Supplementary Information for

Synthesis of Highly Reactive Polyisobutylene by $FeCl_3$/Ether Complexes in Hexanes; Kinetic and Mechanistic Studies

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Table S1. Polymerization of [IB] = 1.0 M by [$FeCl_3$•*i*-Pr_2O] = 0.02 M and [*t*-BuCl] = 0.02M in hexanes at 0 °C. Complex was prepared in DCM.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	2	53	900	800	4.6	76	6	7	9	2
2	5	71	800	1100	2.0	79	7	7	6	2
3	10	84	700	1100	1.9	84	7	8	0	2
4	20	95	700	900	2.0	80	8	9	0	3
5	40	95	700	900	2.3	81	7	10	0	3
6	60	100	800	900	2.1	80	9	9	0	2

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S2. Polymerization of [IB] = 1.0 M by [$FeCl_3$•*i*-Pr_2O] = 0.01 M and [*t*-BuCl] = 0.02 M in hexanes at 0 °C. Complex was prepared in DCM.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	2	25	1200	1800	2.0	65	9	9	17	1
2	5	37	1100	1900	2.1	66	8	9	16	2
3	10	50	1000	1500	2.5	75	7	8	8	2
4	20	64	900	1400	2.7	75	6	9	7	3
5	40	79	1000	1300	2.5	78	9	11	0	2
6	60	92	700	1100	2.3	77	9	11	0	3

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S3. Polymerization of [IB] = 1.0 M by [$FeCl_3$•*i*-Pr_2O] = 0.005 M and [*t*-BuCl] = 0.02 M in hexanes at 0 °C.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	2	15	1500	2100	2.5	60	10	13	15	2
2	5	19	1400	2000	2.2	65	9	12	13	1
3	10	26	1300	2000	2.2	68	9	9	12	2
4	20	27	1100	1500	3.0	70	9	10	9	2
5	40	37	1100	1300	2.9	70	8	11	9	2
6	60	44	1000	1200	3.0	70	9	12	5	4
7	120	52	800	1000	3.1	77	10	12	0	1
8	180	63	700	900	2.8	73	11	14	0	3

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S4. Polymerization of [IB] = 1.0 M by [$FeCl_3$•CEEE] = 0.02 M and [*t*-BuCl] = 0.02M in hexanes at 0 °C.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	1	70	400	700	2.4	74	12	9	0	4
2	2	75	350	700	2.4	75	11	10	0	4
3	5	77	350	500	2.3	71	12	9	0	8
4	10	85	300	400	1.9	71	11	10	0	8
5	20	87	300	500	2.2	73	11	7	0	9
6	40	90	300	500	2.3	60	16	9	0	15
7	60	91	200	400	2.5	55	18	9	0	18

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S5. Polymerization of [IB] = 1.0 M by [$FeCl_3$•CEEE] = 0.01 M and [*t*-BuCl] = 0.02 M in hexanes at 0 °C.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	1	46	700	800	2.8	65	15	11	3	5
2	2	59	600	700	2.7	68	14	12	2	4
3	5	69	500	600	2.9	67	15	13	0	5
4	10	74	500	600	2.7	72	13	12	0	4
5	20	80	450	500	2.6	69	13	12	0	6
6	40	92	400	500	2.8	66	14	13	0	7
7	60	100	300	400	2.9	63	14	13	0	10

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S6. Polymerization of [IB] = 1.0 M by [$FeCl_3$•CEEE] = 0.005 M and [*t*-BuCl] = 0.02 M in hexanes at 0 °C.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	1	30	800	1200	2.9	68	15	10	0	6
2	2	36	1000	1100	2.7	65	18	12	0	6
3	5	50	900	1000	2.7	67	16	14	0	3
4	10	55	800	1000	2.6	66	15	15	0	5
5	20	64	700	900	2.6	68	14	15	0	3
6	40	78	600	800	2.5	69	12	16	0	3
7	60	99	500	600	2.6	64	13	15	0	7
8	1	30	800	700	2.8	68	15	10	0	6

