Electronic Supplementary Information

for

Role of the ligand and activator in selective Cr–PNP ethene tri- and tetramerization catalysts – a spectroscopic study

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Contents

1. General laboratory methods 3
1.1 Laboratory methods and materials 3
1.2 Stopped-flow UV–VIS measurements 3
1.3 EPR measurements 4
1.4 Cr K-edge measurements 4
1.5 Selective ethene oligomerization experiments 4
1.5.1 Experiments performed under 1 bar of ethene pressure 4
1.5.2 Experiments performed under 45 bar of ethene pressure 5
1.6 Computational methods 5
2. Spectroscopic results for the reaction of complex 1 and complex 2 with alkylaluminium compounds 6
2.1 Characterization of complex 1 6
2.2 Reaction of complex 1 with excess $AlMe_3$ 9
2.2.1 Cr K-edge XAS data 9
2.2.2 X-Band EPR data 12
2.2.3 UV–VIS data 13
2.3 Reaction of complex 1 with excess MMAO 14
2.3.1 Cr K-edge XAS data 14
2.3.2 X-Band EPR data 17
2.3.3 UV–VIS data 18
2.4 Characterization of complex 2 19
2.5 Reaction of complex 2 with excess $AlMe_3$ 22
2.5.1 Cr K-edge XAS data 22
2.5.2 X-Band EPR data 25
2.5.3 UV–VIS data 26
2.6 Reaction of complex 2 with excess MMAO 27
2.6.1 Cr K-edge XAS data 27
2.6.2 X-band EPR results 27
3. DFT calculations of the activation pathway of complex 1 and complex 2 29
3.1 Benchmarking study of basis set and functional 29
3.2 Thermochemistry for the reaction of complex 1 with $AlMe_3$ and MMAO. 30
3.3 Thermochemistry for the reaction of complex 2 with $AlMe_3$ 35
4. Spectroscopic results for activation experiments performed in the presence of substrates 41
4.1 Activation experiments for complex 2 in the presence of substrates 41
``4.2 Activation experiments for complex 1 in the presence of substrates 42
5. DFT calculations of the mechanism of selective ethene oligomerization 45

5.1 Mechanism for the selective ethene oligomerization catalyzed by monocationic chromium PNP (PNP = $((C_6H_5)_2P)_2N^{iPr}$) complexes 45
5.2 Mechanism for the selective ethene oligomerization catalyzed by dicationic chromium PNP (PNP = $((C_6H_5)_2P)_2N^{iPr}$) complexes 48
5.3 Mechanism for the selective ethene oligomerization catalyzed by monocationic chromium PNP (PNP = $((o\text{-}C_6H_4OMe)P)_2N^{Me}$) complexes 50
6. DFT coordinates 54
6.1 Benchmarking 54
6.2 Activation of complex 1 60
6.3 Activation of complex 2 88
6.4 Monocationc Cr^{II}/Cr^{IV} mechanism for complex 1 114
6.5 Dicationic Cr^{II}/Cr^{IV} mechanism for complex 1 135
6.6 Dicationic Cr^{II}/Cr^{IV} mechanism for complex 2 161
7. References 192

1. General laboratory methods

1.1 Laboratory methods and materials

All manipulations were performed under inert atmosphere (N_2 or Ar) using standard glovebox and Schlenk techniques. Solvents were dried, degassed and distilled prior to use. Trimethylaluminium (2M in toluene) was purchased from Sigma-Aldrich and MMAO-12 (7 wt.% in toluene) was purchased from Sigma-Aldrich and Akzo Nobel and were used as received. $CrCl_3(THF)_3$ was purchased from Strem.

NMR measurements were performed on a Bruker 300 MHz spectrometer, operating on Topspin software. Chemical shifts were referenced to TMS (^1H and ^{13}C) and H_3PO_4 (^{31}P).

The ligands, $((C_6H_5)_2P)_2N^{iPr}$ and $((o\text{-}C_6H_4OMe)_2P)_2N^{Me}$, and their corresponding complexes were synthesized according to previously published methods.[1–4]

1.2 Stopped-flow UV–VIS measurements

Stopped-flow UV–VIS experiments were performed using a modified SFM-400 stopped-flow UV–VIS from Biologic. The SFM-400 was modified so that the SFM-400 could be put under an argon atmosphere and Schlenk vessels could be connected. Below, an example is given for the activation of complex **1** and $AlMe_3$ (30 eq.). Other stopped-flow UV–VIS measurements have been performed in a similar fashion.

