a transmetallation process for the formation of complex **11** was calculated. The results suggested that the process is unfavor, since the free energy of **11** is much higher than that of **1**. In Figure S5, a second transmetallation between **5** and phenylzinc chloride is also unfavor, as the complex **5** is more stable than complex **12**.

Mechanistic investigation of the reduction of Ph(THF)FeCl$_2$ to a Fe(II) species via single-electron transfer.

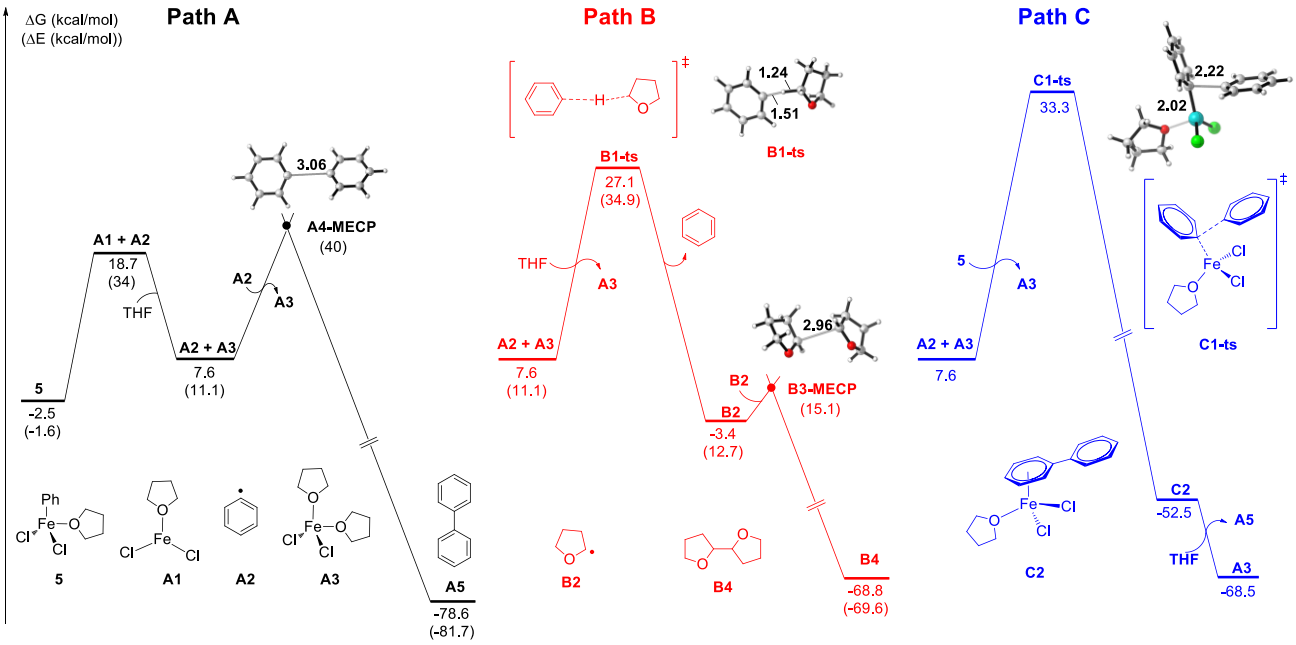


Figure S7. Free energy profile for the generation of biphenyl **A5** from **5** via radical pathways, and optimized structure of several key intermediates and transition states.

In the experiment, when the mixture of $FeCl_3$ and phenylzinc chloride was allowed to stir at room temperature for 1 min, 60% yield of biphenyl could be obtained, and the Fe(III) will be reduced to Fe(II). To determinate the reduction mechanism, DFT calculation was performed. Firstly, three mono-nuclear Fe(III) reduction pathways were considered in calculation. As shown in Figure S6, Path A, the active Fe(III) species **5** suffers a single-electron-transfer reduction to form a Fe(II) species **A1** and the phenyl radical **A2** with a free energy increase of 18.7 kcal/mol. The three coordination Fe(II) species **A1** could further coordinate with a THF to form **A3** by releasing 11.1 kcal/mol of free energy. Finally, radical-radical coupling of phenyl radical **A2** occurs to afford the corresponding product **A5**, this process is highly exergonic by 71.0 kcal/mol. Meanwhile, a minimum energy crossing point **A4-MECP** was obtained for this radical coupling process, the relative energy of **A4-MECP** is determined to be 40.0 kcal/mol. In Path B, the phenyl radical **A2** abstracts a hydrogen atom of THF to produce the THF radical **B2** via transition state B1-ts with an overall energy barrier of 29.6 kcal/mol. Then, radical-radical coupling of **B2** takes place to give B4 with a free energy decrease of 65.4 kcal/mol. A minimum energy crossing point **B3-MECP** was also obtained for this radical coupling

process, the relative energy of **B3-MECP** is determined to be 15.1 kcal/mol. In path C, the phenyl radical **A2** reacts with **5** to afford **C2** through transition state **C1-ts** with an overall energy barrier of 35.8 kcal/mol. **A3** and **A5** are obtained after a ligand exchange process, and the decrease of free energy is 66.0 kcal/mol in all.

Meanwhile, two dinuclear Fe(III) reduction pathways were also considered in our calculation. As shown in Figure S7, Path D, the Fe(III) dimer **D1** is produced from **5** by dissociating a THF ligand with a free energy increase of 12.8 kcal/mol. Then, reduction elimination of **D1** affording **D3** occurs via transition state **D2-ts** with an overall energy barrier of 42.9 kcal/mol. A ligand exchange process takes place between **D3** and THF to obtain the coupling product **A5** with a free energy increase of 11.4 kcal/mol. **D4** undergoes a depolymerization process to **A3** through **D5** by releasing 41.4 kcal/mol of free energy in all. Compared with Path D, Path E suffers two single-electron-transfer reduction processes. Initially, **D1** affords phenyl radical **A2** and **E1**, which quickly produce **D3** through transition state **E2-ts** with an overall energy barrier of 42.4 kcal/mol. Then, **D3** undergoes the same reaction with that in Path D.

Since the overall energy barriers of Path A, B, C, D, E are 21.2 kcal/mol, 29.6 kcal/mol, 35.8 kcal/mol, 42.9 kcal/mol, 41.4 kcal/mol, respectively, we could concluded that Path A is more favorable. In the meantime, the Fe(III) species **5** is reduced to the Fe(II) species **A3**.

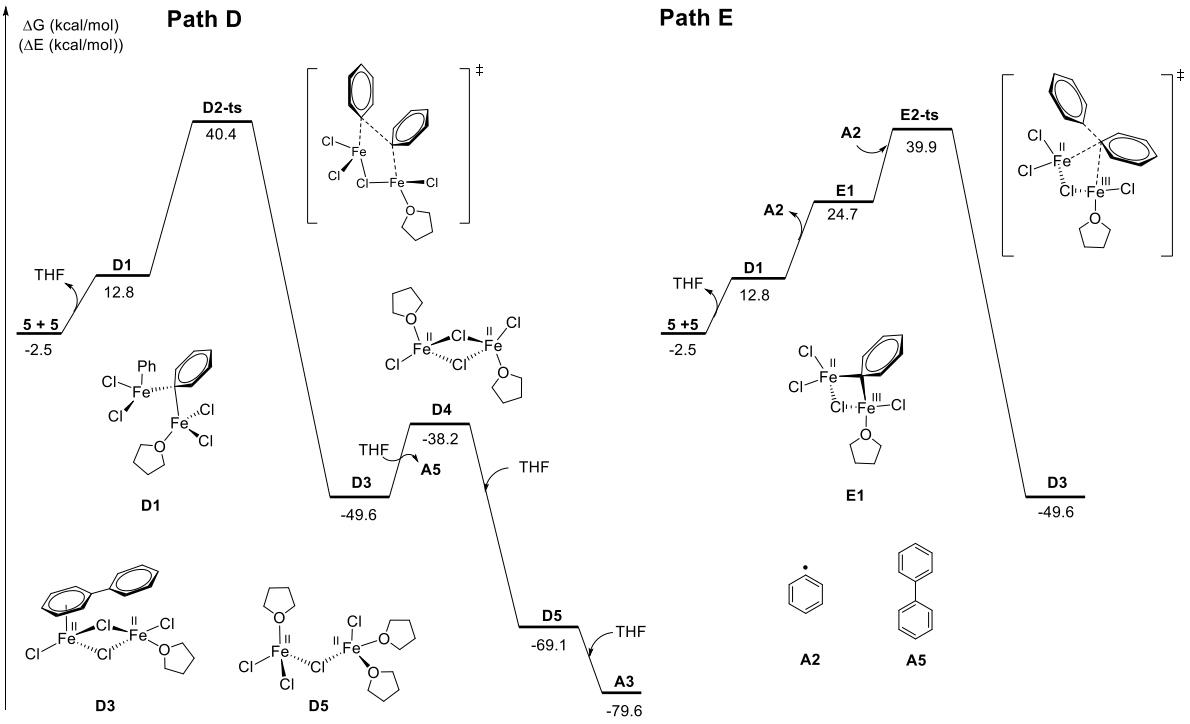


Figure S8. Free energy profile for the generation of biphenyl **A5** from **5** via a dinuclear Fe(III) reduction pathway.

