Supporting Information

Transition Metal-Catalyzed and MAO-Assisted Olefin Polymerization. Cyclic Isomers of Sinn's Dimer Are Excellent Ligands in Iron Complexes and Great Methylating Reagents

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Table S1. Computed Energies of MAO Species

Molecule	E_{tot}	**TE**	S	S_{tr}	$S_{tr,W}$	S_W	ν_1	μ
Methane	-40.337043	30.89	44.44	34.26	25.08	35.26	1413.9	0.000
Water	-76.199244	15.27	45.13	34.61	25.27	35.79	1734.2	2.242
OMe_2	-154.515545	54.29	64.21	37.41	26.78	53.59	222.4	1.594
TMA, **1**	-361.228480	74.02	92.08	40.21	28.29	98.97	28.9	0.000
DMAH, **2**	-397.158987	59.37	92.62	40.26	28.32	95.25	1.3	1.658
MeAlO, **3**	-356.756670	27.65	66.34	38.09	27.15	55.40	158.4	6.308
Al_2OMe_4, **4**	-718.128741	104.00	127.71	40.50	28.45	115.60	21.6	0.000
5a	-1075.027255	133.89	166.11	41.60	29.04	153.55	14.6	0.081
5b	-1075.042973	133.50	133.85	41.60	29.04	121.29	33.8	1.445
5c	-1075.044494	133.41	127.77	41.60	29.04	115.21	76.9	2.892
TSRF(**5a**,**5b**)	-1075.024754	133.12	149.89	41.60	29.04	137.34	-51.6	1.079
TSMT(**5b**,**5c**)	-1075.042775	132.81	126.70	41.60	29.04	114.14	-61.9	1.672
ATS(**5c**)	-1075.010100	132.76	141.83	41.60	29.04	129.27	-31.1	4.951
$(MeAlO)_2$, **7**	-713.725766	57.70	100.70	40.16	28.26	88.81	6.2	0.000

Table S2. Computed Energies of Iron Pre-catalyst

Molecule	E_{tot}	VZPE	TE	S	ν_1	μ	U_0	U_{298}	G_{298}
$L(Me)_2FeCl_2$, C_{2v}	-2697.944566	122.65	132.25	124.32	32.10	6.58	-2697.749111	-2697.733812	-2697.792881
$[L(Me)_2FeCl]^+$, C_s	-2237.466193	122.25	130.72	114.79	45.70	7.13	-2237.271375	-2237.257878	-2237.312418
$L(Ph)_2FeCl_2$, C_2	-3081.420395	188.63	202.17	157.24	34.60	5.48	-3081.119794	-3081.098217	-3081.172927
$L(Ph)_2FeCl_2$, C_s	-3081.420358	188.64	202.18	157.94	30.70	5.55	-3081.119741	-3081.098164	-3081.173206
$[L(Ph)_2FeCl]^+$, C_s, I	-2620.952644	188.23	200.63	149.28	34.00	6.80	-2620.652681	-2620.632920	-2620.703848
$[L(Ph)_2FeCl]^+$, C_s, II	-2620.946946	187.73	200.30	154.87	6.92	7.32	-2620.647777	-2620.627754	-2620.701338
$[L(Ph)_2FeCl]^+$, C_1, III	-2620.951697	188.07	200.51	148.79	32.40	6.86	-2620.651989	-2620.632164	-2620.702859

Table S3. Vibration Modes Involving Bonding Between $[L(R)_2FeCl]^-$ and MAO Moieties

Mode Number	Mode name	Frequency	Infrared intensity	Raman activity
$L(Me)_2FeCl_{ax}(\mathbf{4})_{eq}$				
22	Cl−Fe	214.9	16.2	1.4
28	Fe−Cl, Al−Cl	295.9	21.5	3.6
40	Fe−O	500.9	25.0	5.7
$L(Ph)_2FeCl_{ax}(\mathbf{4})_{eq}$				
30	Cl−Al	253.7	29.3	2.5
34	Fe−Cl	304.1	11.2	5.2
46	Fe−O	536.9	36.0	14.9
$L(Me)_2FeCl_{ax}(\mathbf{7})_{eq}$				
21	Fe−Cl	271.6	17.5	0.8
23	Cl−Al	311.0	10.4	4.4
47	Fe−O	761.9	266.5	19.8
48	Fe−O	801.0	605.0	5.3
$L(Ph)_2FeCl_{ax}(\mathbf{7})_{eq}$				
17	Cl−Al	164.8	7.1	2.6
18	Fe−Cl	168.0	0.7	3.7
25	Cl−Al, Fe−Al	260.9	12.4	3.3
27	Fe−Cl	291.7	2.5	1.5
28	Cl−Al	316.5	16.2	8.2
30	Al−O	352.6	25.8	1.9
39	Fe−O	488.9	23.2	3.4
61	Fe−O	752.1	318.2	5.4
$L(Me)_2FeCl_{ax}(\mathbf{5b})_{eq}$				
26	Fe−Cl	201.8	7.4	1.1
34	Cl−Al	307.2	10.0	4.6
40	Cl−Al	392.0	14.6	5.8
42	Fe−O	413.9	8.4	2.8
44	Fe−Cl	463.1	25.2	2.5
47	Fe−O, Cl−Al	505.9	60.5	18.8
57	Fe−O	673.6	55.5	20.1
61	Fe−O	698.8	69.2	7.4
$L(Ph)_2FeCl_{ax}(\mathbf{5b})_{eq}$				
36	Fe−Cl	261.0	18.1	1.5
39	Al−Cl	306.5	7.8	4.9
44	Cl−Al	385.3	28.0	5.7
49	Fe−O	431.4	12.8	8.6
52	Cl−Al, Fe−O	498.4	51.1	8.5
69	Fe−O	676.0	26.1	13.9
71	Fe−O	694.8	76.1	3.0
73	Fe−O	701.1	28.7	3.7
91	Fe−O	875.6	321.0	3.3

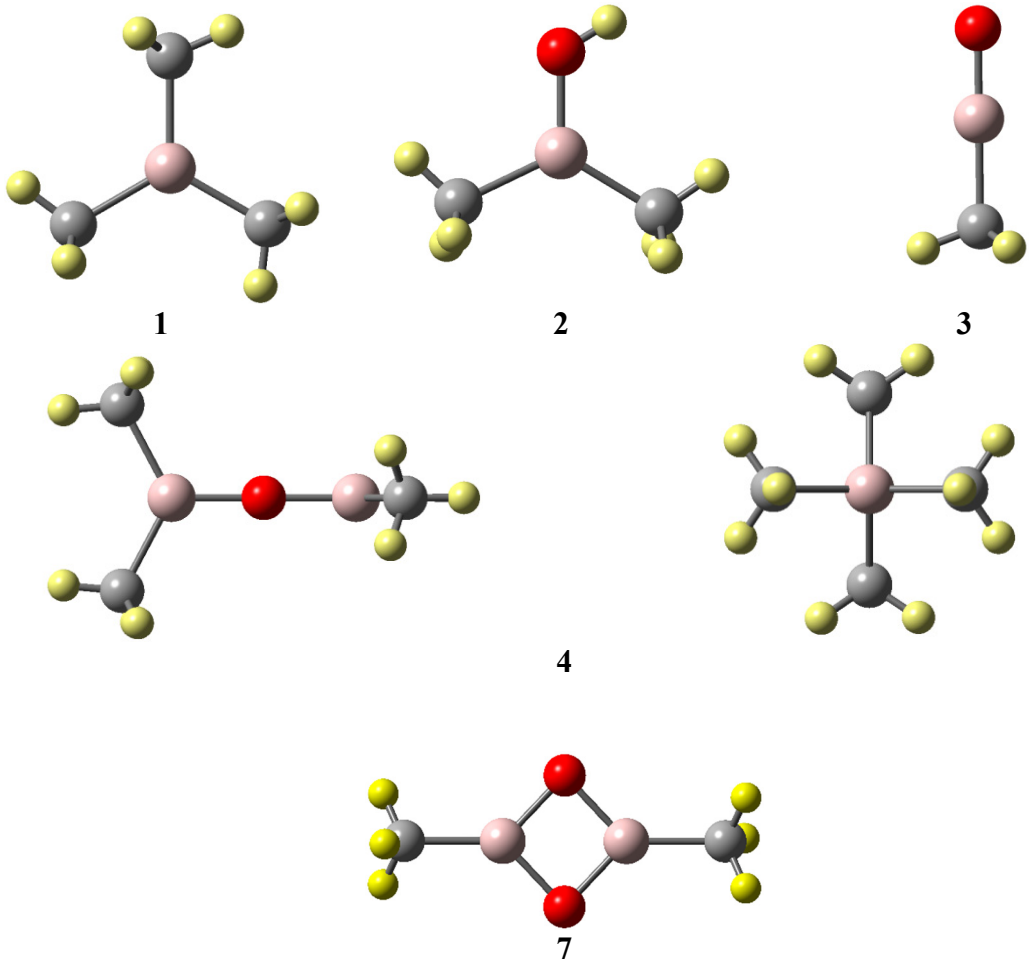


Figure S1. Computed structures of trimethylaluminum **1**, of dimethylaluminumhydroxide **2**, of methylaluminum oxide **3**, of permethyldialuminoxane **4**, and of cyclodialuminoxane **7**.