The SFM-400 consists of four separate syringes. Via microchannels, these syringes are connected to a cuvette. Prior to the experiment, the syringes were flushed with HCl (1M in H_2O), isopropanol and toluene, to remove any potential residues from previous experiments. Next, the syringes are flushed with argon, to ensure the microchannels are devoid of air. In two syringes, toluene solutions were loaded. In the third syringe, a 3.25 mM solution of complex **1** in toluene was loaded and in the fourth syringe, a solution containing $AlMe_3$ (500 mM) in toluene was loaded. Next, the microchannels were flushed with $AlMe_3$, followed by toluene, to ensure the microchannels contained no residual oxygen and moisture. Finally, complex **1** and $AlMe_3$ were reacted with one another. Mixing ratios were chosen to ensure a molar ratio of 1:30 of complex **1** and $AlMe_3$ respectively.

The obtained data was processed using an in-house MATLAB® script.

1.3 EPR measurements

EPR experiments were performed on a Bruker EMXplus EPR spectrometer running on XENON software. The EPR spectrometer was operating at a frequency of 9.4 GHz or 9.65 MHz. For all measurements, the modulation frequency was set to 100 kHz and the modulation amplitude was set to 4.0G unless otherwise stated. EPR experiments were performed either at room temperature or at cryogenic temperatures (10 or 20K). Below, the experiments are derscribed for the reaction between complex **1** and MMAO; other experiments were performed in a similar fashion.

Room temperature. The experiment was performed inside a glovebox. Complex **1** (9.0 mg, 13.7 µmol, 1 eq.) was dissolved into toluene (3 mL) and was reacted with MMAO in toluene (7 wt.% in Al, 3mL, 6.97 mmol, ~500 eq.). The solution was transferred to an EPR tube, was taken out of the glovebox and was rapidly loaded into the EPR cavity. The first measurement was performed after 6 minutes. Over the course of ~1 hour, multiple spectra were acquired. The amount of Cr^{I} was quantified by comparison of the double integral to the double integral of a TEMPO solution with a known concentration.

The obtained data was processed using an in-house MATLAB® script in combination with EasySpin.[5]

Cryogenic temperatures (20-30K). Experiments were performed similar to the experiment described above. After a reaction time of 10 minutes, the solution was frozen into liquid nitrogen and was loaded into the cavity, which was cooled to 20-30K.

Complex **1** and **2** were measured in a 1:1 mixture of DCM and toluene due to their limited solubility in solely toluene.

1.4 Cr K-edge measurements

Cr K-edge XAS measurements were performed at B18 (Diamond) in Didcot, United Kingdom and at BM26A (ESRF) in Grenoble, France. Complex **1** and complex **2** were measured as pellets, diluted with boron nitride. Other measurements were performed on frozen toluene solutions. Samples were kept frozen via the use of a Cryojet, which was set to a temperature of 100K.

Measurements at ESRF were performed with a Si(111) double crystal monochromator in transmission mode. A typical measurement required 2 minutes. 2 to 3 scans were required to obtain good signal-to-noise. All acquired spectra were calibrated to a Cr foil. XAS data processing was performed in Athena and EXAFS analysis was performed in Artemis. The amplitude reduction factor was determined using the Cr foil and was found to be 0.90.[6] Measurements at Diamond were performed with a Si(111) double crystal monochromator in fluoresence mode. Fluoresecence from the sample was detected with a 36 element Ge solid State detector. A typical measurement required 2 minutes. 30 to 50 scans were required to obtain good signal-to-noise. All acquired spectra were calibrated to a Cr foil. XAS data processing was performed in Athena and EXAFS analysis was performed in Artemis. The amplitude reduction factor was determined using the Cr foil and was found to be 0.84.[6] Below, a typical experiment is described; other experiments were performed in a similar fashion.

Experiments were performed inside a glovebox. Complex 1 (23.4 mg, 35.6 µmol, 1 eq.) was dissolved in toluene (0.25 mL). MMAO in toluene (7 wt.% Al, 6.9 mL, ~400 eq.) was added to this solution. The solution was put inside a Kapton® tube. After 2 minutes, the sample was taken out of the glovebox, rapidly frozen in liquid nitrogen and transferred to the beamline for measurement. Additional samples were taken after 10 minutes and 60 minutes.