Geometries for all the optimized compounds and transition states

1

0 6

Fe	-0.90842100	-0.00008200	0.00380800
Cl	-1.19264800	-0.24197100	2.15502700
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Cl	-1.49319500	1.94196800	-0.79157900
C	1.92850300	-1.19064900	-0.19130300
O	1.10221200	0.02917300	-0.16868000
C	1.93717400	1.21646300	0.05935800
C	3.34319400	0.74568200	-0.27737800
C	3.32786900	-0.71814400	0.18829500
H	1.49154500	-1.90088900	0.50925700
H	1.86471400	-1.59191300	-1.20311500
H	1.54728900	2.00641100	-0.57924000
H	1.82786300	1.50209700	1.10823000
H	3.51852000	0.80984500	-1.35445900
H	4.10329300	1.34403900	0.22730100
H	4.10005300	-1.32387100	-0.28822700
H	3.47157400	-0.77697000	1.27010900

2

0 6

Fe	2.45910900	0.34175700	-0.31483000
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Cl	1.92570300	2.44714400	0.07682800
Cl	2.61249900	-0.17262900	-2.43378200
Zn	-0.69144800	0.22160600	-0.56450800
C	0.75083400	-0.77380200	0.44976100
C	0.79027800	-0.51881800	1.84380800
C	1.05553800	-2.09854100	0.04403900
C	1.11283000	-1.50842700	2.76691000
H	0.57733100	0.48532200	2.19702500
C	1.38386400	-3.09225000	0.96068400
H	1.05165500	-2.34024200	-1.01417000
C	1.41207500	-2.79594000	2.32349800
H	1.14876800	-1.27557300	3.82608200
H	1.62907700	-4.09138900	0.61581400
H	1.68499300	-3.56499600	3.03893100
C	-2.58948600	1.33510100	1.72770000
O	-1.55035300	1.63343400	0.76100700
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C	-2.81394400	3.61655200	1.08907900
C	-3.01052300	2.68609800	2.29429700

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H	-2.17114400	0.65293500	2.47011000
H	-0.63657500	3.49031700	0.88820800
H	-1.50302800	3.17003500	-0.63205200
H	-2.70919000	4.66523600	1.37208900
H	-3.65802700	3.53496500	0.39840200
H	-2.35146200	2.97907100	3.11652600
H	-4.03569800	2.67463900	2.66944700
Cl	-1.35158900	1.03455200	-2.51606300
C	-3.16571700	-1.58914500	-1.47607300
O	-2.31575500	-1.23568300	-0.33454900
C	-2.47586000	-2.21644100	0.72350800
C	-3.13055400	-3.42141500	0.05903200
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H	-3.12040300	-1.78858400	1.49911000
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H	-3.68389600	-4.03815400	0.76981200
H	-4.29935600	-3.42342700	-1.81189500
H	-4.94956500	-2.39148700	-0.53495300

3-ts

0 6

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Zn	0.80001100	0.23532300	-0.72444400
C	-1.85914800	0.56123600	-0.21496200
C	-2.26186200	1.51843400	0.73925100
C	-1.85189900	0.95838700	-1.56466600
C	-2.64609200	2.80067200	0.36179300
H	-2.29716700	1.25003500	1.79128500
C	-2.21035300	2.25395900	-1.94750300
H	-1.59721000	0.24663100	-2.34395800
C	-2.61827400	3.17115800	-0.98610300
H	-2.97907300	3.51102500	1.11314700
H	-2.17835000	2.53282200	-2.99532500
H	-2.92050700	4.17106500	-1.28151500
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O	2.48785000	-0.79048300	0.05109600
C	2.52018100	-1.75834200	1.14649500

C	3.38289800	-2.90536700	0.64054900
C	4.39327000	-2.17803300	-0.25744000
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H	4.05544100	-0.18920900	-1.16784300
H	2.96952800	-1.26384200	2.01286600
H	1.49683900	-2.04137800	1.38524100
H	3.85068800	-3.45818200	1.45719900
H	2.77815400	-3.60350600	0.05635800
H	5.18283000	-1.71886400	0.34485200
H	4.86708700	-2.83455200	-0.98911800
Cl	1.52046200	1.11518700	-2.64483000
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O	1.03640000	1.68050400	0.69482100
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C	1.14077400	2.91083200	2.70738500
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H	1.70983600	3.02336600	3.63184300
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H	2.75656400	3.79616000	1.54942200

4

0 6

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C	-3.15001300	-1.63764700	-0.35760000
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H	-3.15629500	-1.64584900	-1.44431900
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H	-3.22545100	-1.65631200	3.51092900
H	-3.93343500	-3.63948900	-0.23453100
H	-3.96609600	-3.66267200	2.24947700
Zn	2.02028600	0.01689400	-0.67144100
C	0.57470600	-2.47856400	0.60501200
O	1.78553000	-1.86898100	0.04564000

C	2.71956900	-2.91319000	-0.40088300
C	2.12618000	-4.21919200	0.11313000
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C	1.45440200	2.19811700	3.06012000
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H	2.45740900	4.06735400	2.47591200
H	3.54759100	2.68762600	2.67762700
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5

0 6

Fe	-0.15592300	-0.88275600	0.00372700
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O	-1.49431900	0.65728800	0.04605900
C	-2.93950700	0.42902500	0.18297200
C	-3.58000600	1.75743400	-0.20398400
C	-2.50207300	2.78389500	0.17704800
H	-0.34268900	2.34183300	0.38344400
H	-0.97912600	2.17953200	-1.27136200
H	-3.20357900	-0.40271200	-0.46917800
H	-3.12032700	0.15055700	1.22221600
H	-3.77691300	1.78961900	-1.27881700
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H	-2.61453800	3.73495800	-0.34617400

H	-2.52031000	2.98264000	1.25205800
C	1.65986500	-0.03982700	0.00657600
C	2.27647200	0.33799500	1.21282600
C	2.34364200	0.22634800	-1.19294300
C	3.51476600	0.97802800	1.22005100
H	1.79342200	0.12360600	2.16231700
C	3.58302800	0.86427000	-1.18959800
H	1.91181500	-0.07425900	-2.14342400
C	4.16876400	1.24281500	0.01750600
H	3.97339500	1.26056500	2.16308100
H	4.09485000	1.05846400	-2.12758700
H	5.13672600	1.73451300	0.02173700

6

0 6

Zn	-1.67653400	0.13443100	0.10805800
Cl	0.47434800	-0.46192300	1.18808600
C	-1.10001800	-2.74252800	-1.23901400
C	-2.27294500	-1.10056400	-2.54197500
C	-0.88507500	-3.03126800	-2.71834300
H	-1.74535400	-3.48644000	-0.76296200
H	-0.17746500	-2.64225500	-0.67249700
C	-2.10774000	-2.36779000	-3.36903800
H	-1.64315200	-0.28745900	-2.90599300
H	-3.30136700	-0.75174300	-2.44713700
H	0.03880700	-2.56217700	-3.06225300
H	-0.82013000	-4.10217100	-2.91789500
H	-1.95718400	-2.14279900	-4.42613600
H	-2.99095700	-3.00773900	-3.28071200
C	-2.59448700	-2.20188800	2.06807200
C	-2.59604500	-0.00916200	3.01941700
C	-2.77373800	-2.31341300	3.58024200
H	-1.62699400	-2.59391000	1.74744600
H	-3.39077700	-2.67226800	1.48972200
C	-2.15257200	-1.00213800	4.08369700
H	-3.60582400	0.37029600	3.19904800
H	-1.91665600	0.83166400	2.88413800
H	-3.83453500	-2.36267200	3.84249300
H	-2.28420500	-3.20108600	3.98420600
H	-2.49548800	-0.72095200	5.08094300
H	-1.06238500	-1.07403600	4.09866900
O	-1.80486400	-1.45894700	-1.19689500
O	-2.61944500	-0.77420900	1.77568000
C	-2.33123300	1.91569400	-0.32592600