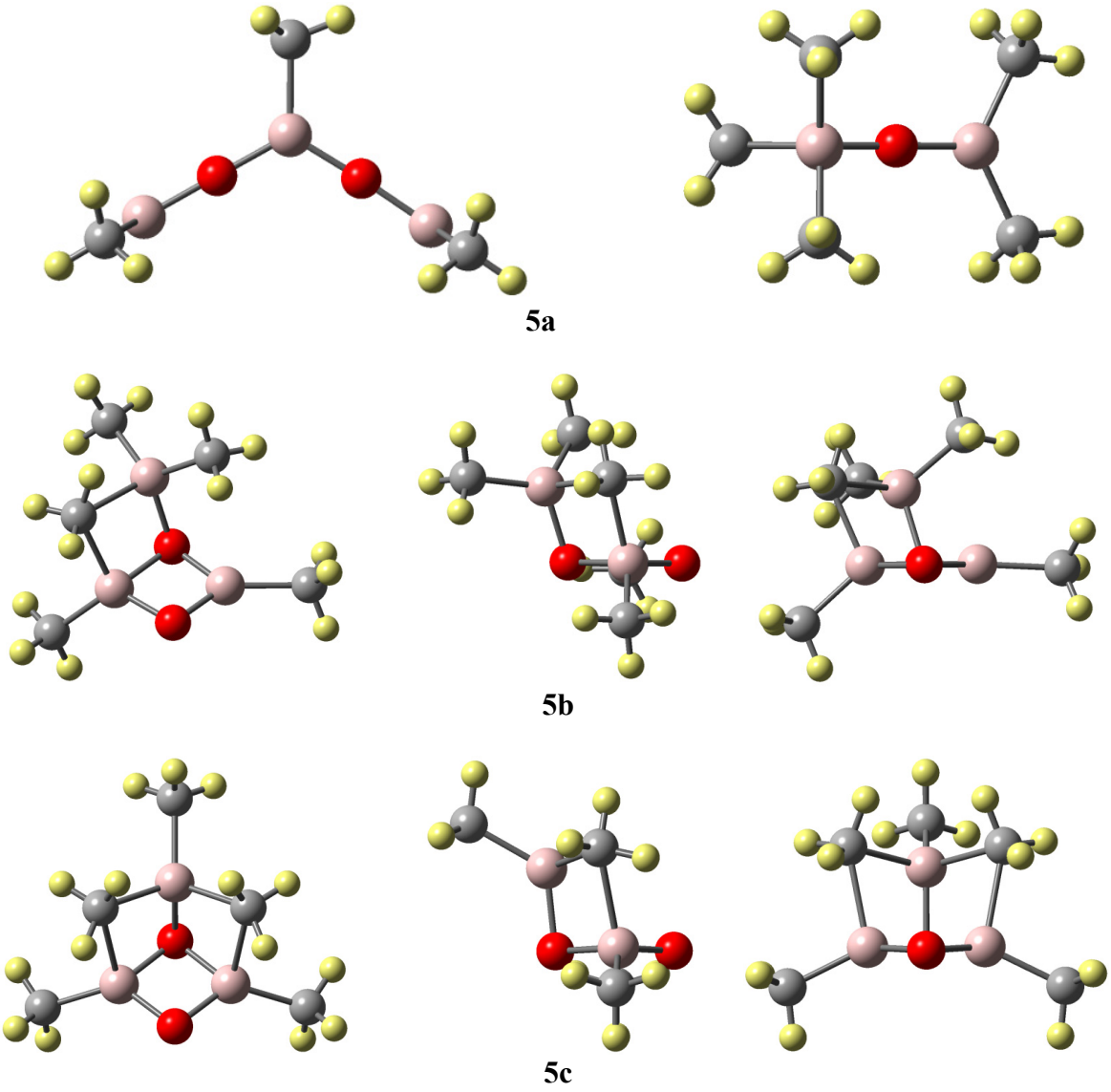
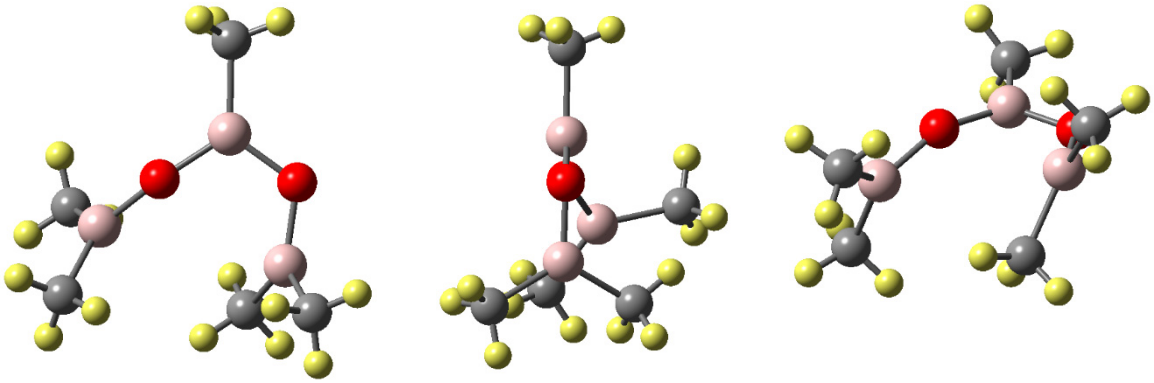
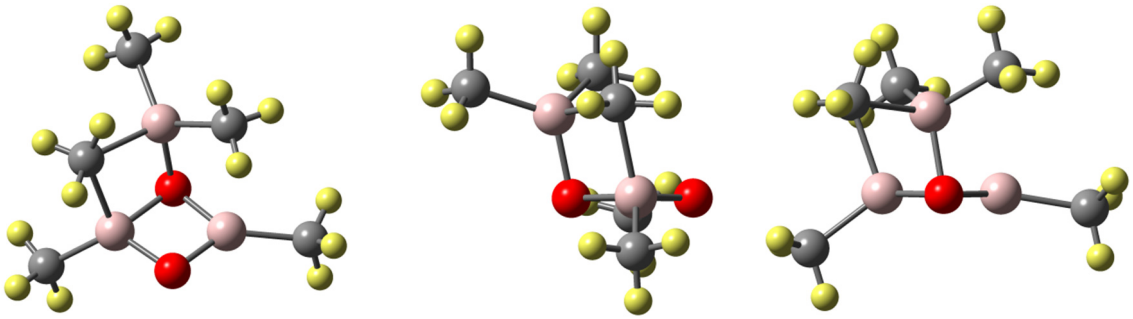


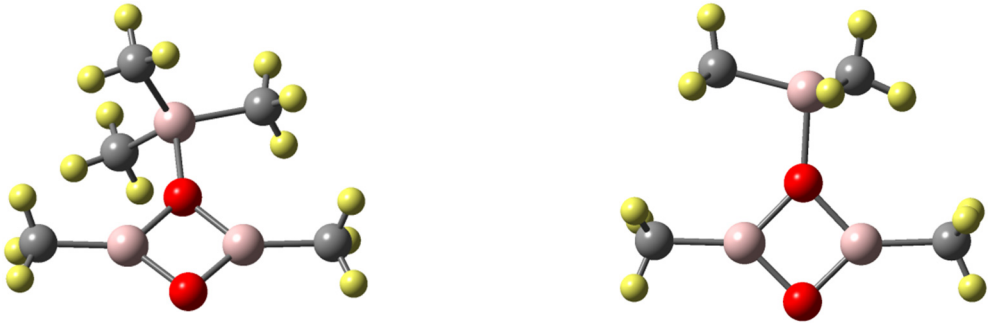
Figure S2. Computed structures of permethyltrialuminoxane **5**: Acyclic allene structure **5a**, cyclic, monobridged structure **5b**, and cyclic, dibridged structure **5c**.



TSRF(**5a**,**5b**)

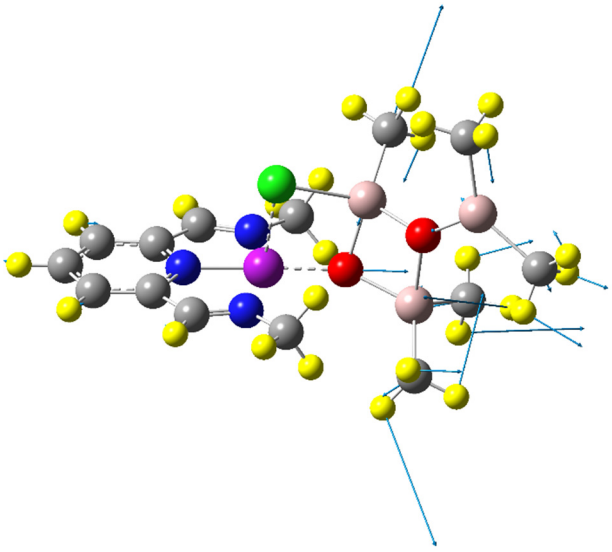


TSMT(**5b**,**5c**)

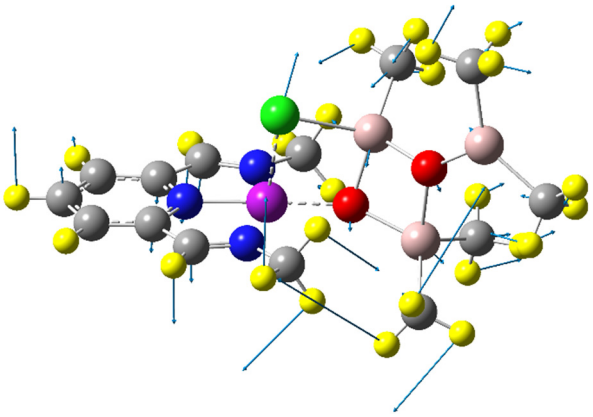


ATS(**5c**)

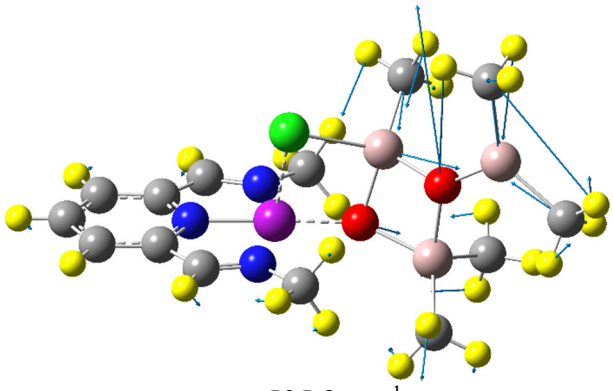
Figure S3. Computed structures of the transition state structures TSRF(**5a**,**5b**) for ring formation, of the transition state structure TSMT(**5b**,**5c**) for methyl transfer between **5b** and **5c**, and of the transition state structure ATS(**5c**) for automerization **5c** ⇄ **5c**.



ν_{61}= 698.8 cm^{-1}



ν_{26}= 201.8 cm^{-1}



ν_{47}= 505.9 cm^{-1}

Figure S4. Computed structure of $L(Me)_2FeCl_{ax}$(**5b**)$_{eq}$ with vibrational displacement vectors for modes ν_{61} (Fe−O bond), ν_{26} (Fe−Cl bond), and ν_{47} (Fe−O and Cl−Al bonds).