1.5 Selective ethene oligomerization experiments

1.5.1 Experiments performed under 1 bar of ethene pressure

Below, a typical experiment is described for a selective ethene oligomerization experiment performed under 1 bar of ethene pressure.

Inside a glovebox, a stock solution of complex **1** (10.0 mg) in toluene (3 mL) was prepared. Outside the glovebox, a gastight balloon is attached to a three-necked Schlenk. The three-necked Schlenk was heated under vacuum and was backfilled with ethene. A septum was attached to the three-necked Schlenk and toluene (10 mL) and MMAO in toluene (7 wt.% Al, 1 mL) were injected. The stock solution of complex **1** was taken out of the glovebox and 1 mL of this solution was injected into the three-necked Schlenk. Catalysis was allowed to proceed for an hour, after which mesitylene (40.2 mg) in toluene (1 mL). The reaction was terminated by injecting MeOH (1 mL) and HCl in H_2O (1M, 10 mL). The solids (261.1 mg PE) were collected through filtration. The organic layer was dried with $MgSO_4$, filtered and its contents were analyzed through GC analysis.

1.5.2 Experiments performed under 45 bar of ethene pressure

Additional catalytic experiments were performed under increased ethene pressure. For these experiments, a Parr Hastelloy® autoclave (450 mL), equipped with an additional funnel was used.

A special drying protocol was developed, to ensure the autoclave was completely devoid of residual oxygen and moisture. The autoclave was subjected to vacuum and backfilled with nitrogen. This was repeated two more times. Next, MMAO in toluene (7 wt.% Al, 10 mL) was injected into the autoclave, together with 150 mL of toluene. The autoclave was heated to 120ºC and stirred for 3 hours. Afterwards, the autoclave was taken into a glovebox and the contents of the autoclave were removed.

Next, the autoclave was filled with toluene (94 mL), mesitylene (449.8 mg) and MMAO in toluene (7 wt.% Al, 6 mL) and the addition funnel was loaded with 18.5 mg of complex **1** in toluene (50 mL). The autoclave was removed from the glovebox, was heated to 45 ºC and was put under an ethene pressure of 45 bar. Next, complex **1** was injected into the autoclave and catalysis was allowed to proceed for 30 minutes. Afterwards, the reaction was quenched with MeOH (10 mL) and HCl in H_2O (1M, 100 mL). The solids were collected through filtration. The organic layer was dried with $MgSO_4$, filtered and its contents were analyzed through GC analysis.

1.6 Computational methods

DFT calculations were performed using the Amsterdam Density Functional (ADF) software package using version 2017.201.[7,8] In all calculations, BP86 was employed as a functional, TZ2P was employed as a basis set, and no frozen core approximation was used. BP86 was chosen as a functional, as a previous benchmarking study has shown that BP86 can accurately predict relative energies of the spin states of chromium.[9] Calculations were performed in the gas phase. Spin multiplicities of 1, 3 and 5 were considered for Cr^{I}, spin multiplicities of 0, 2 and 4 were considered for $Cr^{II,}$ and spin multiplicities of 1 and 3 were considered for Cr^{III}. Frequency calculations were performed to verify whether the optimized geometry had no imaginary frequencies and the transition state had a single imaginary frequency.