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S7. Polymerization of [IB] = 1.0 M by [$FeCl_3$•CEE] = 0.020 M and [*t*-BuCl] = 0.02 M in hexanes at 0 °C.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	1	75	500	700	2.8	65	20	15	0	0
2	2	80	600	600	2.7	60	21	19	0	0
3	5	82	500	600	2.7	61	21	17	0	1
4	10	90	500	600	2.4	63	18	18	0	1
5	20	92	500	600	2.4	64	18	18	0	0
6	40	95	450	500	2.4	63	19	17	0	1
7	60	95	500	500	2.4	62	20	16	0	2

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S8. Polymerization of [IB] = 1.0 M by [$FeCl_3$•CEE] = 0.01 M and [*t*-BuCl] = 0.02 M in hexanes at 0 °C.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	1	50	800	900	2.6	56	21	22	0	2
2	2	60	800	900	2.5	55	23	23	0	0
3	5	74	700	800	2.4	57	22	21	0	0
4	10	79	700	800	2.4	56	22	22	0	0
5	20	84	700	700	2.3	55	21	22	0	2
6	40	93	700	700	2.3	55	21	23	0	1
7	60	100	600	700	2.3	55	23	22	0	1

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S9. Polymerization of [IB] = 1.0 M by [$FeCl_3$•CEE] = 0.005 M and [*t*-BuCl] = 0.02 M in hexanes at 0 °C.

#	Time (min)	Conv. (%)[a]	$M_{n,NMR}$[b] (g/mol)	$M_{n,GPC}$[c] (g/mol)	PDI[c]	exo[d] (%)	tri+endo[d] (%)	tetra[d] (%)	PIB-Cl[d] (%)	Coupled-PIB[d] (%)
1	1	33	1500	1700	2.9	56	18	26	0	0
2	2	40	1500	1600	2.8	54	20	26	0	0
3	5	54	1100	1300	2.8	53	21	26	0	1
4	10	59	1100	1300	2.8	52	21	27	0	1
5	20	70	1000	1200	2.7	52	22	25	0	1
6	40	84	1000	1100	2.5	51	21	27	0	1
7	60	100	900	1000	2.4	50	22	26	0	1

[a]Determined gravimetrically based on monomer feed. [b]Determined from NMR analysis. [c]Obtained from SEC measurements. [d]Calculated from NMR spectroscopic study.

Table S10. The calculated energies with different spin multiplicities.

	Energy (Hartree)		
	S=2	S=4	S=6
$FeCl_3$	-2644.278841	-2644.315117	-2644.344873
$FeCl_3$*CEE	-3797.053857	-3797.079687	-3797.129836
$FeCl_3$*CEEE	-3337.451070	-3337.481759	-3337.527307
$FeCl_3$* *i*-Pr_2O	-2956.432747	-2956.458146	-2956.506762
$FeCl_3$*Et_2O	-2877.85407	-2877.880051	-2877.927426

S=6 is located as the ground state.The sextet results are summarized below.

Gas phase results:

Iron trichloride ($FeCl_3$)

Sum of electronic and zero-point Energies= -2644.310699
Sum of electronic and thermal Energies= -2644.304812
Sum of electronic and thermal Enthalpies= -2644.303868
Sum of electronic and thermal Free Energies= -2644.344873

Fe	-0.00085600	-0.00013800	-0.00030800
Cl	0.96766100	1.90694600	0.00015700
Cl	-2.13671800	-0.11681000	0.00015700
Cl	1.17036600	-1.78992500	0.00015700

Bis-(2-chloroethyl) ether(CEE)

Sum of electronic and zero-point Energies= -1152.729308
Sum of electronic and thermal Energies= -1152.720572
Sum of electronic and thermal Enthalpies= -1152.719627
Sum of electronic and thermal Free Energies= -1152.765164