Cartesian Coordinates of Stationary Structures

MAO Species Calculated at MP2(full)/6-31G*

Trimethylaluminum (TMA), Me_3Al (de facto C_3), 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.000069	-0.000073	-0.000384
2	6	0	0.477963	1.910146	0.000130
3	1	0	0.061628	2.421647	0.875819
4	1	0	1.557134	2.087226	-0.000708
5	1	0	0.060254	2.422707	-0.874292
6	6	0	1.415494	-1.368878	0.000129
7	1	0	2.065785	-1.264791	0.876524
8	1	0	1.029622	-2.392158	-0.001989
9	1	0	2.068863	-1.262365	-0.873686
10	6	0	-1.893368	-0.541207	-0.000060
11	1	0	-2.131621	-1.144882	0.883518
12	1	0	-2.586257	0.304771	-0.014926
13	1	0	-2.125045	-1.171573	-0.866455

Dimethylaluminumhydroxide (DMAH), Me_2AlOH, 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.001104	0.045491	0.000199
2	8	0	-0.057981	1.773609	-0.001360
3	6	0	1.711977	-0.913670	0.000871
4	1	0	1.839706	-1.473796	-0.932168
5	1	0	2.584646	-0.263895	0.111441
6	1	0	1.745582	-1.650121	0.810897
7	6	0	-1.739016	-0.849663	-0.000833
8	1	0	-1.819734	-1.583681	-0.809130
9	1	0	-1.906852	-1.395779	0.933661
10	1	0	-2.556311	-0.133166	-0.115242
11	1	0	0.753403	2.300190	0.008607

Methylaluminumoxide, MeAlO (de facto C_{3v}), 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.188025	0.000304	0.000021
2	8	0	1.818507	-0.000269	-0.000018
3	6	0	-1.760432	-0.000085	-0.000017
4	1	0	-2.143573	1.022611	-0.019614
5	1	0	-2.143091	-0.528934	-0.875881
6	1	0	-2.143119	-0.494965	0.895470

$Me_2Al–O–AlMe_2$, *C_2*, Sinn-Monomer, Permethyldialuminoxane, 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000000	0.000000	-1.717991
2	13	0	0.000000	0.000000	1.718016
3	8	0	0.000000	0.000000	0.000012
4	6	0	1.732368	0.000632	2.637615
5	1	0	2.323346	0.881245	2.364300
6	1	0	1.632452	-0.005192	3.726733
7	1	0	2.329284	-0.873011	2.355135
8	6	0	0.000000	1.732349	-2.637629
9	1	0	0.017668	1.632455	-3.726622
10	1	0	-0.887045	2.318083	-2.373806
11	1	0	0.866951	2.334460	-2.345861
12	6	0	0.000000	-1.732349	-2.637629
13	1	0	-0.017668	-1.632455	-3.726622
14	1	0	0.887045	-2.318083	-2.373806
15	1	0	-0.866951	-2.334460	-2.345861
16	6	0	-1.732368	-0.000632	2.637615
17	1	0	-1.632452	0.005192	3.726733
18	1	0	-2.329284	0.873011	2.355135
19	1	0	-2.323346	-0.881245	2.364300

$Me_2Al–O–AlMe–O–AlMe_2$, Sinn-Dimer, Permethyltrialuminoxane, 5
Acyclic, 5a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.944640	-0.526462	0.000016
2	13	0	-2.930534	-0.546943	0.000019
3	13	0	0.001836	1.227717	-0.000015
4	8	0	1.491139	0.388770	0.000000
5	8	0	-1.462586	0.344449	0.000020
6	6	0	-0.051104	3.179344	-0.000119
7	1	0	0.948073	3.621242	0.000386
8	1	0	-0.584787	3.554868	-0.878669
9	1	0	-0.585748	3.554970	0.877799
10	6	0	3.723884	-1.012044	-1.732546
11	1	0	4.646483	-1.590991	-1.633562
12	1	0	3.022236	-1.605738	-2.328008
13	1	0	3.954544	-0.119947	-2.324448
14	6	0	3.723952	-1.011872	1.732596
15	1	0	4.646779	-1.590460	1.633632
16	1	0	3.954213	-0.119743	2.324602
17	1	0	3.022489	-1.605901	2.327944
18	6	0	-3.718040	-1.019993	1.732386
19	1	0	-3.959089	-0.122976	2.312762
20	1	0	-4.636461	-1.605532	1.633233
21	1	0	-3.016780	-1.602254	2.339339
22	6	0	-3.717959	-1.020121	-1.732351

23	1	0	-3.958945	-0.123149	-2.312823
24	1	0	-3.016683	-1.602461	-2.339210
25	1	0	-4.636404	-1.605622	-1.633198

Rotational constants (GHZ): 1.0297717 0.3181704 0.3009739
Standard basis: 6-31G(d) (6D, 7F)

Cyclic, Monobridged, 5b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.566125	1.360551	0.154272
2	13	0	0.778139	-1.313117	-0.083021
3	13	0	-1.754027	0.359317	-0.153344
4	8	0	-1.066050	1.581879	0.856720
5	8	0	-0.180885	-0.013632	-0.962094
6	6	0	-3.514228	-0.360981	-0.518292
7	1	0	-4.172926	0.402478	-0.942310
8	1	0	-3.464305	-1.194017	-1.223637
9	1	0	-3.982625	-0.721276	0.401855
10	6	0	1.625186	2.822622	-0.581201
11	1	0	2.496931	2.462675	-1.136430
12	1	0	1.026357	3.430331	-1.266834
13	1	0	1.992077	3.494343	0.202029
14	6	0	1.814901	0.109349	1.272172
15	1	0	2.846643	0.277057	0.949067
16	1	0	1.619650	0.814146	2.097423
17	1	0	1.806778	-0.841472	1.824436
18	6	0	-0.518283	-2.294865	1.052310
19	1	0	-1.273886	-2.829103	0.463228
20	1	0	-0.010540	-3.059487	1.652831
21	1	0	-1.056374	-1.668685	1.778041
22	6	0	2.236569	-2.168971	-1.068109
23	1	0	1.855061	-2.890733	-1.798411
24	1	0	2.833762	-1.437687	-1.622524
25	1	0	2.920940	-2.715247	-0.409843

Rotational constants (GHZ): 0.9441023 0.8246476 0.5421935
Standard basis: 6-31G(d) (6D, 7F)

Cyclic, Dibridged, 5c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.452753	-0.804067	1.273405
2	13	0	-0.762363	1.185811	0.000000
3	13	0	0.452753	-0.804067	-1.273405
4	8	0	1.630318	-1.093579	0.000000
5	8	0	-0.912089	-0.623934	0.000000
6	6	0	0.240537	-1.638355	-3.015960
7	1	0	0.040620	-2.708518	-2.904420
8	1	0	-0.589522	-1.207937	-3.584017
9	1	0	1.144149	-1.541438	-3.625982
10	6	0	0.240537	-1.638355	3.015960

11	1	0	-0.589522	-1.207937	3.584017
12	1	0	0.040620	-2.708518	2.904420
13	1	0	1.144149	-1.541438	3.625982
14	6	0	0.452753	1.414136	1.684402
15	1	0	-0.158945	1.625632	2.567820
16	1	0	1.406083	1.008837	2.058746
17	1	0	0.792415	2.386756	1.298176
18	6	0	0.452753	1.414136	-1.684402
19	1	0	-0.158945	1.625632	-2.567820
20	1	0	0.792415	2.386756	-1.298176
21	1	0	1.406083	1.008837	-2.058746
22	6	0	-2.250518	2.447113	0.000000
23	1	0	-2.886636	2.310307	-0.880468
24	1	0	-2.886636	2.310307	0.880468
25	1	0	-1.919395	3.490954	0.000000

TSRF(5a,5b)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.073454	-0.302520	-0.277417
2	13	0	-1.813911	-0.965592	0.380302
3	13	0	-0.632419	1.699885	-0.148178
4	8	0	0.695414	0.689101	-0.576718
5	8	0	-1.979421	0.766156	0.380829
6	6	0	-0.611242	3.641615	-0.275365
7	1	0	-0.239417	3.975398	-1.248246
8	1	0	-1.610117	4.059615	-0.129390
9	1	0	0.046628	4.076415	0.483652
10	6	0	2.376349	-1.829277	-1.466504
11	1	0	2.825764	-2.677292	-0.940228
12	1	0	1.454590	-2.176113	-1.942367
13	1	0	3.067632	-1.557197	-2.272827
14	6	0	3.257907	0.176698	1.209742
15	1	0	4.174366	-0.420460	1.224093
16	1	0	3.548028	1.231754	1.170832
17	1	0	2.756689	0.024413	2.172233
18	6	0	-0.558490	-1.823146	1.630214
19	1	0	-1.077668	-2.486725	2.331559
20	1	0	0.152895	-2.462887	1.091416
21	1	0	0.011781	-1.108690	2.232128
22	6	0	-2.903079	-2.011998	-0.866410
23	1	0	-3.911040	-1.598560	-0.966955
24	1	0	-2.455652	-1.996135	-1.867193
25	1	0	-2.993696	-3.061997	-0.572847

Rotational constants (GHZ): 0.7890599 0.6182381 0.4253710
Standard basis: 6-31G(d) (6D, 7F)

TSMT, TS(5b,5c)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	13	0	-0.839530	-1.255996	0.101194
2	13	0	-0.497539	1.389529	-0.073754
3	13	0	1.602939	-0.582866	-0.115754
4	8	0	0.709768	-1.699544	0.865045
5	8	0	0.120318	-0.051514	-1.029477
6	6	0	3.468117	-0.263514	-0.528144
7	1	0	3.884055	-1.089913	-1.112278
8	1	0	3.598973	0.653696	-1.107910
9	1	0	4.063650	-0.176307	0.384774
10	6	0	-2.161129	-2.511845	-0.583797
11	1	0	-2.967306	-2.010538	-1.128059
12	1	0	-1.694475	-3.224234	-1.271313
13	1	0	-2.622188	-3.097229	0.218454
14	6	0	-1.857589	0.248853	1.193637
15	1	0	-2.885727	0.322547	0.826186
16	1	0	-1.854216	-0.531691	1.972145
17	1	0	-1.679177	1.139227	1.814563
18	6	0	1.061345	1.891070	1.078533
19	1	0	1.855622	2.412462	0.531449
20	1	0	0.685113	2.614169	1.814719
21	1	0	1.544885	1.123890	1.702795
22	6	0	-1.601081	2.742833	-0.953372
23	1	0	-1.006813	3.363009	-1.632773
24	1	0	-2.396391	2.284845	-1.550405
25	1	0	-2.080978	3.421481	-0.239952

Rotational constants (GHZ): 0.9470907 0.8560931 0.5520116
Standard basis: 6-31G(d) (6D, 7F)