C	-3.59875400	2.32692000	0.11752600
C	-1.59472700	2.83968800	-1.08424100
C	-4.10975400	3.59194900	-0.17381300
H	-4.21549000	1.64666200	0.70206100
C	-2.09373600	4.10806300	-1.38015500
H	-0.61107600	2.56997300	-1.45746100
C	-3.35423700	4.48869900	-0.92496300
H	-5.09509400	3.87702600	0.18483000
H	-1.49735700	4.79930400	-1.96893000
H	-3.74482800	5.47553700	-1.15491800
Fe	2.26488000	-0.51154900	-0.36975000
Cl	1.21612200	0.29544000	-2.18310000
Cl	2.78808600	-2.65926800	-0.59617000
C	3.77887800	0.62060500	0.28032300
C	3.74581500	2.01504500	0.11835500
C	4.89093200	0.05323300	0.92287700
C	4.78055300	2.81757900	0.59511400
H	2.90655000	2.48765300	-0.38439300
C	5.92742800	0.85329200	1.40078800
H	4.95560700	-1.02311200	1.05296800
C	5.87268100	2.23660700	1.23783000
H	4.73588500	3.89460100	0.46205300
H	6.77907000	0.39645800	1.89651300
H	6.68117000	2.86027700	1.60719700

7

0 6

Fe	-1.77285300	-0.65457900	-0.74285400
Cl	-1.12030200	-2.71229500	-0.19037100
Cl	-1.55759200	-0.09014600	-2.87125100
Zn	1.35368400	-0.17403100	-0.45424800
C	-0.30569200	0.64281300	0.33551200
C	-0.57366800	0.34531200	1.69380600
C	-0.73722900	1.91235800	-0.12335800
C	-1.22992100	1.24185100	2.53265800
H	-0.26079000	-0.61510000	2.09061300
C	-1.39627500	2.81394900	0.70759300
H	-0.56431600	2.18557800	-1.15950700
C	-1.64255400	2.47797500	2.03839400
H	-1.42782900	0.97599800	3.56611700
H	-1.72547200	3.77227000	0.31876000
H	-2.16956400	3.17257600	2.68470500
C	3.46646400	-1.05856100	1.69291400
O	2.22680000	-1.44495600	1.03880900

C	2.20539600	-2.89763600	0.83216400
C	3.63699200	-3.35185800	1.07590500
C	4.11927100	-2.36135600	2.14442200
H	4.08098900	-0.52491100	0.96440900
H	3.21376900	-0.38415300	2.51326200
H	1.50037800	-3.32006900	1.55107200
H	1.84593400	-3.08804500	-0.17604900
H	3.68826600	-4.39242600	1.40153500
H	4.22509100	-3.24765200	0.16059400
H	3.75481100	-2.65438400	3.13352700
H	5.20659800	-2.27777400	2.19634800
Cl	2.51387500	-0.96458600	-2.17275600
C	3.48855300	2.13371600	-1.15524300
O	2.69439000	1.55064200	-0.07363900
C	2.61263500	2.47734200	1.03935600
C	3.06249300	3.82234800	0.48028200
C	4.10339400	3.39982800	-0.56554800
H	4.20729500	1.38602400	-1.48329400
H	2.81433700	2.34969200	-1.98734700
H	1.58858900	2.46738100	1.41119300
H	3.28453500	2.12760200	1.83080300
H	2.22348200	4.33745400	0.00352900
H	3.46671400	4.47891700	1.25327700
H	4.28264500	4.16084100	-1.32714200
H	5.05990100	3.17682100	-0.08319600
C	-3.62318500	-0.24915800	-0.04652900
C	-4.43624200	0.71635800	-0.66220000
C	-4.14511900	-0.93482300	1.06255900
C	-5.71349000	0.99903900	-0.17956400
H	-4.07805200	1.25062300	-1.53745600
C	-5.42150000	-0.65582500	1.54932400
H	-3.55731900	-1.70674900	1.55148900
C	-6.20721000	0.31455600	0.92967900
H	-6.32620700	1.74710900	-0.67475400
H	-5.80596300	-1.20209600	2.40612000
H	-7.20401600	0.52908300	1.30332800

8-ts

0 6

Fe	1.53943200	-1.06857800	-0.06026200
Cl	0.23318700	-0.34812400	-1.93661700
Cl	1.26116600	-3.26734600	0.20130900
Zn	-1.55491500	0.31838200	-0.51504900
C	0.55556400	-0.05195900	1.43581100

C	1.07330600	1.21150600	1.79038900
C	-0.27511800	-0.67982100	2.38409500
C	0.76868400	1.81985700	3.00633900
H	1.74402300	1.72612400	1.10824800
C	-0.60457400	-0.07047500	3.59730100
H	-0.65098600	-1.67582700	2.17767600
C	-0.07906800	1.18025300	3.91228900
H	1.20097800	2.78510900	3.25532200
H	-1.24811700	-0.58349600	4.30632300
H	-0.31478500	1.64790500	4.86342000
C	-1.63638300	3.17928600	0.63318000
O	-0.96018700	2.29000600	-0.30393100
C	-0.60829300	3.02898400	-1.52210100
C	-1.01817500	4.47958600	-1.25656900
C	-1.10486200	4.55707500	0.27600500
H	-2.71459900	3.09859900	0.47217100
H	-1.37586300	2.83541600	1.63308200
H	0.46467100	2.89970800	-1.66461800
H	-1.14178100	2.58337700	-2.36169200
H	-0.30173700	5.18690700	-1.67745100
H	-1.99541900	4.68409000	-1.69984700
H	-0.11608700	4.70953800	0.71753500
H	-1.76213000	5.35631000	0.62334600
Cl	-3.63538600	0.92431100	-1.23358400
C	-2.24000600	-2.58909900	-1.06313200
O	-2.18088500	-1.58628600	0.01297500
C	-3.30547000	-1.78083600	0.93291400
C	-4.21653900	-2.79183800	0.25030600
C	-3.22483000	-3.63401800	-0.56379900
H	-2.59925200	-2.08761500	-1.96468200
H	-1.22927700	-2.95923600	-1.21328000
H	-2.89380500	-2.16071200	1.87032100
H	-3.77984200	-0.81435600	1.09877100
H	-4.78791600	-3.37827600	0.97237500
H	-4.91769900	-2.27750800	-0.41110400
H	-2.71647000	-4.36396200	0.07197200
H	-3.69683100	-4.17082200	-1.38857900
C	3.44151600	-0.47558900	-0.36672100
C	4.37401200	-0.49008900	0.68244900
C	3.87971200	-0.03916500	-1.62767800
C	5.69327500	-0.08447700	0.48371000
H	4.07726500	-0.82553400	1.67351600
C	5.19802200	0.36814400	-1.83196000
H	3.19026100	-0.01808500	-2.46775100

C	6.10683300	0.34652400	-0.77565200
H	6.39819000	-0.10784900	1.30993000
H	5.51573700	0.69810600	-2.81706900
H	7.13415900	0.66051900	-0.93390600