O	0.00093600	0.44505400	0.00000000
C	0.00096400	-0.33543500	1.18284600
C	0.00096400	-0.33543500	-1.18284600
C	-0.00044800	0.64563700	-2.34608700
C	-0.00044800	0.64563700	2.34608700
H	0.88922900	1.27667800	-2.32679000
H	-0.89134400	1.27494400	-2.32563000
H	-0.88845100	-0.98245500	-1.22920800
H	0.88922900	1.27667800	2.32679000
H	-0.89134400	1.27494400	2.32563000
H	-0.88845100	-0.98245500	1.22920800
H	0.89133900	-0.98105600	-1.22994100
H	0.89133900	-0.98105600	1.22994100
Cl	-0.00044800	-0.24879600	-3.91919300
Cl	-0.00044800	-0.24879600	3.91919300

2-Chloroethyl ethyl ether(CEEE)
Sum of electronic and zero-point Energies= -693.128137
Sum of electronic and thermal Energies= -693.120376
Sum of electronic and thermal Enthalpies= -693.119432
Sum of electronic and thermal Free Energies= -693.161134

O	-1.10959300	0.30187600	0.00013800
C	0.11924400	-0.39470600	-0.00016300
C	-2.24050800	-0.55895800	0.00040200
C	-3.49521100	0.29788900	-0.00038500
C	1.21475800	0.66187200	0.00034100
H	-3.52277900	0.93781300	-0.88814100
H	-3.52300100	0.93912800	0.88641300
H	-2.21519500	-1.21270600	0.88840800
H	1.15301800	1.28987500	-0.88950900
H	1.15312200	1.28893800	0.89085200
H	0.21380600	-1.03854600	0.88894600
H	-2.21484000	-1.21377500	-0.88679300
H	0.21381000	-1.03770600	-0.88987200
Cl	2.84812600	-0.12171700	-0.00015100
H	-4.38903100	-0.33542900	-0.00001500

Di-isopropyl ether (*i*-Pr_2O)
Sum of electronic and zero-point Energies= -312.103071
Sum of electronic and thermal Energies= -312.093715
Sum of electronic and thermal Enthalpies= -312.092771
Sum of electronic and thermal Free Energies= -312.136710

O	0.00002900	-0.00017600	-0.52418600
C	-1.20526100	0.14086500	0.23320300
C	-1.75605900	-1.23206400	0.63176400
C	-2.18194700	0.92389300	-0.63974500
H	-0.99974300	0.72333000	1.14561400
H	-1.03154100	-1.79394400	1.23170100
H	-2.67333800	-1.12978400	1.22376300
H	-1.98412100	-1.81970000	-0.26458400
H	-1.76981400	1.90652600	-0.88979900
H	-2.36624900	0.38370300	-1.57526100
H	-3.14009200	1.06425800	-0.12693000
C	1.20531200	-0.14092400	0.23324100
C	1.75573700	1.23214700	0.63182400
C	2.18220600	-0.92378600	-0.63963900
H	0.99992300	-0.72347600	1.14562900
H	1.03111400	1.79378100	1.23186500

H	2.67311400	1.13013700	1.22371800
H	1.98350400	1.81986500	-0.26454300
H	1.77001300	-1.90629700	-0.89006400
H	2.36689900	-0.38338200	-1.57495600
H	3.14016600	-1.06440000	-0.12654300

Diethyl ether (Et_2O)

Sum of electronic and zero-point Energies= -233.525950
Sum of electronic and thermal Energies= -233.519167
Sum of electronic and thermal Enthalpies= -233.518223
Sum of electronic and thermal Free Energies= -233.556021

O	-0.00027000	-0.25725500	0.00000000
C	0.00004900	0.52213200	1.18280000
C	0.00004900	0.52213200	-1.18280000
C	0.00004900	-0.41646800	-2.37882000
C	0.00004900	-0.41646800	2.37882000
H	-0.88700900	-1.05817200	-2.36193400
H	0.88689900	-1.05845500	-2.36171900
H	0.88730300	1.17890300	-1.20627200
H	-0.88700900	-1.05817200	2.36193400
H	0.88689900	-1.05845500	2.36171900
H	0.88730300	1.17890300	1.20627200
H	-0.88695200	1.17923700	-1.20654300
H	-0.88695200	1.17923700	1.20654300
H	0.00024900	0.15352100	3.31465000
H	0.00024900	0.15352100	-3.31465000