ATS(5c)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.079942	1.524084	-0.007159
2	13	0	1.762134	-0.403376	0.004471
3	13	0	-1.696318	-0.895579	-0.011580
4	8	0	-2.585775	0.620744	0.009370
5	8	0	-0.139698	-0.005635	-0.034318
6	6	0	-2.143785	-2.773189	-0.001928
7	1	0	-1.624536	-3.296746	-0.808637
8	1	0	-1.828596	-3.235850	0.937479
9	1	0	-3.219387	-2.924993	-0.117693
10	6	0	-0.525668	3.372861	-0.002221
11	1	0	0.160166	3.559505	0.828744
12	1	0	0.010153	3.612108	-0.925025
13	1	0	-1.377779	4.050083	0.089434
14	6	0	2.298820	0.389828	1.753323
15	1	0	2.114641	1.471298	1.810595
16	1	0	1.776648	-0.067817	2.603194
17	1	0	3.370296	0.258740	1.947626
18	6	0	1.744352	-2.395274	-0.092064
19	1	0	1.278335	-2.774339	-1.011164
20	1	0	2.760226	-2.808561	-0.078119
21	1	0	1.218780	-2.862584	0.751227
22	6	0	2.408178	0.556642	-1.618281

23	1	0	1.938814	0.189323	-2.539652
24	1	0	2.228776	1.639545	-1.577861
25	1	0	3.489505	0.437534	-1.758061

Rotational constants (GHZ): 0.8454027 0.7249727 0.4609456
Standard basis: 6-31G(d) (6D, 7F)

$(MeAlO)_2$, Cyclodialuminoxane, 7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000000	1.212085	0.000000
2	13	0	0.000000	-1.212085	0.000000
3	8	0	0.000000	0.000000	-1.286748
4	8	0	0.000000	0.000000	1.286748
5	6	0	-0.018824	3.153646	0.000000
6	1	0	0.477996	3.555094	0.886725
7	1	0	0.477996	3.555094	-0.886725
8	1	0	-1.045916	3.530749	0.000000
9	6	0	0.018824	-3.153646	0.000000
10	1	0	-0.477996	-3.555094	-0.886725
11	1	0	-0.477996	-3.555094	0.886725
12	1	0	1.045916	-3.530749	0.000000

Rotational constants (GHZ): 8.5281474 1.2724059 1.1225766
Standard basis: 6-31G(d) (6D, 7F)

Iron Complexes Calculated at B3LYP/6-31G*

$L(Me)_2FeCl_2$, C_{2v}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.774939	0.000067	0.000110
2	7	0	0.506709	1.935042	-0.000337
3	17	0	1.566283	0.000699	2.098195
4	7	0	-1.021149	-0.000001	0.000003
5	7	0	0.506891	-1.934989	0.000342
6	6	0	-0.741588	2.286444	-0.000555
7	6	0	-3.082798	1.211766	-0.000400
8	1	0	-3.609853	2.160616	-0.000744
9	6	0	-1.688585	-1.189093	0.000328
10	6	0	-1.688705	1.189028	-0.000358
11	6	0	-0.741396	-2.286431	0.000439
12	6	0	-3.780879	-0.000145	-0.000063
13	1	0	-4.865968	-0.000195	-0.000091
14	6	0	-3.082676	-1.211985	0.000327
15	1	0	-3.609625	-2.160893	0.000620
16	1	0	-1.059833	-3.328878	0.000513
17	1	0	-1.060082	3.328870	-0.000767
18	17	0	1.566445	-0.000672	-2.097950
19	6	0	1.556402	2.940343	-0.000415
20	1	0	2.177709	2.787131	-0.888297

21	1	0	1.151739	3.959310	-0.000343
22	1	0	2.177946	2.787062	0.887283
23	6	0	1.556570	-2.940303	-0.000078
24	1	0	2.178580	-2.786861	0.887270
25	1	0	1.151903	-3.959254	0.000400
26	1	0	2.177461	-2.787191	-0.888277

Rotational constants (GHZ): 0.5537204 0.4389644 0.3504898
Standard basis: 6-31G(d) (6D, 7F)

[L(Me)$_2$FeCl]$^+$, C_s

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.885599	-0.000005	-0.379101
2	7	0	-0.606349	1.954988	-0.351570
3	17	0	-2.419063	0.000000	1.137972
4	7	0	0.937122	0.000001	-0.075791
5	7	0	-0.606341	-1.954990	-0.351565
6	6	0	0.621652	2.292553	-0.132296
7	6	0	2.953269	1.217446	0.243064
8	1	0	3.478471	2.162987	0.326176
9	6	0	1.576415	-1.183474	0.020588
10	6	0	1.576410	1.183479	0.020584
11	6	0	0.621661	-2.292551	-0.132291
12	6	0	3.635881	0.000008	0.356270
13	1	0	4.706774	0.000010	0.531603
14	6	0	2.953274	-1.217434	0.243067
15	1	0	3.478481	-2.162973	0.326180
16	1	0	0.940444	-3.331450	-0.048939
17	1	0	0.940430	3.331453	-0.048944
18	6	0	-1.635761	2.984234	-0.479346
19	6	0	-1.635747	-2.984241	-0.479349
20	1	0	-2.127998	-2.874799	-1.451576
21	1	0	-2.385565	2.811481	0.297986
22	1	0	-1.220590	-3.992462	-0.388538
23	1	0	-2.385552	-2.811497	0.297985
24	1	0	-1.220609	3.992457	-0.388529
25	1	0	-2.128011	2.874796	-1.451574

Rotational constants (GHZ): 0.7394821 0.5523166 0.3469014
Standard basis: 6-31G(d) (6D, 7F)

L(Ph)$_2$FeCl$_2$, C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000126	0.047030	0.001315
2	7	0	-1.958878	0.315983	-0.170750
3	17	0	0.270044	-0.612602	-2.129522
4	7	0	0.000069	1.840653	0.000684
5	7	0	1.959061	0.316149	0.170877
6	6	0	-2.790651	-1.862437	-0.854387
7	6	0	-2.281935	1.579506	-0.208922

8	6	0	-1.204055	3.904550	-0.124870
9	1	0	-2.148885	4.429817	-0.221706
10	6	0	1.181763	2.508959	0.118799
11	6	0	-2.981959	-0.669476	-0.143982
12	6	0	2.981886	-0.669485	0.143257
13	6	0	-1.181557	2.508887	-0.118578
14	6	0	2.282239	1.579674	0.208569
15	6	0	-4.154634	-0.479576	0.603343
16	6	0	4.154092	-0.479792	-0.604767
17	6	0	0.000126	4.603368	-0.000845
18	1	0	0.000108	5.688445	-0.001409
19	6	0	-5.138937	-1.465062	0.613317
20	1	0	-6.037753	-1.318474	1.205826
21	6	0	1.204272	3.904667	0.123711
22	1	0	2.149168	4.429966	0.219740
23	6	0	-3.786289	-2.836482	-0.844236
24	1	0	-3.639631	-3.752775	-1.409044
25	6	0	5.138177	-1.465521	-0.615462
26	1	0	6.036638	-1.319073	-1.208542
27	6	0	2.790864	-1.862406	0.853871
28	6	0	-4.961809	-2.643156	-0.115126
29	6	0	4.961275	-2.643609	0.113001
30	1	0	5.728994	-3.412196	0.100324
31	6	0	3.786204	-2.836700	0.842949
32	1	0	3.639715	-3.752965	1.407839
33	1	0	1.883189	-1.993268	1.432799
34	1	0	4.268846	0.412335	-1.213045
35	1	0	3.313134	1.916707	0.297859
36	1	0	-4.269475	0.412525	1.211632
37	1	0	-5.729720	-3.411568	-0.103098
38	1	0	-1.882580	-1.993523	-1.432617
39	1	0	-3.312696	1.916592	-0.299603
40	17	0	-0.269956	-0.613296	2.131600

Rotational constants (GHZ): 0.2591002 0.1523043 0.1124670
Standard basis: 6-31G(d) (6D, 7F)

L(Ph)$_2$FeCl$_2$, *C*$_s$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.000042	0.053592	0.118585
2	7	0	1.963849	0.321246	0.060327
3	17	0	0.000199	-0.415840	2.324859
4	7	0	-0.000022	1.846214	0.052075
5	7	0	-1.963928	0.321404	0.060296
6	6	0	2.869382	-1.832032	0.727458
7	6	0	2.291002	1.584059	0.032941
8	6	0	1.210671	3.910078	0.020027
9	1	0	2.160430	4.435310	0.011220
10	6	0	-1.187762	2.514625	0.038244
11	6	0	2.976986	-0.668761	-0.046426
12	6	0	-2.977024	-0.668659	-0.046408
13	6	0	1.187767	2.514510	0.038225
14	6	0	-2.291058	1.584195	0.032910

15	6	0	4.054674	-0.512283	-0.930822
16	6	0	-4.054465	-0.512465	-0.931135
17	6	0	0.000109	4.608823	0.012229
18	1	0	0.000134	5.693810	-0.001717
19	6	0	5.031153	-1.502075	-1.017232
20	1	0	5.855219	-1.382391	-1.715082
21	6	0	-1.210537	3.910167	0.020051
22	1	0	-2.160233	4.435512	0.011290
23	6	0	3.857285	-2.809830	0.640379
24	1	0	3.777677	-3.703094	1.253436
25	6	0	-5.030918	-1.502301	-1.017493
26	1	0	-5.854795	-1.382850	-1.715604
27	6	0	-2.869594	-1.831662	0.727901
28	6	0	4.939805	-2.650151	-0.227946
29	6	0	-4.939764	-2.650105	-0.227800
30	1	0	-5.700748	-3.422159	-0.299162
31	6	0	-3.857476	-2.809488	0.640875
32	1	0	-3.778053	-3.702546	1.254257
33	1	0	-2.034507	-1.935831	1.412003
34	1	0	-4.097218	0.355760	-1.581901
35	1	0	-3.326278	1.918756	0.004993
36	1	0	4.097603	0.356117	-1.581342
37	1	0	5.700830	-3.422158	-0.299369
38	1	0	2.034137	-1.936420	1.411330
39	1	0	3.326230	1.918593	0.005155
40	17	0	-0.000201	-0.825435	-1.935298

Rotational constants (GHZ): 0.2558028 0.1529561 0.1132552
Standard basis: 6-31G(d) (6D, 7F)