9

0 6

Fe	1.87001300	-0.30399000	0.35527200
Cl	0.16889000	-0.67529900	-1.35308900
Cl	1.32451800	-1.65963300	2.06981200
C	1.14163100	2.04597300	2.16362300
C	1.88630600	2.65232200	-0.03612700
C	0.96134000	3.39414700	2.47827000
H	0.93803400	1.29926500	2.92689200
C	1.70716800	4.00238300	0.26858400
H	2.26432600	2.38808300	-1.02110700
C	1.24001700	4.37590500	1.52837800
H	0.61479100	3.67939800	3.46803000
H	1.94443900	4.76226700	-0.47097800
H	1.10887300	5.42580900	1.77303800
Zn	-2.10940100	-0.86173100	-0.87185100
C	-1.90888600	2.27655500	-0.55449600
O	-2.69963300	1.09171900	-0.90559100
C	-3.85346300	1.47577000	-1.72749900
C	-3.89010200	2.99748000	-1.66720400
C	-2.40867400	3.36397500	-1.49371300
H	-2.11076600	2.51272300	0.49304400
H	-0.85694700	2.02602400	-0.66925200
H	-3.68176800	1.09864000	-2.73727500
H	-4.73274200	0.98262900	-1.31475500
H	-4.33665400	3.42762500	-2.56516700
H	-4.47262000	3.33650700	-0.80572700
H	-1.88313100	3.31223100	-2.45119800
H	-2.25713500	4.36121000	-1.07810500
Cl	-3.48807800	-2.08702900	-2.07185500
C	-2.24449300	-2.71539900	1.53080100
O	-2.22672200	-1.31877100	1.08119000
C	-2.22174700	-0.40978200	2.22571100
C	-2.12488800	-1.31016400	3.45488600
C	-2.73141000	-2.63658200	2.96919900
H	-2.90373000	-3.25957000	0.85510100
H	-1.22575900	-3.10034100	1.46009800
H	-1.37227700	0.26428200	2.11605300
H	-3.15461000	0.15876000	2.18960200

H	-1.07884300	-1.45049800	3.73082200
H	-2.65736500	-0.88861600	4.30943200
H	-2.39538000	-3.49151400	3.55792600
H	-3.82426200	-2.60539300	3.00389800
C	1.59638000	1.64083800	0.89681400
C	3.61297300	-0.71843300	-0.56533300
C	3.66205000	-1.24215000	-1.86755000
C	4.82919800	-0.45498100	0.08391400
C	4.88127600	-1.49506300	-2.49554400
H	2.74141500	-1.45735200	-2.40268900
C	6.05062900	-0.70754900	-0.53933600
H	4.83396500	-0.04790300	1.09246200
C	6.07753400	-1.22876200	-1.83176000
H	4.89601000	-1.90191600	-3.50277400
H	6.97979000	-0.49838100	-0.01679700
H	7.02722300	-1.42747900	-2.31938400

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-1 6

Fe	0.00000100	0.91107900	0.00002600
Cl	-0.07976800	2.15157700	1.90922400
Cl	0.07985400	2.15172500	-1.90908200
C	1.68428000	-0.27162500	0.05137100
C	2.53116000	-0.44383600	-1.05625200
C	2.00459300	-0.99736000	1.21119400
C	3.63731500	-1.29469200	-1.01227200
H	2.32820500	0.10267900	-1.97368400
C	3.10719200	-1.85046600	1.26774700
H	1.38298300	-0.89372100	2.09776000
C	3.92914500	-2.00319200	0.15192700
H	4.27385700	-1.40326300	-1.88825100
H	3.32651100	-2.39567100	2.18359400
H	4.79017400	-2.66627600	0.19078900
C	-1.68429000	-0.27159800	-0.05138600
C	-2.00468100	-0.99717500	-1.21128800
C	-2.53112300	-0.44393900	1.05625400
C	-3.10730300	-1.85024700	-1.26789900
H	-1.38311200	-0.89343700	-2.09787100
C	-3.63729600	-1.29476700	1.01222100
H	-2.32811600	0.10244600	1.97375300
C	-3.92920300	-2.00310600	-0.15205700
H	-3.32668200	-2.39532100	-2.18380900
H	-4.27378900	-1.40344100	1.88822200
H	-4.79024700	-2.66616700	-0.19096400

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-1 6

Fe	0.92379000	-0.00627600	-0.00338000
Cl	1.62281800	1.43308100	-1.58757000
Cl	1.61389500	0.68880800	2.02248500
Cl	1.64877700	-2.09995000	-0.41904900
C	-1.12577600	-0.02142200	-0.01323300
C	-1.86881200	-1.21150000	-0.01070400
C	-1.84436900	1.18409700	-0.00946200
C	-3.26482600	-1.20109300	-0.00045800
H	-1.35176700	-2.16697000	-0.01913000
C	-3.23906700	1.20555000	0.00094900
H	-1.30875400	2.13010500	-0.01693700
C	-3.95513500	0.00933500	0.00565200
H	-3.81378700	-2.14036700	0.00121600
H	-3.76731900	2.15649800	0.00378500
H	-5.04233900	0.02114000	0.01277400

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0 6

Fe	-0.03891000	0.05906200	0.70247000
Cl	0.09820800	-0.61678200	2.83231200
C	-0.46105900	-2.05962400	-1.60113800
O	0.04820300	-1.77731700	-0.26373100
C	0.95313600	-2.84356200	0.18040800
C	1.08040300	-3.77997800	-1.01864700
C	-0.23599000	-3.55434100	-1.77867300
H	-1.50253700	-1.74380800	-1.62343200
H	0.11540300	-1.46846700	-2.31857700
H	1.89063300	-2.37932100	0.48403800
H	0.48771300	-3.31135800	1.04844900
H	1.93236500	-3.49315100	-1.64094900
H	1.22290600	-4.81711000	-0.71081400
H	-0.17632700	-3.83873500	-2.83073500
H	-1.05149200	-4.11944700	-1.31893700
C	-1.83459900	0.80136800	0.14065700
C	-3.01263600	0.07379500	0.38873600
C	-1.96378500	2.03881200	-0.51256700
C	-4.26053600	0.54936500	-0.01268500
H	-2.96393100	-0.87533100	0.91829800
C	-3.20908900	2.52359600	-0.91310200
H	-1.08224900	2.64411200	-0.70853900
C	-4.35960400	1.77697500	-0.66652200
H	-5.15577800	-0.03063500	0.19363600

H	-3.28227000	3.48535300	-1.41299900
H	-5.33036700	2.15332400	-0.97480200
C	1.64668200	0.98669100	0.06002300
C	1.72228600	1.45935400	-1.26211900
C	2.77377500	1.17570000	0.87855100
C	2.87131900	2.08069000	-1.75252100
H	0.86976700	1.35236500	-1.93069500
C	3.92522000	1.79821000	0.39657100
H	2.75534900	0.83514200	1.91015800
C	3.97643500	2.25090100	-0.92088800
H	2.90198700	2.43664900	-2.77864400
H	4.78209900	1.93315500	1.05067900
H	4.87147900	2.73776200	-1.29631300

A1

0 5

Fe	1.08787600	-0.00003800	-0.00103500
Cl	1.76090600	2.08013300	0.01116700
Cl	1.76006700	-2.08046100	-0.00753600
C	-1.78823100	1.19661000	-0.16046500
C	-1.78714400	-1.19710100	0.15208400
C	-3.18877400	0.73718300	0.22296300
H	-1.72087700	1.51239000	-1.20388300
H	-1.36833100	1.97425000	0.47478800
C	-3.19219400	-0.73574400	-0.21318900
H	-1.70756900	-1.51811000	1.19297000
H	-1.37496100	-1.97181700	-0.49177100
H	-3.33722200	0.81919400	1.30320200
H	-3.96094000	1.33030400	-0.26961300
H	-3.95849400	-1.32824000	0.28918500
H	-3.35482800	-0.81745700	-1.29140700
O	-0.95250500	0.00004400	-0.00583200

A2

0 2

C	-1.21189700	0.63148700	-0.00000600
C	-1.22361600	-0.77059300	0.00002300
C	-0.00001300	-1.39675000	-0.00001100
C	1.22361900	-0.77058200	-0.00000800
C	1.21191200	0.63145800	0.00001900
C	-0.00000400	1.32221200	-0.00000600
H	-2.15142700	1.17652700	-0.00002800
H	-2.15857600	-1.32185600	-0.00000900
H	2.15854800	-1.32190100	-0.00002700