$FeCl_3$*CEE

Sum of electronic and zero-point Energies= -3797.076970
Sum of electronic and thermal Energies= -3797.061002
Sum of electronic and thermal Enthalpies= -3797.060058
Sum of electronic and thermal Free Energies= -3797.129836

Cl	1.70287000	-2.10570000	-1.17855700
Cl	-1.96717500	-1.99536300	-0.84554500
O	0.01362800	0.55422700	-0.09423400
C	-1.09455500	1.36977700	-0.58144900
C	1.14260400	1.28876800	0.46863000
C	2.14839100	1.61926100	-0.62641300
C	-2.11703900	1.57905400	0.52806900
H	1.70485400	2.22614100	-1.41829600
H	2.57424100	0.71221200	-1.05659900
H	1.58114800	0.64418200	1.23214800

H	-2.58701100	0.63675000	0.81285100
H	-1.67494300	2.04926200	1.40862700
H	-0.68819500	2.32021700	-0.93561900
H	0.76119900	2.19201800	0.95178300
H	-1.53173100	0.83030700	-1.42164400
Cl	3.49119900	2.57789500	0.10437700
Cl	-3.41053800	2.67645700	-0.08657600
Cl	0.17825500	-1.85779700	2.14387500
Fe	-0.02436100	-1.50805500	0.00418600

$FeCl_3$*CEEE

Sum of electronic and zero-point Energies= -3337.478814
Sum of electronic and thermal Energies= -3337.463855
Sum of electronic and thermal Enthalpies= -3337.462911
Sum of electronic and thermal Free Energies= -3337.527307

Cl	2.51812000	0.80292200	-1.39722700
Cl	0.46910100	-2.21476200	-0.86022000
O	-0.39800900	0.81298300	0.19276600
C	-1.64920800	0.21928400	0.65145900
C	-0.20380300	2.23212400	0.52105800
C	-1.10753000	3.13884100	-0.29244300
C	-2.54900100	-0.07540100	-0.54115500
H	-2.16740200	2.98362800	-0.06620500
H	-0.94342600	2.99135400	-1.36412500
H	0.84540600	2.42459800	0.29397800
H	-2.78211800	0.82812600	-1.10540000
H	-2.09813700	-0.81787600	-1.20001000
H	-1.40144600	-0.69881400	1.18815200
H	-0.35643300	2.34098900	1.59979600
H	-2.12420500	0.91413500	1.34803000
Cl	-4.10631400	-0.75564000	0.07207200
H	-0.86826800	4.18035800	-0.05034200
Cl	2.00854500	-0.50099600	2.00239900
Fe	1.26987200	-0.36059100	-0.04265100

$FeCl_3$*i*-Pr_2O**

Sum of electronic and zero-point Energies= -2956.458874
Sum of electronic and thermal Energies= -2956.442252
Sum of electronic and thermal Enthalpies= -2956.441308
Sum of electronic and thermal Free Energies= -2956.506762

Fe	-1.00769200	-0.13776000	-0.00004900
Cl	-2.03301700	1.78989700	-0.00036300
Cl	-1.35260200	-1.29622800	1.82599100

Cl	-1.35268500	-1.29779400	-1.82505600
O	1.00507200	0.10465600	-0.00026000
C	1.76724500	1.37678700	-0.00048900
C	1.46134000	2.14458600	1.27930300
C	1.46090400	2.14419000	-1.28040900
H	2.81844700	1.07987700	-0.00067700
H	1.69119900	1.54387500	2.16404200
H	2.07411300	3.05236400	1.31092500
H	0.41065900	2.44580400	1.32136000
H	1.69105400	1.54342400	-2.16503700
H	0.41008000	2.44490600	-1.32250000
H	2.07315600	3.05231800	-1.31223000
C	1.77899100	-1.16479300	0.00035300
C	2.58413000	-1.30511900	1.28547200
C	2.58358000	-1.30631100	-1.28498900
H	0.99052800	-1.92068100	0.00091100
H	1.93650000	-1.19718900	2.15993700
H	3.03124200	-2.30465000	1.31428100
H	3.40037800	-0.57770600	1.34978800
H	1.93544900	-1.19967000	-2.15923800
H	3.39936900	-0.57848300	-1.35051300
H	3.03128100	-2.30560100	-1.31286500