2. Spectroscopic results for the reaction of complex 1 and complex 2 with alkylaluminium compounds

2.1 Characterization of complex 1

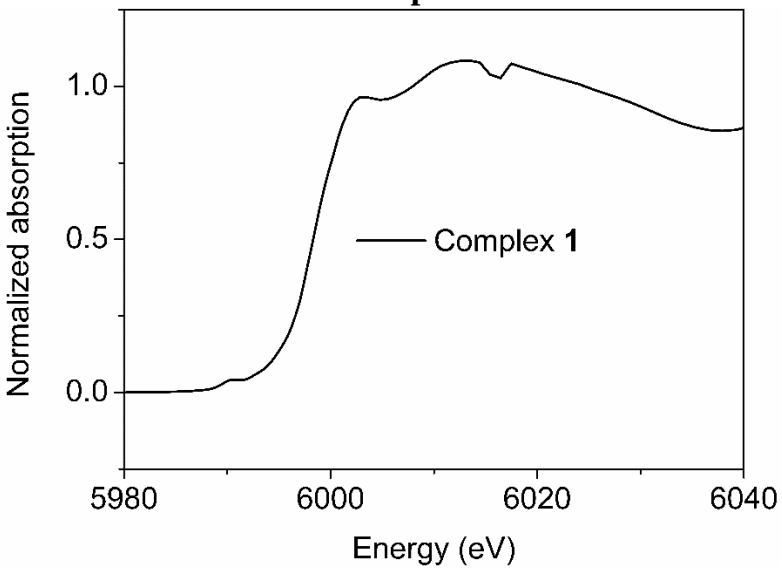


Figure S1. Cr K-edge XANES region of complex 1. The sample was measured as a pellet mixed with boron nitride.

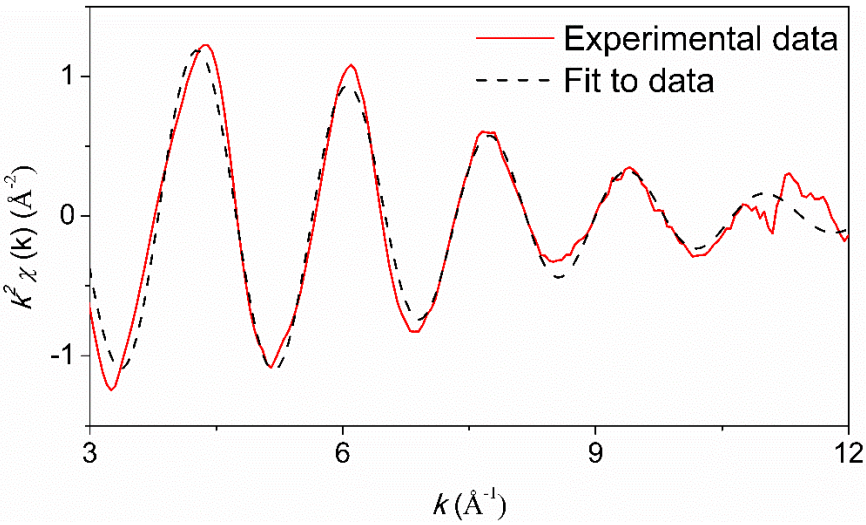


Figure S2. Cr K-edge k^2-weighted EXAFS data of complex 1. The sample was measured as a pellet mixed with boron nitride.

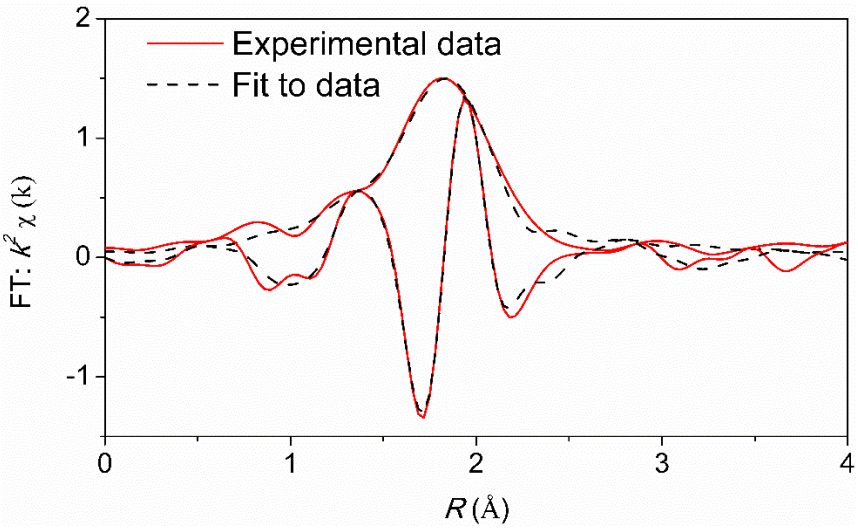


Figure S3. Fourier transform of the Cr K-edge k^2-weighted EXAFS data of complex 1. The sample was measured as a pellet mixed with boron nitride.