H	2.15142000	1.17653700	0.00001300
H	0.00002700	2.40730700	-0.00002200

A3

0 5

Fe	-0.00723500	-0.92769000	0.02389700
Cl	-0.60320700	-1.66308600	2.05887100
Cl	0.60590600	-1.83397000	-1.93540000
C	2.64420400	0.20331300	1.06108000
C	1.86628800	1.48845600	-0.80063700
C	3.66946500	1.28814100	0.76294600
H	2.99428600	-0.78510400	0.74849900
H	2.31286200	0.15258200	2.09748400
C	3.38777500	1.59722300	-0.71566000
H	1.37067600	2.44098700	-0.59235700
H	1.50747400	1.08976100	-1.74907300
H	3.48941000	2.16919400	1.38600500
H	4.69169600	0.95029000	0.94185800
H	3.74825000	2.58000500	-1.02478700
H	3.85722100	0.84710900	-1.35721800
O	1.48376000	0.55549200	0.25349100
C	-1.80557300	1.57469200	0.63462700
O	-1.50536300	0.52028700	-0.32415700
C	-2.71207200	0.13896200	-1.05134600
C	-3.85465900	0.87549900	-0.35788200
C	-3.15871500	2.12548100	0.20197300
H	-1.83805200	1.12664100	1.63086700
H	-0.99112300	2.29806700	0.59195700
H	-2.57957100	0.44734300	-2.09095500
H	-2.80058600	-0.94694900	-1.01397700
H	-4.66992600	1.11032800	-1.04433400
H	-4.25963700	0.27028500	0.45721100
H	-3.03626600	2.88194400	-0.57889200
H	-3.70192900	2.58058600	1.03209900

A4-MECP

0 1

C	2.15434900	-1.14106600	0.43932100
C	3.55669400	-1.13158200	0.43337300
C	4.24829200	0.00002200	-0.00000700
C	3.55670200	1.13154800	-0.43335700
C	2.15435300	1.14110100	-0.43933300
C	1.52801300	-0.00002200	0.00000900
H	1.60347000	-2.01257700	0.77965000

H	4.09984400	-2.01016300	0.76965200
H	5.33364300	0.00000000	0.00000200
H	4.09984700	2.01017400	-0.76965300
H	1.60347300	2.01257100	-0.77964500
C	-1.52802000	-0.00002800	-0.00000900
C	-2.15432700	1.14112900	0.43934500
C	-2.15431800	-1.14108600	-0.43932800
C	-3.55675400	1.13150800	0.43334100
H	-1.60348500	2.01255700	0.77964300
C	-3.55674300	-1.13155200	-0.43336200
H	-1.60347800	-2.01256600	-0.77964300
C	-4.24823300	0.00002700	0.00000700
H	-4.09985300	2.01018200	0.76965500
H	-4.09984400	-2.01017000	-0.76965600
H	-5.33366800	-0.00000200	-0.00000600

A5

0 1

C	1.46405800	-1.12573500	0.42396900
C	2.85584800	-1.12608700	0.42431500
C	3.55832600	-0.00000100	0.00000100
C	2.85584700	1.12608800	-0.42431700
C	1.46405800	1.12573700	-0.42397000
C	0.74262400	0.00000000	0.00000400
H	0.92811200	-1.99880200	0.78200100
H	3.39286300	-2.00579300	0.76514100
H	4.64358700	0.00000100	-0.00000200
H	3.39286500	2.00579000	-0.76514900
H	0.92811000	1.99880000	-0.78200900
C	-0.74262400	0.00000000	0.00000000
C	-1.46405900	1.12573600	0.42397200
C	-1.46405700	-1.12573500	-0.42396900
C	-2.85584800	1.12608800	0.42431500
H	-0.92811200	1.99880000	0.78201000
C	-2.85584800	-1.12608800	-0.42431500
H	-0.92811000	-1.99880200	-0.78200100
C	-3.55832600	-0.00000100	-0.00000300
H	-3.39286700	2.00579000	0.76514400
H	-3.39286200	-2.00579300	-0.76514500
H	-4.64358700	0.00000100	-0.00000400

B1-ts

0 2

C	-2.78471900	-1.30119200	-0.09862000

C	-1.44736500	-1.07090300	0.24002200
C	-1.00017800	0.23655300	0.32234300
C	-1.82659000	1.32216600	0.08686700
C	-3.16301700	1.08366700	-0.25181100
C	-3.63720500	-0.22475300	-0.34385800
H	-3.15895100	-2.31873700	-0.16872100
H	-0.77351400	-1.90019800	0.43720300
H	-1.45781400	2.34188300	0.16237000
H	-3.83121300	1.91910200	-0.44175600
H	-4.67496000	-0.40581700	-0.60599400
C	1.66765700	0.33267200	0.94071400
O	2.09618000	-0.98397300	0.69560900
C	2.63942100	-1.02641500	-0.62902700
C	3.35089200	0.31687500	-0.79153900
C	2.41617200	1.27282900	-0.01864200
H	0.45338900	0.38274800	0.69474100
H	1.75693300	0.54230000	2.00807200
H	3.29346200	-1.89728400	-0.68575900
H	1.82936300	-1.14199100	-1.36191400
H	4.33509400	0.27485200	-0.31744000
H	3.48861200	0.60281800	-1.83637600
H	2.96433600	2.05577100	0.50990000
H	1.71541300	1.76735100	-0.69789600

B2

0 2

C	-1.10797500	0.46553700	-0.17469300
O	-0.84896900	-0.91810100	0.12040000
C	0.49648000	-1.14114800	-0.05033100
C	1.26384700	0.14915400	-0.13482600
C	0.17993500	1.19667200	0.21205900
H	-1.32523200	0.56796600	-1.24514500
H	-1.98865300	0.76199100	0.39551100
H	0.84209400	-2.06334100	0.39979400
H	2.11861300	0.18686200	0.54889200
H	1.66446000	0.32315100	-1.14329600
H	0.18356100	1.40365800	1.28569300
H	0.30318600	2.14323400	-0.31789400

B3-MECP

0 1

C	-2.84423300	-0.80007500	0.51809800
O	-1.93446500	-1.16154400	-0.53148500
C	-1.20628200	-0.04445700	-0.86040500

C	-1.85698100	1.20909400	-0.34313900
C	-3.17608300	0.67383100	0.26364300
H	-3.69949300	-1.47366100	0.45776800
H	-2.34771700	-0.94076300	1.48562300
H	-0.68781300	-0.13925200	-1.80640000
H	-1.24495500	1.70292400	0.42355200
H	-2.03444300	1.95757900	-1.12425200
H	-3.47918000	1.19898700	1.17152400
H	-3.98842000	0.75596300	-0.46339100
C	1.20657500	-0.04391600	0.86092100
O	1.93442000	-1.16139500	0.53201000
C	1.85747500	1.20927800	0.34326400
H	0.68857200	-0.13842000	1.80724300
C	2.84365300	-0.80050800	-0.51823200
C	3.17596700	0.67350700	-0.26452900
H	2.03576600	1.95761600	1.12418400
H	1.24498900	1.70343300	-0.42300700
H	3.69885000	-1.47413000	-0.45813900
H	2.34649600	-0.94143200	-1.48542000
H	3.98892300	0.75585000	0.46171100
H	3.47825300	1.19829900	-1.17291800

B4

0 1

C	2.80005300	-0.79413300	-0.29160300
O	1.43538000	-1.15402800	-0.05174900
C	0.67431800	-0.00785900	0.35216300
C	1.55729400	1.20674600	0.03083800
C	2.96797100	0.63895500	0.22401100
H	3.44696000	-1.51382600	0.21821600
H	3.00506000	-0.85554000	-1.36849000
H	0.49038700	-0.07641200	1.43503500
H	1.41095700	1.51504100	-1.01086300
H	1.34348900	2.06645400	0.66899700
H	3.73757800	1.19668400	-0.31443000
H	3.23399600	0.63816900	1.28560800
C	-0.67438400	-0.00785600	-0.35257200
O	-1.43542700	-1.15413500	0.05114100
C	-1.55735500	1.20673600	-0.03110300
H	-0.49044000	-0.07632600	-1.43543600
C	-2.79981600	-0.79408600	0.29227900
C	-2.96808600	0.63884400	-0.22358500
H	-1.34384600	2.06634000	-0.66950100
H	-1.41064100	1.51525100	1.01048000

H	-3.44723100	-1.51391500	-0.21669100
H	-3.00382100	-0.85511300	1.36938900
H	-3.23455000	0.63777300	-1.28507100
H	-3.73750000	1.19665100	0.31505400