$FeCl_3$*Et_2O

Sum of electronic and zero-point Energies= -2877.881982
Sum of electronic and thermal Energies= -2877.867999
Sum of electronic and thermal Enthalpies= -2877.867054
Sum of electronic and thermal Free Energies= -2877.927426

Fe	0.78170800	0.05623100	0.01122400
Cl	1.43283600	-1.13120100	1.72160900
Cl	1.21869300	-0.82516500	-1.93841100
Cl	1.22546200	2.18966700	0.12633800
O	-1.24476200	-0.00747100	0.11637200
C	-1.98819900	-1.05986800	0.81235400
C	-2.15017700	-2.30210900	-0.04590500
H	-2.94996800	-0.62906600	1.10604400
H	-1.40928000	-1.26455300	1.71370200
H	-2.69701200	-3.06107500	0.52493700
H	-2.71485300	-2.09818900	-0.96139300
H	-1.17695500	-2.71743900	-0.32328300
C	-2.04072500	0.86007900	-0.75556900
C	-2.63423600	2.02490600	0.01524100
H	-2.80472800	0.23603400	-1.22872700
H	-1.35489900	1.20076400	-1.53383300
H	-3.20769500	2.65488800	-0.67421700

H	-3.31340500	1.68758800	0.80517300
H	-1.84425800	2.63397000	0.46290100

Results including solvent effects in hexane:

Iron trichloride ($FeCl_3$)

Sum of electronic and zero-point Energies= -2644.321767
Sum of electronic and thermal Energies= -2644.315817
Sum of electronic and thermal Enthalpies= -2644.314872
Sum of electronic and thermal Free Energies= -2644.356063

Fe	-0.00444100	-0.00168600	0.00121500
Cl	0.68289700	2.03559400	-0.00070400
Cl	1.43553800	-1.60215000	-0.00063300
Cl	-2.11164400	-0.43086500	-0.00052100

Bis-(2-chloroethyl) ether(CEE)

Sum of electronic and zero-point Energies= -1152.735963
Sum of electronic and thermal Energies= -1152.727180
Sum of electronic and thermal Enthalpies= -1152.726236
Sum of electronic and thermal Free Energies= -1152.771923

O	0.00024800	0.45172200	0.00000000
C	0.00020000	-0.33284400	1.18296900
C	0.00020000	-0.33284400	-1.18296900
C	-0.00010200	0.64839900	-2.34611900
C	-0.00010200	0.64839900	2.34611900
H	0.89244000	1.27772000	-2.33333400
H	-0.89286100	1.27740800	-2.33316100
H	-0.89219900	-0.97903900	-1.22669300
H	0.89244000	1.27772000	2.33333400
H	-0.89286100	1.27740800	2.33316100
H	-0.89219900	-0.97903900	1.22669300
H	0.89277800	-0.97877800	-1.22695100
H	0.89277800	-0.97877800	1.22695100
Cl	-0.00010200	-0.25279600	-3.92149000
Cl	-0.00010200	-0.25279600	3.92149000

2-Chloroethyl ethyl ether(CEEE)

Sum of electronic and zero-point Energies= -693.132712
Sum of electronic and thermal Energies= -693.124948
Sum of electronic and thermal Enthalpies= -693.124004
Sum of electronic and thermal Free Energies= -693.165681

O	1.11045900	0.30643000	0.00011700
C	-0.11936600	-0.39296400	0.00006200
C	2.24147300	-0.55862300	-0.00004100
C	3.49907000	0.29426900	0.00030700
C	-1.21441400	0.66436800	-0.00015500
H	3.53057500	0.93440800	0.88879900
H	3.53061400	0.93504600	-0.88772500
H	2.21296700	-1.21197300	-0.88878800
H	-1.15837000	1.29177900	0.89220600
H	-1.15826100	1.29152500	-0.89268700
H	-0.21187200	-1.03647500	-0.89189600
H	2.21282700	-1.21249500	0.88831600
H	-0.21204300	-1.03630400	0.89212600
Cl	-2.85062300	-0.12382700	-0.00014200
H	4.38990900	-0.34418200	0.00009300