[L(Ph)$_2$FeCl]$^+$, disrot. I, C_s

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000000	-0.283216	-0.619730
2	7	0	-1.755874	-0.370641	0.182598
3	17	0	-0.000002	0.942776	-2.357838
4	7	0	0.000000	-2.031724	-0.087695
5	7	0	1.755873	-0.370641	0.182598
6	6	0	-2.209735	-1.605178	0.256978
7	6	0	-1.216911	-3.978482	0.532961
8	1	0	-2.159061	-4.477506	0.734286
9	6	0	1.186216	-2.622689	0.191893
10	6	0	-1.186216	-2.622689	0.191894
11	6	0	2.209734	-1.605179	0.256976
12	6	0	0.000000	-4.660763	0.657750
13	1	0	0.000000	-5.713402	0.919951
14	6	0	1.216911	-3.978482	0.532960
15	1	0	2.159061	-4.477506	0.734283
16	1	0	3.259458	-1.822840	0.433419
17	1	0	-3.259458	-1.822841	0.433424
18	6	0	-2.638332	0.742489	0.289805
19	6	0	-2.187839	1.875465	0.978800
20	6	0	-3.919622	0.720757	-0.280055
21	6	0	-3.032134	2.971730	1.127642

22	1	0	-1.194537	1.879169	1.416767
23	6	0	-4.752090	1.827586	-0.134787
24	1	0	-4.243820	-0.132571	-0.868345
25	6	0	-4.314298	2.950328	0.572187
26	1	0	-2.688723	3.844448	1.674138
27	1	0	-5.738595	1.818066	-0.587593
28	1	0	-4.965936	3.811986	0.678396
29	6	0	2.638332	0.742487	0.289806
30	6	0	2.187845	1.875459	0.978813
31	6	0	3.919617	0.720759	-0.280064
32	6	0	3.032142	2.971723	1.127655
33	1	0	1.194547	1.879160	1.416789
34	6	0	4.752087	1.827586	-0.134797
35	1	0	4.243810	-0.132566	-0.868362
36	6	0	4.314301	2.950324	0.572188
37	1	0	2.688736	3.844437	1.674159
38	1	0	5.738588	1.818069	-0.587611
39	1	0	4.965940	3.811981	0.678397

Rotational constants (GHZ): 0.2476709 0.1910491 0.1244089
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl]^+$, disrot. II, C_s

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.000123	0.018748	0.077896
2	7	0	1.961725	0.274338	-0.089669
3	17	0	-0.000051	-0.389165	2.212889
4	7	0	0.000136	1.837653	-0.110924
5	7	0	-1.961582	0.274370	-0.090039
6	6	0	2.686405	-1.981609	0.381028
7	6	0	2.292892	1.535126	-0.120740
8	6	0	1.216114	3.882037	-0.094911
9	1	0	2.162138	4.412782	-0.087806
10	6	0	-1.185457	2.485097	-0.102605
11	6	0	2.929264	-0.749886	-0.247899
12	6	0	-2.929323	-0.749741	-0.248078
13	6	0	1.185765	2.485056	-0.102162
14	6	0	-2.292625	1.535177	-0.121319
15	6	0	4.078768	-0.575374	-1.038841
16	6	0	-2.686624	-1.981386	0.381035
17	6	0	0.000184	4.574102	-0.090748
18	1	0	0.000192	5.659133	-0.082217
19	6	0	4.986821	-1.620515	-1.170621
20	1	0	5.867454	-1.490064	-1.791935
21	6	0	-1.215777	3.882068	-0.095407
22	1	0	-2.161779	4.412856	-0.088735
23	6	0	3.609051	-3.016208	0.249843
24	1	0	3.430848	-3.959775	0.756053
25	6	0	-3.609473	-3.015844	0.250125
26	1	0	-3.431378	-3.959360	0.756469
27	6	0	-4.078888	-0.575150	-1.038908
28	6	0	4.758862	-2.839470	-0.522853
29	6	0	-4.759354	-2.839027	-0.522445

30	1	0	-5.472412	-3.650595	-0.629823
31	6	0	-4.987167	-1.620135	-1.170386
32	1	0	-5.867846	-1.489619	-1.791621
33	1	0	-4.237470	0.351397	-1.582663
34	1	0	-1.814335	-2.093628	1.016227
35	1	0	-3.326825	1.869305	-0.166333
36	1	0	4.237441	0.351267	-1.582415
37	1	0	5.471760	-3.651147	-0.630471
38	1	0	1.814165	-2.093778	1.016302
39	1	0	3.327129	1.869161	-0.165650

Rotational constants (GHZ): 0.2697574 0.1671828 0.1154883
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl]^+$, conrot., III , C_1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.004115	0.028981	-0.002811
2	7	0	1.958696	0.299383	-0.250667
3	17	0	0.200577	-0.521416	2.085986
4	7	0	-0.008717	1.853672	-0.163721
5	7	0	-1.963575	0.284739	-0.018507
6	6	0	4.244579	-0.580403	0.142901
7	6	0	2.283201	1.558824	-0.309597
8	6	0	1.199106	3.901174	-0.245140
9	1	0	2.141587	4.434728	-0.306376
10	6	0	-1.192648	2.498134	-0.079917
11	6	0	2.922286	-0.735123	-0.301392
12	6	0	-2.947303	-0.733224	-0.117347
13	6	0	1.172645	2.504846	-0.238050
14	6	0	-2.296783	1.545719	-0.025662
15	6	0	2.491776	-1.968430	-0.811020
16	6	0	-2.694656	-1.958526	0.520578
17	6	0	-0.016412	4.590426	-0.162130
18	1	0	-0.018995	5.675503	-0.161792
19	6	0	3.385845	-3.027552	-0.924522
20	1	0	3.051997	-3.975340	-1.334615
21	6	0	-1.227138	3.895455	-0.078617
22	1	0	-2.172308	4.423604	-0.012126
23	6	0	5.128490	-1.650297	0.042831
24	1	0	6.147302	-1.537713	0.400147
25	6	0	-3.639480	-2.979027	0.447530
26	1	0	-3.453547	-3.916997	0.961385
27	6	0	-4.128682	-0.552482	-0.858922
28	6	0	4.706451	-2.869851	-0.496733
29	6	0	-4.820180	-2.796189	-0.275699
30	1	0	-5.549787	-3.597781	-0.337450
31	6	0	-5.058128	-1.584416	-0.933106
32	1	0	-5.963517	-1.449433	-1.516749
33	1	0	-4.296377	0.368430	-1.409609
34	1	0	-1.795737	-2.076195	1.116110
35	1	0	-3.332346	1.877777	-0.000845
36	1	0	1.462171	-2.082757	-1.143734
37	1	0	5.402125	-3.700225	-0.567129

38	1	0	4.568242	0.348138	0.602770
39	1	0	3.309725	1.899915	-0.424310

Rotational constants (GHZ): 0.2750528 0.1681839 0.1145757
Standard basis: 6-31G(d) (6D, 7F)

Active Catalysts, Iron-MAO Adducts

$[L(Me)_2FeCl_{ax}(\mathbf{4})_{eq}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.196149	-0.033089	0.257255
2	7	0	-0.537726	-2.003129	0.072849
3	17	0	0.072971	0.186466	-2.078274
4	7	0	-2.068849	-0.010583	0.142455
5	7	0	-0.511108	1.937861	0.446752
6	6	0	-1.786903	-2.292618	-0.089896
7	6	0	-4.106991	-1.175994	-0.271874
8	1	0	-4.634750	-2.107718	-0.446637
9	6	0	-2.708440	1.176537	0.147666
10	6	0	-2.724393	-1.168371	-0.075690
11	6	0	-1.755964	2.270351	0.345179
12	6	0	-4.788366	0.045190	-0.248431
13	1	0	-5.862558	0.067048	-0.399636
14	6	0	-4.090445	1.239504	-0.041707
15	1	0	-4.605589	2.194410	-0.036972
16	8	0	1.808418	-0.035086	0.217392
17	6	0	0.245210	-0.258142	2.689732
18	1	0	0.141380	0.569684	3.402696
19	1	0	-0.698525	-0.214833	2.105283
20	1	0	0.142694	-1.189883	3.260928
21	6	0	3.145552	1.950414	-1.876005
22	1	0	3.749771	2.337482	-1.043218
23	1	0	3.814355	1.907326	-2.745615
24	1	0	2.389896	2.711417	-2.110522
25	1	0	-2.089349	3.307494	0.389800
26	1	0	-2.134721	-3.314319	-0.244924
27	13	0	2.075445	-0.200696	1.906725
28	13	0	2.394154	0.163880	-1.513946
29	6	0	3.211521	-1.452204	-2.281452
30	1	0	2.578803	-2.348449	-2.286753
31	1	0	3.485072	-1.264142	-3.328492
32	1	0	4.144347	-1.720147	-1.765119
33	6	0	3.761947	-0.330183	2.864765
34	1	0	4.111918	-1.370234	2.903636
35	1	0	4.549719	0.253651	2.374849
36	1	0	3.674846	0.018707	3.900258
37	6	0	0.484596	2.990149	0.630502
38	1	0	0.034098	3.987787	0.626507
39	1	0	0.996190	2.838499	1.587722
40	1	0	1.228139	2.916560	-0.166528
41	6	0	0.441997	-3.085334	0.047619
42	1	0	1.188741	-2.865791	-0.718821
43	1	0	0.952546	-3.133777	1.016114
44	1	0	-0.021944	-4.055945	-0.154636

Rotational constants (GHZ): 0.3509934 0.1895342 0.1881838

Standard basis: 6-31G(d) (6D, 7F)

$[L(Me)_2FeCl_{eq}(\mathbf{4})_{ax}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.148937	-0.917759	0.266990
2	7	0	-0.530692	-0.345193	2.146935
3	17	0	1.830842	-2.085275	0.679962
4	7	0	-1.890541	-0.304810	0.035561
5	7	0	-0.425338	-1.471637	-1.638798
6	6	0	-1.715313	0.152157	2.296458
7	6	0	-3.895848	0.576555	0.983494
8	1	0	-4.432481	0.970144	1.840437
9	6	0	-2.496381	-0.481717	-1.159153
10	6	0	-2.562204	0.182093	1.101790
11	6	0	-1.590326	-1.147611	-2.097854
12	6	0	-4.523026	0.440238	-0.259424
13	1	0	-5.558445	0.741953	-0.378148
14	6	0	-3.827538	-0.104510	-1.344472
15	1	0	-4.311346	-0.243863	-2.305641
16	8	0	0.926579	0.641358	-0.182797
17	6	0	2.202617	3.373192	-1.098515
18	1	0	2.625585	3.886281	-0.224164
19	1	0	3.010795	2.786469	-1.548918
20	1	0	1.925293	4.156593	-1.815377
21	6	0	3.595362	-0.250496	-1.737034
22	1	0	4.550368	0.291366	-1.755512
23	1	0	3.839624	-1.307492	-1.904481
24	1	0	3.028223	0.095634	-2.611965
25	1	0	-1.904704	-1.382385	-3.115287
26	1	0	-2.085658	0.503373	3.260143
27	13	0	0.626090	2.326783	-0.601833
28	13	0	2.685504	0.036196	-0.011236
29	6	0	3.614949	0.827093	1.533645
30	1	0	2.967574	1.224768	2.326281
31	1	0	4.278410	0.090258	2.005618
32	1	0	4.257115	1.657503	1.210468
33	6	0	-1.199448	3.040699	-0.519172
34	1	0	-1.917035	2.486638	-1.136429
35	1	0	-1.595840	3.051506	0.504462
36	1	0	-1.205235	4.078901	-0.872078
37	6	0	0.505152	-2.186495	-2.511731
38	1	0	0.072672	-2.374218	-3.499682
39	1	0	1.420651	-1.598232	-2.611706
40	1	0	0.776387	-3.133841	-2.037326
41	6	0	0.344991	-0.453316	3.313084
42	1	0	1.275726	0.080793	3.107731
43	1	0	-0.126896	-0.050667	4.214972
44	1	0	0.601993	-1.505486	3.465220