Table S1. Cr K-edge EXAFS data fitting results for complex 1. These parameters were used to obtain the fits shown in Figure S2 and Figure S3.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–O	1	0.002(5)	2.15(3)
Cr–Cl	3	0.011(2)	2.32(2)
Cr–P	2	0.011(2)	2.32(2)

General fitting parameters: $S_0^2 = 0.90$, $E_0 = 0(2)$ eV, $\Delta k = 3.40 – 11.60$ Å^{-1}, $\Delta R = 1– 3$ Å, $R^2 = 0.013$, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

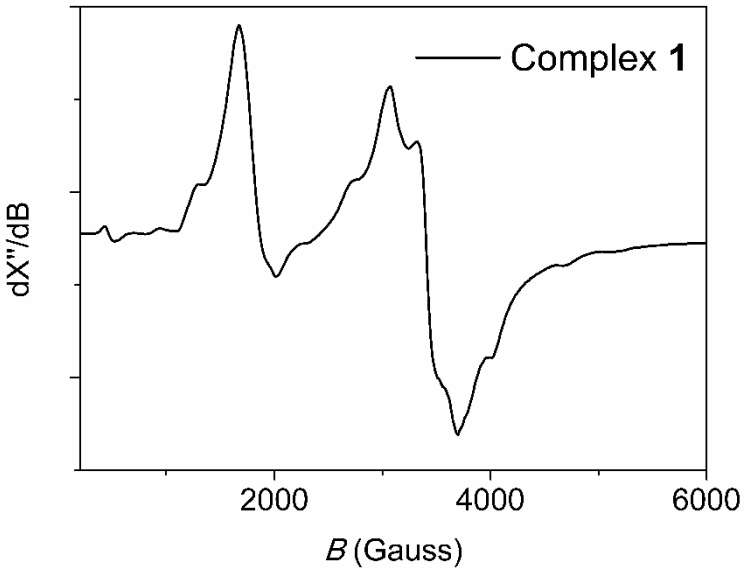


Figure S4. X-Band EPR spectrum of complex 1, measured in a 1:1 mixture of toluene and DCM, acquired at a temperature of 20K. The spectrometer was operating at a frequency of 9.4 GHz.

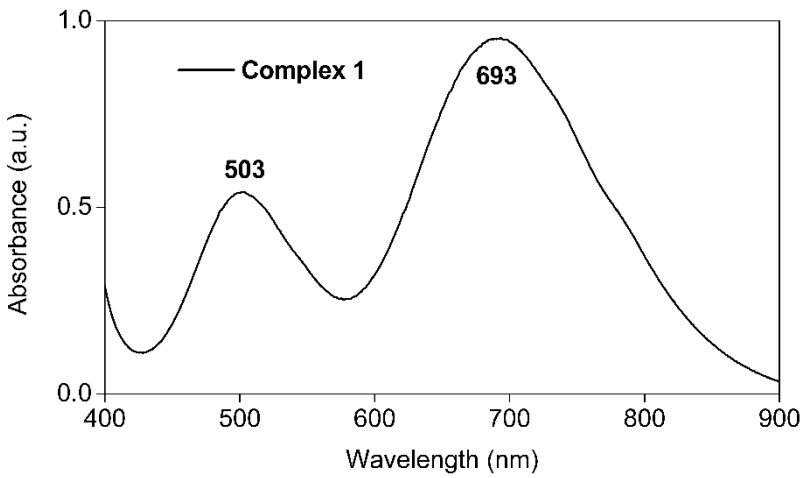


Figure S5. UV–VIS spectrum of complex 1, measured in toluene.