Di-isopropyl ether (*i*-Pr_2O)

Sum of electronic and zero-point Energies= -312.106343
Sum of electronic and thermal Energies= -312.096980
Sum of electronic and thermal Enthalpies= -312.096036
Sum of electronic and thermal Free Energies= -312.139981

O	0.00002000	-0.00002300	-0.52939700
C	-1.20580600	0.13841800	0.23260500
C	-1.75518500	-1.23644700	0.62621500
C	-2.18605600	0.92597700	-0.63230900
H	-0.99528200	0.71701700	1.14769300
H	-1.02744800	-1.80154800	1.21999100
H	-2.66980800	-1.13524400	1.22334400
H	-1.98921600	-1.81969400	-0.27232900
H	-1.77559500	1.91094200	-0.87909000
H	-2.37686300	0.39030400	-1.57001500
H	-3.14151800	1.06349900	-0.11281100
C	1.20579000	-0.13843500	0.23269300
C	1.75510100	1.23643300	0.62638800
C	2.18613600	-0.92593100	-0.63217200
H	0.99522000	-0.71707200	1.14774800
H	1.02731300	1.80149900	1.22013300
H	2.66968500	1.13522900	1.22357700
H	1.98918300	1.81971600	-0.27211900
H	1.77572400	-1.91089700	-0.87902900
H	2.37700700	-0.39021300	-1.56983900
H	3.14155700	-1.06344700	-0.11259700

Diethyl ether (Et_2O**)**
Sum of electronic and zero-point Energies= -233.528629
Sum of electronic and thermal Energies= -233.521832
Sum of electronic and thermal Enthalpies= -233.520888
Sum of electronic and thermal Free Energies= -233.558721

O	-0.00009100	-0.26159800	0.00000000
C	0.00001700	0.52086800	1.18375600
C	0.00001700	0.52086800	-1.18375600
C	0.00001700	-0.41392200	-2.38283600
C	0.00001700	-0.41392200	2.38283600
H	-0.88781500	-1.05586200	-2.37031500
H	0.88778000	-1.05595500	-2.37024500
H	0.88798100	1.17750200	-1.20418900
H	-0.88781500	-1.05586200	2.37031500
H	0.88778000	-1.05595500	2.37024500
H	0.88798100	1.17750200	1.20418900
H	-0.88786400	1.17761500	-1.20428000
H	-0.88786400	1.17761500	1.20428000
H	0.00008200	0.16141800	3.31578700
H	0.00008200	0.16141800	-3.31578700

$FeCl_3$*CEE
Sum of electronic and zero-point Energies= -3797.091620
Sum of electronic and thermal Energies= -3797.075824
Sum of electronic and thermal Enthalpies= -3797.074880
Sum of electronic and thermal Free Energies= -3797.140952

Cl	1.07106300	-2.58653600	-1.03720900
Cl	-2.39854000	-1.39975600	-0.99778800
O	0.20079600	0.51888400	-0.10910200
C	-0.62445000	1.62411500	-0.59799200
C	1.48935300	0.90514600	0.46685700
C	2.54087200	0.97280300	-0.63244500
C	-1.54865700	2.10641100	0.51243800
H	2.28036300	1.69836400	-1.40693700
H	2.70720300	-0.00716000	-1.08457300
H	1.73848900	0.14331300	1.21221100
H	-2.27282300	1.33771200	0.79250800
H	-0.99520600	2.43182700	1.39678900
H	0.04435000	2.42074200	-0.94013100
H	1.36520400	1.86841500	0.97346800
H	-1.19158800	1.23726500	-1.44865900
Cl	4.10240400	1.51211600	0.10480700
Cl	-2.48167400	3.53109700	-0.09676100

Cl	-0.55499700	-1.76190400	2.17055500
Fe	-0.45915200	-1.42187200	0.00921900

$FeCl_3$*CEEE

Sum of electronic and zero-point Energies= -3337.491343
Sum of electronic and thermal Energies= -3337.476499
Sum of electronic and thermal Enthalpies= -3337.475554
Sum of electronic and thermal Free Energies= -3337.538218