Rotational constants (GHZ): 0.3244497 0.1993401 0.1914118

Standard basis: 6-31G(d) (6D, 7F)

$[L(Me)_2FeCl_{ax}(7)_{eq}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.247028	-0.016463	-0.349585
2	7	0	-0.781920	1.794831	-0.989994
3	17	0	0.226437	0.555337	1.869272
4	7	0	-2.099910	-0.174361	-0.171668
5	7	0	-0.369039	-1.953948	0.204751
6	6	0	-2.058866	2.000585	-0.949019
7	6	0	-4.264221	0.822225	-0.311518
8	1	0	-4.886781	1.680989	-0.540095
9	6	0	-2.632951	-1.342803	0.243852
10	6	0	-2.878078	0.891697	-0.459370
11	6	0	-1.580078	-2.332885	0.459765
12	6	0	-4.828107	-0.377883	0.134876
13	1	0	-5.902908	-0.455930	0.260567
14	6	0	-4.012250	-1.479035	0.413128
15	1	0	-4.436639	-2.418332	0.752082
16	8	0	1.626630	0.184035	-0.728525
17	13	0	3.051887	-0.903004	-0.648741
18	8	0	3.506704	-0.317864	0.904433
19	6	0	3.715387	-2.171094	-1.958963
20	1	0	2.946893	-2.485246	-2.673742
21	1	0	4.531560	-1.719476	-2.536487
22	1	0	4.125664	-3.064030	-1.473849
23	13	0	2.296626	0.969252	0.884495
24	6	0	2.746297	2.847822	1.153142
25	1	0	1.885175	3.502465	1.328075
26	1	0	3.394882	2.932194	2.034726
27	1	0	3.317413	3.253267	0.308189
28	1	0	-1.813012	-3.332119	0.828576
29	1	0	-2.511267	2.934894	-1.282168
30	6	0	0.088821	2.843057	-1.520607
31	1	0	-0.485900	3.680671	-1.928092
32	1	0	0.741672	3.203372	-0.721023
33	1	0	0.724582	2.411145	-2.297275
34	6	0	0.717797	-2.899142	0.451683
35	1	0	1.234450	-3.112918	-0.491527
36	1	0	1.424617	-2.449663	1.158801
37	1	0	0.359127	-3.845505	0.869324

Rotational constants (GHZ): 0.4289178 0.2070700 0.1727672
Standard basis: 6-31G(d) (6D, 7F)

$[L(Me)_2FeCl_{eq}(7)_{ax}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.061419	0.506797	0.699769
2	7	0	-0.305304	2.328528	-0.088365
3	17	0	2.128451	0.732464	1.610955
4	7	0	-1.819011	0.339818	0.148061

5	7	0	-0.461698	-1.291310	1.493361
6	6	0	-1.459900	2.480613	-0.648496
7	6	0	-3.698763	1.242525	-1.007179
8	1	0	-4.155252	2.054588	-1.563423
9	6	0	-2.495463	-0.794969	0.431489
10	6	0	-2.387114	1.351088	-0.542185
11	6	0	-1.667360	-1.694922	1.235380
12	6	0	-4.408423	0.067694	-0.734631
13	1	0	-5.429446	-0.039818	-1.085515
14	6	0	-3.811944	-0.964277	-0.002453
15	1	0	-4.356647	-1.874073	0.227581
16	8	0	0.762887	-0.158594	-0.900550
17	13	0	1.080422	-1.892115	-1.247211
18	8	0	2.722535	-1.761401	-0.756372
19	6	0	-0.099860	-3.275135	-1.929586
20	1	0	-1.137445	-2.937469	-2.022739
21	1	0	0.234795	-3.591579	-2.925016
22	1	0	-0.078756	-4.167337	-1.292885
23	13	0	2.626531	-0.004832	-0.542001
24	6	0	3.838309	1.259251	-1.396267
25	1	0	3.736436	2.292859	-1.047567
26	1	0	4.873936	0.955683	-1.196351
27	1	0	3.713736	1.257048	-2.486275
28	1	0	-2.060544	-2.639476	1.612816
29	1	0	-1.748150	3.401582	-1.156009
30	6	0	0.658163	3.426529	-0.135868
31	1	0	1.540881	3.096926	-0.691381
32	1	0	0.237787	4.317851	-0.612095
33	1	0	0.978613	3.665570	0.882183
34	6	0	0.397857	-2.117151	2.348752
35	1	0	0.655290	-1.545670	3.245452
36	1	0	-0.092572	-3.052810	2.635118
37	1	0	1.335877	-2.328930	1.825886

Rotational constants (GHZ): 0.3662699 0.2403827 0.1967072
Standard basis: 6-31G(d) (6D, 7F)

$[L(Me)_2FeCl_{ax}(\mathbf{5})_{eq}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.210086	0.008713	-0.374490
2	7	0	-1.864652	1.879669	-0.673575
3	17	0	-0.440927	0.187577	1.858425
4	7	0	-3.035899	-0.243308	-0.019079
5	7	0	-1.242133	-1.997162	-0.116471
6	6	0	-3.134229	2.021680	-0.469216
7	6	0	-5.224485	0.681524	0.220671
8	1	0	-5.885597	1.541318	0.189991
9	6	0	-3.497651	-1.478810	0.262956
10	6	0	-3.864413	0.822647	-0.059144
11	6	0	-2.408068	-2.451678	0.207440
12	6	0	-5.711253	-0.591478	0.535592
13	1	0	-6.764126	-0.727648	0.759417
14	6	0	-4.846824	-1.690405	0.553247

15	1	0	-5.211610	-2.685878	0.783905
16	8	0	0.592594	0.415204	-0.900757
17	13	0	2.204759	-0.193531	-1.617269
18	8	0	2.795972	-0.036677	0.244750
19	6	0	2.364188	-2.031031	-2.326960
20	1	0	1.514432	-2.333488	-2.955806
21	1	0	3.243133	-2.065430	-2.985194
22	1	0	2.509727	-2.816786	-1.575118
23	13	0	1.350397	0.991157	0.631709
24	6	0	1.741513	2.780592	1.307131
25	1	0	0.851409	3.339049	1.618813
26	1	0	2.388132	2.714944	2.192461
27	1	0	2.279176	3.386760	0.567048
28	1	0	-2.579239	-3.502864	0.440933
29	1	0	-3.648372	2.970920	-0.622679
30	6	0	-1.095691	3.026934	-1.156304
31	1	0	-1.744235	3.873416	-1.403183
32	1	0	-0.380947	3.330334	-0.386553
33	1	0	-0.522587	2.721407	-2.034487
34	6	0	-0.121943	-2.931452	-0.148043
35	1	0	0.268582	-2.988854	-1.165439
36	1	0	0.674556	-2.543128	0.492200
37	1	0	-0.413431	-3.929953	0.193925
38	13	0	4.347293	-0.404531	1.018638
39	6	0	3.036229	1.271114	-2.646224
40	1	0	2.572264	1.372329	-3.637759
41	1	0	2.962684	2.256435	-2.165661
42	1	0	4.103915	1.087280	-2.830058
43	6	0	5.718879	-1.153203	-0.152228
44	1	0	5.340267	-1.991193	-0.750762
45	1	0	6.086689	-0.401380	-0.863349
46	1	0	6.585305	-1.513104	0.414479
47	6	0	4.448610	-0.005598	2.931397
48	1	0	3.476288	-0.031716	3.438142
49	1	0	5.110323	-0.711072	3.448836
50	1	0	4.870519	0.995083	3.099452

Rotational constants (GHZ): 0.3257879 0.1121246 0.1065782
Standard basis: 6-31G(d) (6D, 7F)

$[L(Me)_2FeCl_{eq}(\mathbf{5})_{ax}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.203098	0.748368	0.722319
2	7	0	-1.996080	2.095735	-0.540914
3	17	0	0.640275	2.021676	1.644487
4	7	0	-2.622573	-0.255058	0.085386
5	7	0	-1.073547	-0.795322	1.983216
6	6	0	-2.964375	1.604734	-1.242014
7	6	0	-4.390874	-0.534403	-1.486979
8	1	0	-4.987186	-0.145535	-2.305701
9	6	0	-2.853297	-1.473785	0.616456
10	6	0	-3.364688	0.231006	-0.929831
11	6	0	-1.943713	-1.720432	1.737850

12	6	0	-4.631686	-1.807949	-0.960844
13	1	0	-5.422207	-2.423304	-1.377516
14	6	0	-3.866896	-2.287788	0.108174
15	1	0	-4.053505	-3.267897	0.534374
16	8	0	0.051174	0.180988	-0.612558
17	13	0	1.042906	-1.358287	-0.971646
18	8	0	2.516213	-0.279476	-0.295293
19	6	0	0.755914	-2.967365	0.144230
20	1	0	-0.251310	-3.388661	0.013080
21	1	0	1.448006	-3.753846	-0.187408
22	1	0	0.922087	-2.842654	1.221232
23	13	0	1.495533	1.224325	-0.344214
24	6	0	2.210537	2.706255	-1.393546
25	1	0	1.653562	3.644267	-1.292850
26	1	0	3.240295	2.925119	-1.081440
27	1	0	2.247033	2.454163	-2.460987
28	1	0	-2.014539	-2.630771	2.332876
29	1	0	-3.489793	2.184901	-2.001340
30	6	0	-1.601715	3.485725	-0.760959
31	1	0	-2.264495	3.991926	-1.470107
32	1	0	-1.612200	4.015738	0.196062
33	1	0	-0.576871	3.509956	-1.141368
34	6	0	-0.163724	-0.961459	3.115361
35	1	0	0.865177	-0.928262	2.748510
36	1	0	-0.294700	-0.122342	3.805074
37	1	0	-0.337831	-1.904111	3.643527
38	13	0	4.238959	-0.637814	-0.080709
39	6	0	1.247231	-1.590124	-2.919035
40	1	0	0.338700	-2.014524	-3.369375
41	1	0	1.448158	-0.650696	-3.451406
42	1	0	2.063125	-2.281623	-3.170697
43	6	0	4.787990	-2.450263	-0.558505
44	1	0	4.309258	-3.201969	0.082828
45	1	0	4.514276	-2.698975	-1.591856
46	1	0	5.871869	-2.582914	-0.463914
47	6	0	5.326337	0.830661	0.616736
48	1	0	4.762397	1.538247	1.236348
49	1	0	6.160575	0.453222	1.220756
50	1	0	5.773884	1.409101	-0.203446