2.2 Reaction of complex 1 with excess $AlMe_3$

2.2.1 Cr K-edge XAS data

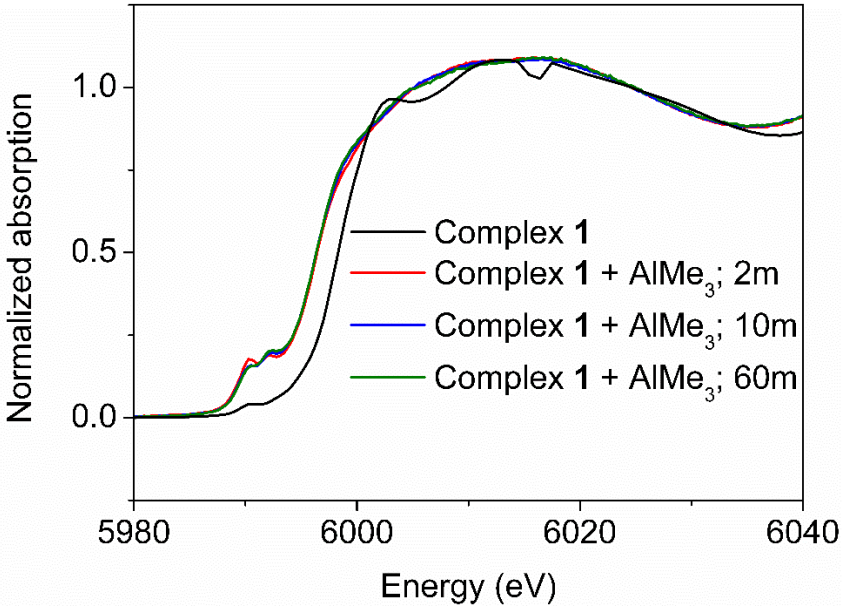


Figure S6. Cr K-edge XANES region for the reaction between complex 1 and $AlMe_3$ (40 eq.) in toluene, frozen after reaction times of 2 minutes, 10 minutes and 60 minutes. The final concentration in Cr after mixing was ~25.5 mM.

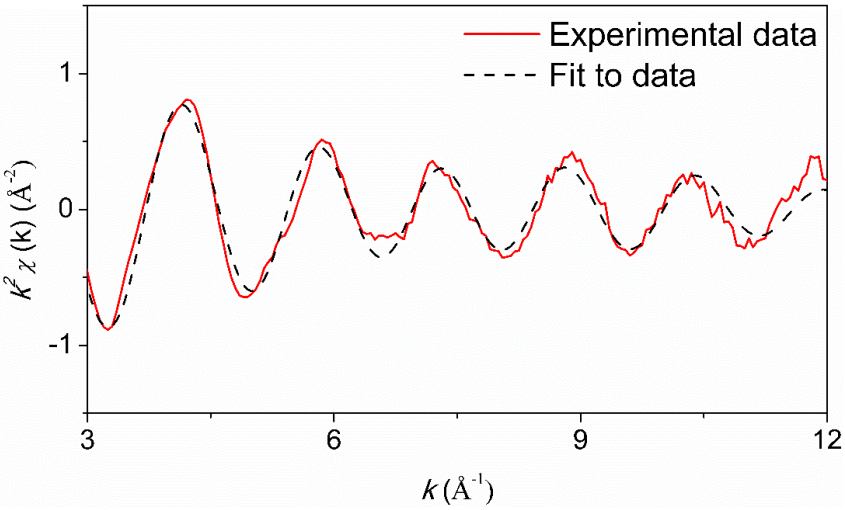


Figure S7. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and $AlMe_3$ (40 eq.) in toluene, frozen after 2 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

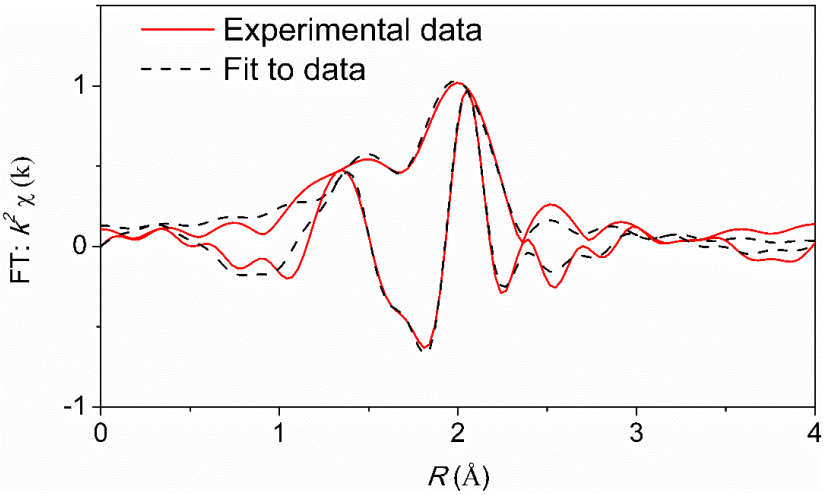


Figure S8. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and $AlMe_3$ (40 eq.) in toluene, frozen after 2 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