C1-ts

0 7

Fe	-0.43127300	-0.65633300	-0.01268100
Cl	-0.33255300	-1.93824800	-1.81445500
Cl	-0.64763200	-1.58173000	1.99468200
C	-3.03839400	0.96780200	0.56229100
O	-2.44467100	-0.11765700	-0.22314100
C	-3.47966900	-1.05774400	-0.65831700
C	-4.77556400	-0.27153600	-0.53140300
C	-4.51341300	0.59989700	0.70564200
H	-2.50951100	1.02581700	1.51274000
H	-2.87745700	1.88941800	0.00074300
H	-3.22355600	-1.36811500	-1.66876400
H	-3.45012700	-1.92481300	0.00670300
H	-4.93419000	0.34898500	-1.41785400
H	-5.64107400	-0.92634200	-0.41594000
H	-5.15084000	1.48471900	0.74936700
H	-4.67449900	0.02159200	1.61903000
C	0.40545800	1.17945600	-0.06648200
C	0.57751800	1.98701300	1.10596000
C	0.54924800	1.85525000	-1.32294100
C	0.97591600	3.30947000	1.02391700
H	0.41108500	1.54669600	2.08472400
C	0.94885500	3.17845800	-1.39403600
H	0.35254600	1.31470400	-2.24459600
C	1.17921300	3.91347600	-0.22392000
H	1.11985800	3.88686900	1.93273400
H	1.06836000	3.65477600	-2.36307000
H	1.49023300	4.95124500	-0.28370000
C	3.94517600	-1.12995900	1.33980600
C	4.64279100	-1.41148100	0.16609900
C	4.12097700	-1.03193800	-1.07120100
C	2.89580700	-0.36667000	-1.13900800
C	2.20725400	-0.11827600	0.03921000
C	2.71982600	-0.46073800	1.28252600
H	4.35284500	-1.42603000	2.30195400
H	5.59768800	-1.92517900	0.21513300
H	4.66627000	-1.25341700	-1.98403200
H	2.48881800	-0.07161000	-2.10028500

H	2.18117000	-0.23866100	2.19723700

C2

0 5

Fe	-1.78785300	-0.26810400	0.01668700
Cl	-1.68507400	-0.54663400	2.22666600
C	-1.85606800	2.80132300	-0.18620800
O	-0.93291800	1.67444100	-0.10216900
C	0.32275600	2.09778300	0.51371800
C	0.10099200	3.54842600	0.93809900
C	-0.97280700	4.03215900	-0.04745600
H	-2.38521600	2.71442600	-1.13297700
H	-2.57463400	2.72019700	0.63535800
H	0.53273700	1.42757800	1.34607500
H	1.10597200	1.99650800	-0.23994500
H	-0.27717900	3.59229900	1.96294100
H	1.02189300	4.13251100	0.89208100
H	-1.52816800	4.89882100	0.31571400
H	-0.52682100	4.29352900	-1.01152400
C	1.29462600	-2.66308300	0.73896700
C	1.32860300	-1.61815700	-0.18916100
C	0.23427500	-1.47818600	-1.06986700
C	-0.83491800	-2.38508000	-1.02934500
C	-0.83849400	-3.42812000	-0.09424000
C	0.22203300	-3.55366400	0.79117800
H	2.13254000	-2.80336800	1.41281800
H	0.25951700	-0.71929500	-1.84494700
H	-1.61142000	-2.32996400	-1.78298900
H	-1.66497800	-4.12915600	-0.06970100
H	0.22780400	-4.35516200	1.52183700
C	2.49453700	-0.70284300	-0.26371100
C	2.98122400	-0.25436500	-1.50066600
C	3.14158900	-0.26473800	0.90179300
C	4.07452400	0.60454000	-1.57004300
H	2.52039700	-0.60464800	-2.41830200
C	4.23350900	0.59537700	0.83247200
H	2.76855900	-0.57776500	1.87131700
C	4.70415200	1.03484100	-0.40366500
H	4.44151200	0.92929400	-2.53836300
H	4.71423600	0.92718000	1.74719400
H	5.55757000	1.70279100	-0.45767700
Cl	-3.28845600	-0.06735900	-1.63823200

D1

0 11

Fe	1.89240700	1.04535900	0.03397000
Cl	-0.20890600	-1.81041500	-1.73260500
Cl	-0.25111800	-1.55436100	1.97428700
C	-3.06501700	-0.78475800	0.02990300
C	-3.80010200	-0.73844200	1.22656300
C	-3.77491100	-0.84883900	-1.18094500
C	-5.19351600	-0.72806100	1.21311200
H	-3.28537700	-0.71623400	2.18269900
C	-5.16829500	-0.83741000	-1.19771900
H	-3.24067700	-0.91503400	-2.12431700
C	-5.87932600	-0.77434300	0.00002000
H	-5.74375400	-0.69164500	2.14876800
H	-5.69892900	-0.88676700	-2.14407400
H	-6.96496700	-0.77213100	-0.01148800
Fe	-1.05944700	-0.77701500	0.05067500
C	3.25430100	-1.52596500	1.15589800
C	3.25430600	-1.39490300	-1.26480000
C	4.13353300	-2.62773000	0.57405700
H	2.36853600	-1.90342900	1.66262500
H	3.77893300	-0.82375900	1.80093800
C	3.57881100	-2.81589400	-0.84571200
H	4.13066500	-0.83281000	-1.59319000
H	2.45784800	-1.31108600	-1.99879400
H	5.17917800	-2.31043700	0.53786300
H	4.07747400	-3.53717400	1.17418900
H	4.29568600	-3.28313700	-1.52328000
H	2.66824400	-3.41934700	-0.83546700
O	2.76913100	-0.76452200	-0.02158300
Cl	2.77246600	1.98008800	-1.74883800
C	-0.72956600	1.68374000	-1.31614400
C	-0.16630900	1.31531700	-0.06304100
C	-0.80592200	1.83924000	1.09475200
C	-1.92218100	2.66494700	1.00534700
C	-2.43848800	3.00403400	-0.24400000
C	-1.84658600	2.50758100	-1.40466000
H	-0.27525900	1.31982100	-2.23112800
H	-0.41240900	1.59384300	2.07502000
H	-2.38577500	3.04601700	1.90900900
H	-3.30820900	3.64902900	-0.31346200
H	-2.25089900	2.76709000	-2.37727200
Cl	2.64139800	1.88676500	1.91524200

D2-ts

0 11

Fe	-1.66205000	0.65995200	-0.58216800
Cl	0.84598800	-2.71425100	0.94532700
Cl	2.60404600	-1.58245600	-2.23734300
C	2.82418700	0.60795500	0.68744600
C	3.78494500	1.24530200	-0.07183600
C	3.07960700	0.00176700	1.90176000
C	5.09535900	1.25660800	0.41383300
H	3.54680700	1.71226000	-1.02100400
C	4.39749900	0.01981500	2.37209900
H	2.30162200	-0.48978500	2.47452900
C	5.39748000	0.64641000	1.63128500
H	5.87746800	1.73830200	-0.16516700
H	4.63493600	-0.45962300	3.31691700
H	6.41732100	0.65714700	2.00162400
Fe	1.06221000	-1.28811600	-0.72728800
C	-3.22596000	-1.72586100	0.81173400
C	-3.93827400	0.47135500	1.49670200
C	-4.27507800	-1.85705200	1.90742100
H	-2.29013300	-2.24347700	1.01612200
H	-3.59837300	-2.02941200	-0.16788100
C	-5.04384500	-0.53237900	1.79940100
H	-4.25347200	1.30919600	0.87572900
H	-3.45937800	0.84641000	2.40561900
H	-4.90933100	-2.73226700	1.75802100
H	-3.79838500	-1.94916600	2.88740600
H	-5.75950300	-0.56902800	0.97387900
H	-5.58992000	-0.27795400	2.70938800
O	-2.93473800	-0.28605500	0.74775800
C	0.05435300	0.91962500	1.18909200
C	0.74580400	0.64509900	-0.04553600
C	0.77960800	1.75128200	-0.96624800
C	0.42717900	3.03879500	-0.58344900
C	-0.07172200	3.29292800	0.70085200
C	-0.28754700	2.22039800	1.56841200
H	-0.10168800	0.11071100	1.89532500
H	1.14586900	1.58741500	-1.97506800
H	0.50397900	3.84892000	-1.30103500
H	-0.34056400	4.30079400	0.99446100
H	-0.73538700	2.39183100	2.54269600
Cl	-2.94493100	2.06242800	-1.72485200
Cl	-1.03332000	-1.36241800	-1.80875500