Rotational constants (GHZ): 0.2693386 0.1364382 0.1202377
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl_{ax}(\mathbf{4})_{eq}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.076627	0.634695	-0.034953
2	7	0	2.052167	0.783006	-0.478480
3	17	0	0.525677	0.667937	2.240524
4	7	0	0.231845	2.497580	-0.150002
5	7	0	-1.894745	1.147917	0.013314
6	6	0	4.242087	-0.260764	-0.065017
7	6	0	2.469090	2.014922	-0.458940
8	6	0	1.634350	4.429162	-0.166397

9	1	0	2.625187	4.864710	-0.241730
10	6	0	-0.867103	3.262263	0.017469
11	6	0	3.008555	-0.244330	-0.730236
12	6	0	-3.049992	0.329089	-0.171802
13	6	0	1.461693	3.044345	-0.240465
14	6	0	-2.067323	2.438353	0.051583
15	6	0	2.699067	-1.238927	-1.667094
16	6	0	-3.223423	-0.821203	0.612769
17	6	0	0.504422	5.233328	0.010246
18	1	0	0.612342	6.310992	0.075038
19	6	0	3.636642	-2.226869	-1.958485
20	1	0	3.406741	-2.982642	-2.703554
21	6	0	-0.764427	4.653344	0.100945
22	1	0	-1.651093	5.263793	0.236326
23	6	0	5.165941	-1.264773	-0.350435
24	1	0	6.113877	-1.285664	0.178333
25	6	0	-4.349959	-1.623621	0.419013
26	1	0	-4.495291	-2.494966	1.050350
27	6	0	-3.991099	0.650433	-1.163171
28	6	0	4.868994	-2.245246	-1.299023
29	6	0	-5.288280	-1.303678	-0.565938
30	1	0	-6.156904	-1.936946	-0.717264
31	6	0	-5.104447	-0.166194	-1.355338
32	1	0	-5.823396	0.083196	-2.129857
33	8	0	-0.106561	-1.298650	0.186896
34	6	0	-1.136942	-1.319431	-2.746191
35	1	0	-2.189952	-1.322330	-3.055464
36	1	0	-0.813002	-0.267428	-2.754671
37	1	0	-0.579923	-1.823176	-3.547912
38	6	0	-1.084504	-2.312083	3.100584
39	1	0	-1.662142	-3.151483	2.688270
40	1	0	-0.640504	-2.683472	4.034563
41	1	0	-1.799848	-1.533249	3.392794
42	1	0	-3.829373	1.512280	-1.804293
43	1	0	-2.521534	-1.045862	1.405119
44	1	0	-3.059511	2.886494	0.075249
45	1	0	1.751559	-1.206029	-2.195338
46	1	0	5.591200	-3.025292	-1.519016
47	1	0	4.453819	0.478166	0.702082
48	1	0	3.510606	2.274248	-0.641789
49	13	0	-0.913746	-2.266016	-1.032630
50	13	0	0.381991	-1.705199	1.924756
51	6	0	2.150414	-2.530496	2.135711
52	1	0	2.839323	-2.381385	1.298728
53	1	0	2.648581	-2.155367	3.040216
54	1	0	2.039531	-3.615094	2.276227
55	6	0	-1.282240	-4.155620	-0.703917
56	1	0	-0.415115	-4.770834	-0.981152
57	1	0	-1.506739	-4.376686	0.345599
58	1	0	-2.125919	-4.509524	-1.308841

Rotational constants (GHZ): 0.1544748 0.1243025 0.0895312
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl_{eq}(\mathbf{4})_{ax}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.017502	0.334397	-0.705260
2	7	0	-2.014234	0.629503	-0.777360
3	17	0	0.089230	-1.884073	-1.441416
4	7	0	-0.033863	2.191106	-0.485988
5	7	0	2.035559	0.734485	-0.698210
6	6	0	-3.162797	-1.261672	-1.837473
7	6	0	-2.322993	1.887119	-0.650144
8	6	0	-1.295266	4.224509	-0.459836
9	1	0	-2.257633	4.724994	-0.484369
10	6	0	1.123556	2.887689	-0.440192
11	6	0	-3.106397	-0.293522	-0.827096
12	6	0	3.175439	-0.128769	-0.732929
13	6	0	-1.224070	2.830601	-0.517744
14	6	0	2.273618	2.001880	-0.526202
15	6	0	-4.131122	-0.212693	0.129871
16	6	0	3.312161	-1.065289	-1.765177
17	6	0	-0.105083	4.952081	-0.376945
18	1	0	-0.133247	6.035584	-0.327865
19	6	0	-5.206383	-1.096455	0.071640
20	1	0	-5.986813	-1.042874	0.824537
21	6	0	1.122346	4.283422	-0.374577
22	1	0	2.058699	4.830124	-0.333720
23	6	0	-4.252513	-2.127502	-1.896694
24	1	0	-4.301339	-2.867307	-2.689646
25	6	0	4.449611	-1.867957	-1.816362
26	1	0	4.560628	-2.582215	-2.626289
27	6	0	4.167252	-0.018645	0.255174
28	6	0	-5.271739	-2.052415	-0.944175
29	6	0	5.437183	-1.762537	-0.833989
30	1	0	6.312825	-2.403163	-0.872295
31	6	0	5.290775	-0.840344	0.204519
32	1	0	6.045851	-0.765608	0.981096
33	8	0	0.025309	-0.347960	1.118334
34	6	0	0.093120	-0.852081	4.244655
35	1	0	-0.870184	-1.207838	4.634750
36	1	0	0.698084	-1.736659	4.020681
37	1	0	0.582146	-0.314911	5.067783
38	6	0	1.825048	-3.033125	1.362838
39	1	0	1.892326	-3.275431	2.432225
40	1	0	1.924736	-3.986573	0.826020
41	1	0	2.703608	-2.430834	1.108371
42	1	0	4.036185	0.677556	1.078999
43	1	0	2.547902	-1.149376	-2.527586
44	1	0	3.287952	2.395575	-0.484760
45	1	0	-4.062895	0.513111	0.935630
46	1	0	-6.109202	-2.741833	-0.988477
47	1	0	-2.374050	-1.323535	-2.576557
48	1	0	-3.356731	2.228854	-0.664138
49	13	0	-0.170484	0.346929	2.721866
50	13	0	0.097906	-2.210608	0.915319
51	6	0	-1.598718	-3.069286	1.414971
52	1	0	-2.493302	-2.577148	1.017725
53	1	0	-1.614921	-4.105319	1.050304
54	1	0	-1.713670	-3.128844	2.506468

55	6	0	-0.641081	2.245169	2.906963
56	1	0	0.066356	2.923741	2.414618
57	1	0	-1.636223	2.471950	2.502538
58	1	0	-0.661922	2.517686	3.969038

Rotational constants (GHZ): 0.1579543 0.1129569 0.0917468
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl_{ax}(\mathbf{7})_{eq}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.199105	0.608726	-0.282694
2	7	0	2.224305	0.496963	-0.380650
3	17	0	0.021011	0.394281	2.027634
4	7	0	0.600288	2.431468	-0.294829
5	7	0	-1.661463	1.364228	-0.318699
6	6	0	4.234258	-0.698979	0.386940
7	6	0	2.782616	1.674716	-0.370125
8	6	0	2.227194	4.181152	-0.293460
9	1	0	3.267133	4.490610	-0.306607
10	6	0	-0.405555	3.336093	-0.259491
11	6	0	3.071938	-0.649153	-0.400318
12	6	0	-2.881123	0.638515	-0.199639
13	6	0	1.893718	2.824152	-0.311395
14	6	0	-1.695043	2.662760	-0.244194
15	6	0	2.732363	-1.731048	-1.224678
16	6	0	-3.648767	0.728121	0.965298
17	6	0	1.196280	5.124830	-0.254773
18	1	0	1.432245	6.183623	-0.237681
19	6	0	3.578907	-2.835576	-1.290658
20	1	0	3.325287	-3.664815	-1.944085
21	6	0	-0.137642	4.706976	-0.237484
22	1	0	-0.949620	5.426021	-0.206659
23	6	0	5.061896	-1.817224	0.326281
24	1	0	5.950657	-1.860606	0.948336
25	6	0	-4.814087	-0.031175	1.084176
26	1	0	-5.398457	0.031525	1.996898
27	6	0	-3.268622	-0.227368	-1.239044
28	6	0	4.742342	-2.882784	-0.519047
29	6	0	-5.223867	-0.872823	0.048862
30	1	0	-6.132894	-1.457052	0.147362
31	6	0	-4.460339	-0.958770	-1.116883
32	1	0	-4.782595	-1.591644	-1.937744
33	8	0	-0.212805	-1.234082	-0.460426
34	13	0	-1.720899	-2.236085	-0.618078
35	8	0	-1.748242	-2.548869	1.083242
36	6	0	-2.162922	-3.316401	-2.178831
37	1	0	-2.227833	-2.744557	-3.111889
38	1	0	-1.388987	-4.081300	-2.321557
39	1	0	-3.112337	-3.846019	-2.038771
40	13	0	-0.152236	-1.860472	1.347832
41	6	0	1.301978	-2.808633	2.230100
42	1	0	2.264827	-2.291507	2.166628
43	1	0	1.068752	-2.943136	3.294244

44	1	0	1.427540	-3.810960	1.803098
45	1	0	-2.723419	-0.217442	-2.180464
46	1	0	-3.311621	1.356156	1.783607
47	1	0	-2.631411	3.213935	-0.169362
48	1	0	1.817650	-1.696326	-1.802858
49	1	0	5.390513	-3.752562	-0.564765
50	1	0	4.462830	0.111233	1.073316
51	1	0	3.861917	1.801107	-0.430670