Cl	2.41416200	0.81288000	-1.48342800
Cl	0.42079900	-2.22875600	-0.82396600
O	-0.39632200	0.80370900	0.32129000
C	-1.67005600	0.21485400	0.72766900
C	-0.21673700	2.23437400	0.62928100
C	-1.01457200	3.12545200	-0.30200700
C	-2.53787400	-0.04843200	-0.49690800
H	-2.09482000	2.99278100	-0.17913700
H	-0.74448800	2.93825800	-1.34656700
H	0.85596500	2.40884000	0.51724200
H	-2.76027900	0.86772100	-1.04675300
H	-2.07939200	-0.78102400	-1.16350900
H	-1.44505100	-0.71754800	1.25588900
H	-0.48644500	2.36972500	1.68243500
H	-2.15698100	0.90773700	1.42211200
Cl	-4.11535700	-0.74083100	0.06245100
H	-0.77996600	4.17113100	-0.06967700
Cl	2.18502000	-0.52789600	1.91242500
Fe	1.23534000	-0.35025000	-0.05145200

$FeCl_3$*i*-Pr_2O

Sum of electronic and zero-point Energies= -2956.469478
Sum of electronic and thermal Energies= -2956.452880
Sum of electronic and thermal Enthalpies= -2956.451935
Sum of electronic and thermal Free Energies= -2956.516191

Fe	-0.98147000	-0.12787800	-0.00522200
Cl	-2.07110100	1.76854200	-0.16285100
Cl	-1.34576100	-1.10190800	1.93414300
Cl	-1.42640400	-1.45737300	-1.70147400
O	1.01749400	0.09765500	-0.04309100
C	1.78824400	1.37064400	-0.02111400
C	1.45235300	2.13921500	1.25017900
C	1.52381900	2.13933300	-1.30913700
H	2.83811800	1.06487100	0.00772900

H	1.64633800	1.53377300	2.14092800
H	2.07774400	3.03816000	1.30090900
H	0.40488800	2.45846900	1.26105600
H	1.77775500	1.53665900	-2.18680600
H	0.47610100	2.44802200	-1.38338400
H	2.14358500	3.04352900	-1.32062100
C	1.79258800	-1.17752900	-0.01359900
C	2.57593500	-1.30589600	1.28563600
C	2.62095300	-1.32768400	-1.28193200
H	1.00075800	-1.93438100	-0.02144300
H	1.91755000	-1.18179600	2.15086000
H	3.01265900	-2.31018300	1.33086000
H	3.39783700	-0.58466700	1.35214600
H	1.99144600	-1.22684800	-2.17147900
H	3.43780500	-0.59952300	-1.33539600
H	3.06784700	-2.32843600	-1.29195400

$FeCl_3$*Et_2O

Sum of electronic and zero-point Energies= -2877.892574
Sum of electronic and thermal Energies= -2877.878556
Sum of electronic and thermal Enthalpies= -2877.877612
Sum of electronic and thermal Free Energies= -2877.937589

Fe	-0.75501100	0.04996900	-0.00151900
Cl	-1.50410600	-1.27175900	-1.58116800
Cl	-1.20425300	-0.66766300	2.02554500
Cl	-1.23080400	2.16866400	-0.30363400
O	1.25093200	-0.03192900	-0.13971000
C	1.98230500	-1.16825900	-0.71768500
C	2.11926900	-2.30976000	0.27224100
H	2.95229300	-0.78158500	-1.04591800
H	1.40697300	-1.45875600	-1.59950900
H	2.67599000	-3.12614300	-0.20344700
H	2.66700500	-2.00669300	1.17117600
H	1.13905700	-2.69365500	0.57280200
C	2.07230600	0.93484200	0.60286200
C	2.66721500	1.97985100	-0.32139500
H	2.83431500	0.36353200	1.14306300
H	1.39926000	1.38474000	1.33806600
H	3.25792000	2.68490200	0.27584200
H	3.33059800	1.53319900	-1.06981500
H	1.87862300	2.53952500	-0.83385000