D3

0 9

Fe	-1.31751800	1.58184100	0.39964200
Cl	-2.04732500	-3.11526200	-0.13891900
Cl	-0.15114100	0.18140900	-1.28129400
Fe	-0.33143900	-1.73889600	0.12316800
Cl	-0.92044300	-0.20302600	1.96373200
C	-4.29805600	0.66266700	0.73352800
C	-5.30022600	-0.06136400	-0.15277600
C	-5.17222300	0.70045200	-1.48177600
C	-3.67773300	1.00768500	-1.56005900
H	-4.70579800	1.58329100	1.16184800
H	-3.86858900	0.04899900	1.52393900
H	-5.00585300	-1.10678200	-0.27414000
H	-6.31094300	-0.03298600	0.25829000
H	-5.51201000	0.11759400	-2.33932600
H	-5.75446200	1.62554800	-1.45028900
H	-3.11070800	0.23351000	-2.07843600
H	-3.44793500	1.97890800	-1.99980700
O	-3.21383400	1.02636800	-0.17212600
C	1.68693800	-2.49053200	1.23090600
C	1.45491600	-3.28878300	0.09545700
C	2.07600400	-2.94864000	-1.12099900
C	2.89436500	-1.83268600	-1.19841400
C	3.12828600	-1.01752500	-0.07277100
C	2.51775600	-1.36467900	1.13625400
H	1.27369500	-2.77292800	2.19288400
H	0.87908300	-4.20350500	0.17709400
H	1.91548600	-3.56882700	-1.99564300
H	3.37142200	-1.58283800	-2.13931000
H	2.65988500	-0.73954800	2.00999800
C	3.97739000	0.19267000	-0.17910100
C	4.95163200	0.47545000	0.78785300
C	3.80779900	1.08238300	-1.24913600
C	5.74307400	1.61482100	0.68208600
H	5.10721100	-0.21306700	1.61244200
C	4.59514800	2.22547800	-1.34796700
H	3.02325200	0.89956700	-1.97574300
C	5.56691000	2.49287900	-0.38572400
H	6.49995000	1.81600400	1.43316500
H	4.43950800	2.91459500	-2.17133000
H	6.18000100	3.38460700	-0.46421800
Cl	-1.16118000	3.77150900	0.56226800

D4

0 9

Fe	1.38852700	1.11953500	0.03936400
Cl	-0.01523600	0.06495300	-1.64477500
Cl	-2.04903600	-3.16084600	0.05235200
Fe	-1.36021000	-1.06649800	0.05654900
Cl	2.17827900	3.17614200	0.09690100
Cl	0.00934800	0.02730500	1.72418600
C	3.71772100	-0.63234700	1.13354900
C	4.97985500	-1.28862100	0.57616600
C	4.54244700	-1.75024600	-0.82365900
C	3.62249200	-0.62162200	-1.26596200
H	3.08071800	-1.32791900	1.68297000
H	3.91386600	0.24283300	1.75391300
H	5.79003000	-0.55851800	0.50018400
H	5.32521600	-2.10958000	1.20645000
H	5.38180700	-1.89004000	-1.50688700
H	3.98918400	-2.69158000	-0.76673700
H	4.17490900	0.23068400	-1.67215300
H	2.84112600	-0.91597400	-1.96547800
O	2.96346400	-0.19089300	-0.03883000
C	-3.64514900	0.61307100	-1.25703100
O	-2.99855800	0.16463800	-0.02941200
C	-3.81018200	0.51049800	1.13619900
C	-5.08797300	1.12773900	0.56933600
C	-4.63523400	1.67230400	-0.79548600
H	-2.86105800	0.97619900	-1.91993200
H	-4.14030200	-0.24835000	-1.71453400
H	-3.97943900	-0.40202100	1.70911300
H	-3.22765300	1.21135500	1.73719600
H	-5.85761500	0.36256500	0.43758200
H	-5.49215800	1.90179300	1.22351200
H	-5.46100700	1.79923600	-1.49756200
H	-4.13399600	2.63730000	-0.68141200

D5

0 9

Fe	-1.43141800	0.02332400	0.62762500
Cl	3.47545300	1.42760300	-2.53259100
Cl	1.56883100	-2.07610000	-1.37096300
Fe	2.34757100	0.04264500	-1.19739700
Cl	-1.15149700	-0.84386700	2.66690100
Cl	0.26416300	1.26887000	-0.34400200
C	-2.97179600	2.61690500	1.17771300
C	-3.78411600	3.66016200	0.42240100

C	-3.38382600	3.38970200	-1.03605400
C	-3.28798300	1.86870000	-1.07914400
H	-1.95235600	2.95796200	1.37571500
H	-3.42415600	2.26738700	2.10531200
H	-4.85570900	3.49614800	0.56840100
H	-3.54963400	4.67499100	0.74757300
H	-4.10567700	3.77650500	-1.75731500
H	-2.41012300	3.83484400	-1.25407100
H	-4.24863100	1.39454000	-1.29616700
H	-2.53362100	1.49770600	-1.77226600
O	-2.89730100	1.47033000	0.27305800
C	2.86115500	0.34789900	1.96496300
O	3.35407100	0.05509400	0.62403400
C	4.72452100	-0.43075600	0.67362600
C	5.21260700	-0.08460700	2.07532600
C	3.92674600	-0.20411800	2.90769300
H	2.74884200	1.43185400	2.04492000
H	1.88579600	-0.12270800	2.08127200
H	4.70676800	-1.50997600	0.49556900
H	5.27390000	0.06065300	-0.12943800
H	6.00574200	-0.75402700	2.41343800
H	5.59691000	0.93901400	2.10339100
H	3.71921900	-1.25129800	3.14405500
H	3.97004200	0.35053200	3.84679900
C	-3.83801000	-1.83206200	0.23748400
O	-2.58148100	-1.38794500	-0.36719500
C	-2.07865600	-2.40960200	-1.29502600
C	-2.83567700	-3.67228600	-0.91685900
C	-4.20570200	-3.12151800	-0.49198200
H	-3.64981800	-1.99659600	1.30047700
H	-4.56616600	-1.02865500	0.11975500
H	-2.31456900	-2.07472200	-2.30907100
H	-0.99863600	-2.46497300	-1.17676900
H	-2.89711700	-4.37734800	-1.74744000
H	-2.34303700	-4.17337100	-0.07960000
H	-4.82216800	-2.90868300	-1.37021700
H	-4.76179300	-3.80593400	0.15085300

E1

0 10

Fe	0.78047300	0.63983900	0.77231800
Cl	-1.28799100	-2.52040000	-1.34699400
Cl	-3.94089400	-0.64245700	0.52496100
Fe	-1.83341400	-0.90763900	0.05304200

C	-0.35227600	0.92710500	-1.90290900
C	-0.96742300	0.84458900	-0.62937400
C	-1.43718000	2.06295300	-0.07644700
C	-1.27162800	3.28159000	-0.72989900
C	-0.64881400	3.32019100	-1.97567900
C	-0.18362900	2.14268900	-2.56102500
H	-0.00312700	0.01757600	-2.38166500
H	-1.93882900	2.05696600	0.88724500
H	-1.63409300	4.19515600	-0.27120100
H	-0.52453200	4.26760400	-2.48994800
H	0.29308900	2.17098400	-3.53583900
Cl	1.70390100	2.29408000	1.89764100
Cl	-0.49692800	-1.10585000	1.95525600
C	3.46699100	0.05653100	-0.52090400
C	4.22357300	-1.08430200	-1.18574400
C	3.78515800	-2.30183900	-0.35841600
C	2.31264100	-2.02139300	-0.08837400
H	3.98390600	0.45836700	0.35244900
H	3.20681000	0.87592900	-1.19132100
H	3.91427400	-1.19539900	-2.22861800
H	5.30233400	-0.92150600	-1.16759000
H	3.92537500	-3.24692500	-0.88516800
H	4.34607000	-2.35023800	0.57870400
H	1.65473100	-2.37315800	-0.88368000
H	1.95076400	-2.39422300	0.86772100
O	2.21346400	-0.54979300	-0.05781200

E2-ts

0 11

Fe	-1.73979800	0.39376900	-0.63302600
Cl	1.46319400	-2.32466100	1.68479700
Cl	2.49786400	-2.14736600	-1.95231800
Fe	1.20721500	-1.47667100	-0.32119400
C	0.05038900	1.13136100	0.73532600
C	0.86429600	0.56101000	-0.30509200
C	0.97110800	1.34904500	-1.49760100
C	0.49264300	2.64977100	-1.56775800
C	-0.18605200	3.22058400	-0.48433700
C	-0.41742300	2.44965900	0.65871400
H	-0.10500300	0.57126900	1.65370900
H	1.47367300	0.92868300	-2.36251100
H	0.61569500	3.21765600	-2.48391900
H	-0.56276100	4.23461500	-0.54523700
H	-0.96874700	2.87380600	1.49251200