Rotational constants (GHZ): 0.1734971 0.1348213 0.0901252
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl_{eq}(\mathbf{7})_{ax}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-0.109695	0.330837	-0.563817
2	7	0	-2.093229	0.821738	-0.497691
3	17	0	-0.309234	-2.049943	-0.785840
4	7	0	0.047045	2.176033	-0.425376
5	7	0	1.912950	0.509616	-0.815259
6	6	0	-3.392976	-0.933623	-1.586514
7	6	0	-2.259791	2.091739	-0.273182
8	6	0	-0.975524	4.299800	-0.039422
9	1	0	-1.872254	4.888273	0.124141
10	6	0	1.271187	2.745608	-0.462997
11	6	0	-3.262191	0.003820	-0.553605
12	6	0	2.921738	-0.487299	-1.002812
13	6	0	-1.062228	2.916633	-0.219315
14	6	0	2.302235	1.749058	-0.708064
15	6	0	-4.277657	0.142460	0.405913
16	6	0	2.743668	-1.472960	-1.981973
17	6	0	0.285373	4.901944	-0.077944
18	1	0	0.378173	5.974406	0.057670
19	6	0	-5.422975	-0.645369	0.318443
20	1	0	-6.198424	-0.549311	1.072184
21	6	0	1.426342	4.124522	-0.296102
22	1	0	2.412781	4.574769	-0.334377
23	6	0	-4.550687	-1.702613	-1.675080
24	1	0	-4.656844	-2.416359	-2.486054
25	6	0	3.734426	-2.430427	-2.181682
26	1	0	3.600081	-3.183820	-2.951503
27	6	0	4.083718	-0.480736	-0.213074
28	6	0	-5.565348	-1.563722	-0.724343
29	6	0	4.888237	-2.430834	-1.393387
30	1	0	5.647655	-3.192074	-1.542321
31	6	0	5.058339	-1.458233	-0.406678
32	1	0	5.946102	-1.461295	0.218143
33	8	0	-0.034973	-0.008761	1.316691
34	13	0	1.379203	-0.357223	2.366643
35	8	0	0.994171	-2.025197	2.468509
36	6	0	2.667991	0.865078	3.157966
37	1	0	2.810968	1.781646	2.575337
38	1	0	2.324059	1.166942	4.155343
39	1	0	3.641500	0.380480	3.290831

40	13	0	-0.494197	-1.848945	1.525444
41	6	0	-2.198491	-2.577784	2.121458
42	1	0	-3.009224	-2.459947	1.396412
43	1	0	-2.081940	-3.651190	2.318948
44	1	0	-2.515794	-2.116481	3.065158
45	1	0	4.210411	0.266827	0.565450
46	1	0	1.849318	-1.476497	-2.593823
47	1	0	3.346980	2.035669	-0.818219
48	1	0	-4.148354	0.828861	1.237697
49	1	0	-6.458490	-2.177446	-0.789596
50	1	0	-2.606601	-1.043178	-2.324617
51	1	0	-3.249393	2.534764	-0.174379

Rotational constants (GHZ): 0.1805462 0.1166695 0.0942159
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl_{ax}(\mathbf{5})_{eq}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	-1.093097	-0.642296	-0.193533
2	7	0	-2.696271	0.629596	-0.229224
3	17	0	-0.501464	-0.167450	2.036212
4	7	0	-2.489035	-1.877863	0.059078
5	7	0	-0.018208	-2.410257	-0.154767
6	6	0	-3.821132	0.013001	-0.011424
7	6	0	-4.828519	-2.317425	0.310187
8	1	0	-5.844263	-1.943374	0.385534
9	6	0	-2.222974	-3.200909	0.090195
10	6	0	-3.761451	-1.429936	0.147201
11	6	0	-0.794292	-3.444583	-0.025363
12	6	0	-4.558443	-3.687164	0.365347
13	1	0	-5.369731	-4.396246	0.492296
14	6	0	-3.242442	-4.142572	0.247312
15	1	0	-3.010486	-5.202109	0.276430
16	8	0	0.177057	0.691638	-0.694286
17	13	0	1.807135	1.041487	-1.529859
18	8	0	2.381942	1.338036	0.316546
19	6	0	2.736946	-0.390678	-2.507590
20	1	0	2.044250	-1.005896	-3.098734
21	1	0	3.430653	0.063399	-3.228371
22	1	0	3.319436	-1.078789	-1.886789
23	13	0	0.645749	1.495821	0.848605
24	6	0	0.215227	3.174997	1.736020
25	1	0	-0.858198	3.294601	1.914187
26	1	0	0.713540	3.235820	2.712688
27	1	0	0.552684	4.034828	1.144677
28	1	0	-0.393460	-4.455362	0.036818
29	1	0	-4.772858	0.541014	0.009498
30	13	0	3.988680	1.608713	0.996621
31	6	0	1.698194	2.819084	-2.391631
32	1	0	1.162192	2.764427	-3.350604
33	1	0	1.190333	3.584392	-1.789060
34	1	0	2.696564	3.212924	-2.628555
35	6	0	5.438816	1.837093	-0.292171

36	1	0	5.424546	1.064073	-1.070594
37	1	0	5.359977	2.803233	-0.808584
38	1	0	6.423067	1.808546	0.189661
39	6	0	4.097549	1.638448	2.951360
40	1	0	3.219918	1.212904	3.452260
41	1	0	4.980901	1.094190	3.309204
42	1	0	4.205965	2.669548	3.315526
43	6	0	-2.745247	2.049832	-0.370217
44	6	0	-3.509091	2.826519	0.516814
45	6	0	-2.036731	2.662447	-1.412717
46	6	0	-3.577241	4.206993	0.344388
47	1	0	-4.010474	2.355056	1.357309
48	6	0	-2.127035	4.042531	-1.584577
49	1	0	-1.433618	2.061244	-2.080294
50	6	0	-2.893689	4.816820	-0.710533
51	1	0	-4.156553	4.806227	1.040232
52	1	0	-1.589842	4.512068	-2.402772
53	1	0	-2.949414	5.892948	-0.843497
54	6	0	1.386476	-2.712612	-0.217745
55	6	0	1.870737	-3.582341	-1.202801
56	6	0	2.248849	-2.197463	0.756336
57	6	0	3.219266	-3.937615	-1.211044
58	1	0	1.199494	-3.955953	-1.971047
59	6	0	3.590574	-2.577873	0.751307
60	1	0	1.856792	-1.556698	1.536910
61	6	0	4.081123	-3.441938	-0.231755
62	1	0	3.593429	-4.601686	-1.984193
63	1	0	4.251901	-2.213858	1.533111
64	1	0	5.128138	-3.729055	-0.231823

Rotational constants (GHZ): 0.1232287 0.1005973 0.0670417
Standard basis: 6-31G(d) (6D, 7F)

$[L(Ph)_2FeCl_{eq}(\mathbf{5})_{ax}]^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	26	0	0.663001	-0.910441	-0.427082
2	7	0	2.647825	-0.492370	-0.147947
3	17	0	0.051043	0.866912	-1.956080
4	7	0	1.089201	-2.267332	0.764242
5	7	0	-1.038024	-2.014204	-0.574186
6	6	0	3.144254	-1.207531	0.817022
7	6	0	2.597038	-3.173555	2.375531
8	1	0	3.561525	-3.147683	2.871706
9	6	0	0.162224	-3.201075	1.063031
10	6	0	2.286763	-2.239124	1.383301
11	6	0	-1.017482	-3.043439	0.223023
12	6	0	1.641057	-4.137984	2.706763
13	1	0	1.857394	-4.872660	3.475317
14	6	0	0.410802	-4.165603	2.042563
15	1	0	-0.337862	-4.914339	2.279044
16	8	0	0.246589	0.347690	0.958033
17	13	0	-1.177194	0.612311	2.128902
18	8	0	-1.605844	2.064053	0.903339

19	6	0	-2.610263	-0.748041	2.204945
20	1	0	-2.243990	-1.699118	2.618719
21	1	0	-3.393530	-0.409104	2.897288
22	1	0	-3.105802	-0.975199	1.254082
23	13	0	0.021153	1.911414	0.087908
24	6	0	1.110522	3.525616	0.042457
25	1	0	2.085291	3.362220	-0.428395
26	1	0	0.606639	4.317780	-0.526548
27	1	0	1.289504	3.916345	1.052234
28	1	0	-1.833280	-3.763314	0.254124
29	1	0	4.172764	-1.089586	1.154318
30	13	0	-2.895191	3.275851	0.925252
31	6	0	-0.523520	1.384382	3.823867
32	1	0	-0.075592	0.614596	4.468312
33	1	0	0.242965	2.158920	3.685291
34	1	0	-1.334037	1.837902	4.411067
35	6	0	-4.186484	3.111236	2.382173
36	1	0	-4.689444	2.135433	2.371142
37	1	0	-3.701413	3.201949	3.362732
38	1	0	-4.963180	3.882637	2.327673
39	6	0	-2.851966	4.587870	-0.525660
40	1	0	-2.394608	4.204499	-1.445777
41	1	0	-3.860277	4.939427	-0.776300
42	1	0	-2.276666	5.476287	-0.230218
43	6	0	3.475549	0.504223	-0.742699
44	6	0	3.463390	0.649235	-2.136585
45	6	0	4.295536	1.329334	0.043774
46	6	0	4.296492	1.588076	-2.739810
47	1	0	2.822959	0.017397	-2.742331
48	6	0	5.111857	2.277414	-0.568906
49	1	0	4.259249	1.257450	1.126847
50	6	0	5.120193	2.404147	-1.960178
51	1	0	4.296990	1.685814	-3.820954
52	1	0	5.733144	2.924609	0.042597
53	1	0	5.757210	3.144466	-2.434314
54	6	0	-2.112631	-1.944893	-1.517670
55	6	0	-2.410058	-3.058888	-2.317792
56	6	0	-2.859766	-0.767153	-1.646110
57	6	0	-3.458502	-2.995032	-3.233935
58	1	0	-1.798968	-3.954508	-2.246134
59	6	0	-3.916529	-0.721363	-2.551966
60	1	0	-2.628924	0.086184	-1.020944
61	6	0	-4.216934	-1.829103	-3.349139
62	1	0	-3.675906	-3.854159	-3.861185
63	1	0	-4.506488	0.186014	-2.639697
64	1	0	-5.033635	-1.779891	-4.062749

Rotational constants (GHZ): 0.1094523 0.0937778 0.0776555

Standard basis: 6-31G(d) (6D, 7F)