Cl	-3.02605600	1.35867600	-2.15191000
Cl	-1.04682400	-1.93273900	-0.90009000
C	-3.80756800	0.91301800	1.67223500
C	-4.85092600	0.12513400	2.45224700
C	-5.28179000	-0.93832700	1.43110700
C	-3.97710800	-1.27891000	0.71671100
H	-4.25930800	1.66621700	1.02046700
H	-3.04480900	1.38070900	2.29570500
H	-4.39859200	-0.34172300	3.33159600
H	-5.67636400	0.75502200	2.78832800
H	-5.73196900	-1.81659400	1.89632900
H	-6.00615000	-0.51911900	0.72809400
H	-3.42896800	-2.09489500	1.18890000
H	-4.10032600	-1.49562700	-0.34336900
O	-3.14299900	-0.07560000	0.83614800
C	4.36077800	1.31809100	2.33853100
C	3.07198500	1.11193800	1.83723400
C	2.94271700	0.86015800	0.48723400
C	4.00289300	0.81644700	-0.39578500
C	5.28643300	1.02264000	0.12317100
C	5.46115700	1.27391200	1.48259400
H	4.50061500	1.50616000	3.39888300
H	2.21437400	1.13417000	2.50074000
H	3.86634300	0.61520900	-1.45207900
H	6.14424100	0.98267400	-0.54123400
H	6.45899800	1.43236300	1.87831300

THF

0 1

C	1.18271300	-0.46189100	0.00000000
O	0.00001400	-1.25780300	-0.00000100
C	-1.18270100	-0.46191500	0.00000000
C	-0.77314000	1.02613400	0.00000100
C	0.77311800	1.02614800	0.00000000
H	1.77637800	-0.71949400	0.88426100
H	1.77637800	-0.71949400	-0.88426100
H	-1.77636800	-0.71953300	-0.88425700
H	-1.77636800	-0.71953400	0.88425600
H	-1.16858900	1.54239400	-0.87687900
H	-1.16858900	1.54239300	0.87688100
H	1.16855400	1.54241900	-0.87687800
H	1.16855400	1.54241900	0.87688000

PhZn(THF)$_2$Cl

0 1

Zn	-0.04105700	0.16366800	0.57771100
Cl	-1.55635600	0.32691800	2.23752500
C	-1.41407400	-2.78307800	0.53354000
C	-0.05164900	-2.32741200	-1.36773600
C	-0.74366400	-4.08276200	0.10907500
H	-2.47151900	-2.75952400	0.24902500
H	-1.33431200	-2.54290900	1.59196100
C	-0.42829400	-3.81143300	-1.36957800
H	1.02222100	-2.16764400	-1.24946900
H	-0.39138600	-1.78997800	-2.25520300
H	0.17745600	-4.23927700	0.67799800
H	-1.38699900	-4.95216400	0.25827800
H	0.37550300	-4.43823000	-1.75997700
H	-1.31622900	-3.98501200	-1.98448600
C	-2.61424900	0.95458800	-1.09646800
C	-0.94609100	2.56449400	-1.19187200
C	-3.26984500	2.26398700	-0.61170500
H	-2.85581100	0.09299600	-0.47911700
H	-2.85658400	0.73663300	-2.14188300
C	-2.08647800	3.24802100	-0.44058200
H	-0.97187900	2.78225200	-2.26657500
H	0.05144000	2.78098900	-0.81101100
H	-3.99454900	2.62809100	-1.34334500
H	-3.79021600	2.11454500	0.33413100
H	-2.30140400	4.24277000	-0.83612700
H	-1.82989300	3.34912300	0.61520800
O	-0.71151000	-1.75014600	-0.20711500
O	-1.18370100	1.15352000	-1.00016400
C	1.86180300	0.43422900	0.23289600
C	2.35578400	0.60981100	-1.07071200
C	2.81373100	0.46886300	1.26529300
C	3.71260500	0.79983600	-1.33720300
H	1.66440100	0.60140000	-1.91165100
C	4.17340000	0.65792300	1.01796400
H	2.49285300	0.34761200	2.29741400
C	4.62865000	0.82328200	-0.28849500
H	4.05408700	0.93169100	-2.36069700
H	4.87831600	0.67843600	1.84476700
H	5.68618800	0.97147600	-0.48676200

$Zn(THF)_2Cl_2$

0 1

Zn	0.00010000	0.91048700	0.00053300

Cl	0.10984400	1.69609000	2.07170500
C	1.90258600	-1.34669100	1.01161400
C	2.64315000	-0.37682200	-1.05207300
C	3.40542600	-1.56566400	0.86810000
H	1.33994600	-2.28027500	0.91980300
H	1.61117100	-0.83470500	1.92824300
C	3.60953400	-1.48445300	-0.65200900
H	3.08352300	0.61687000	-0.93428400
H	2.23477100	-0.46202600	-2.05748600
H	3.95632700	-0.76657800	1.37158100
H	3.72547000	-2.51767400	1.29548600
H	4.63804100	-1.25396100	-0.93538300
H	3.33102600	-2.42873500	-1.12920800
C	-2.64428100	-0.37653400	1.05150400
C	-1.90394900	-1.34282300	-1.01396900
C	-3.60924500	-1.48532500	0.65128400
H	-3.08609000	0.61660600	0.93438300
H	-2.23534400	-0.46166300	2.05670900
C	-3.40627700	-1.56489700	-0.86907100
H	-1.33938600	-2.27548700	-0.92483200
H	-1.61463100	-0.82837100	-1.92987900
H	-3.32881100	-2.42954900	1.12749300
H	-4.63788200	-1.25674100	0.93571600
H	-3.72480600	-2.51720000	-1.29693500
H	-3.95927400	-0.76653900	-1.37139000
O	1.53182300	-0.49566600	-0.11300400
O	-1.53327300	-0.49354500	0.11203200
Cl	-0.10791000	1.69828400	-2.06997200

$[Zn(THF)_3Cl]^+$

1 1

Zn	0.00772100	-0.00273000	0.61737600
C	1.97372400	-1.37377500	-1.39810600
C	3.01328200	-0.25418400	0.47011300
C	3.33385900	-2.00184300	-1.12820500
H	1.96490100	-0.78311300	-2.31752100
H	1.14486600	-2.08051400	-1.41166100
C	4.08888700	-0.87314300	-0.41002700
H	2.90686100	-0.75804500	1.43199500
H	3.12685900	0.81683600	0.63649400
H	3.23279500	-2.87353100	-0.47666700
H	3.82459300	-2.32302500	-2.04771300
H	4.93200700	-1.23653700	0.17831500
H	4.47092800	-0.14424300	-1.12949900

C	-1.80259400	-2.42514700	0.52886400
C	-2.11759700	-1.05504200	-1.43273800
C	-2.83704300	-3.07310400	-0.37897300
H	-2.23191500	-2.02386400	1.44803900
H	-0.95630500	-3.06439000	0.77887400
C	-3.37188200	-1.88321300	-1.19005000
H	-1.55819000	-1.39711000	-2.30708500
H	-2.29201300	0.01754500	-1.50940600
H	-2.36932500	-3.81023600	-1.03672800
H	-3.61519400	-3.57968200	0.19275600
H	-3.84844300	-2.18487700	-2.12350200
H	-4.10130300	-1.31542800	-0.60669900
C	-1.27368900	2.73022600	0.49092200
C	0.18817700	2.39132000	-1.39900700
C	-1.29613800	3.96747000	-0.39446300
H	-0.77107400	2.89700300	1.44478900
H	-2.25255700	2.28751300	0.67378700
C	0.04897800	3.88320900	-1.13142700
H	-0.33373600	2.08393400	-2.30878300
H	1.21525800	2.02993700	-1.43024700
H	-2.12804400	3.92411500	-1.10219800
H	-1.40152100	4.88123500	0.19116000
H	0.06593700	4.46588700	-2.05324900
H	0.86189600	4.23788500	-0.49263400
O	1.75321700	-0.45227600	-0.27658800
O	-1.27821900	-1.28458600	-0.25123500
O	-0.47663700	1.74053300	-0.26356300
Cl	0.01214300	-0.01243600	2.78975100

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