Table S2. Cr K-edge EXAFS data fitting results for the reaction complex 1 and AlMe3 (40 eq.), frozen after 2 minutes. These parameters were used to obtain the fits shown in Figure S7 and Figure S8.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–C	1.4(5)	0.002(4)	2.03(2)
Cr–Cl	1	0.0060(7)	2.43(1)
Cr–P	2	0.0060(7)	2.43(1)

General fitting parameters: $S_0^2 = 0.84$, $E_0 = 0(1)$ eV, $\Delta k = 2.70 – 11.40$ Å^{-1}, $\Delta R = 1.18 – 3$ Å, $R^2 = 0.020$, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

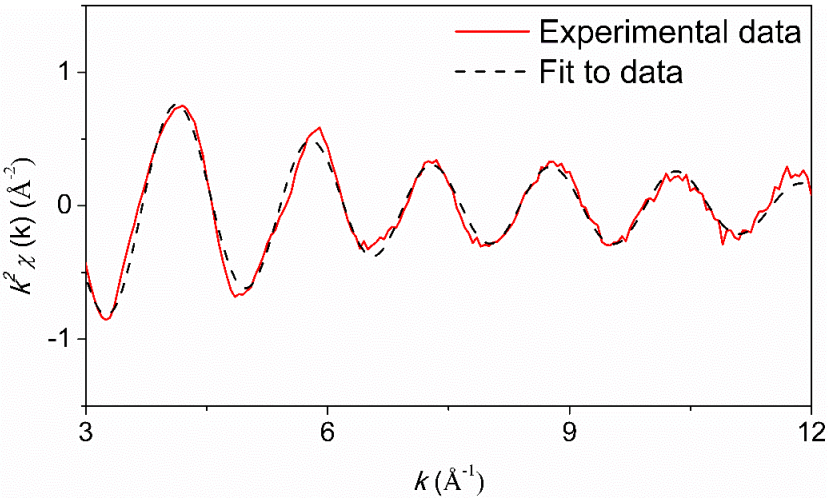


Figure S9. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and $AlMe_3$ (40 eq.) in toluene, frozen after 10 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

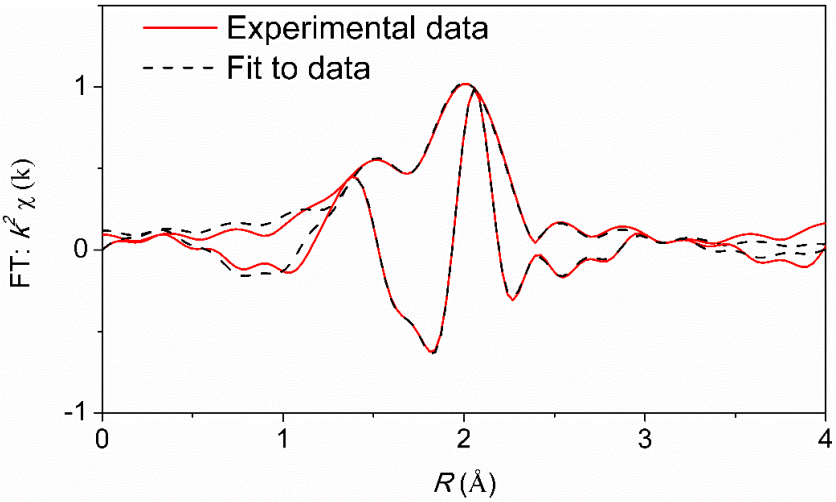


Figure S10. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and $AlMe_3$ (40 eq.) in toluene, frozen after 10 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

Table S3. Cr K-edge EXAFS data fitting results for the reaction complex 1 and $AlMe_3$ (40 eq.), frozen after 10 minutes. These parameters were used to obtain the fits shown in Figure SFigure S9 and Figure S10.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–C	1.0(2)	0.000(2)	2.046(8)
Cr–Cl	1	0.0059(3)	2.443(4)
Cr–P	2	0.0059(3)	2.443(4)

General fitting parameters: S_0^2 = 0.84, E_0 = 1.3(4) eV, Δk = 2.70 – 11.40 Å^{-1}, ΔR = 1.21– 3 Å, R^2 = 0.003, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

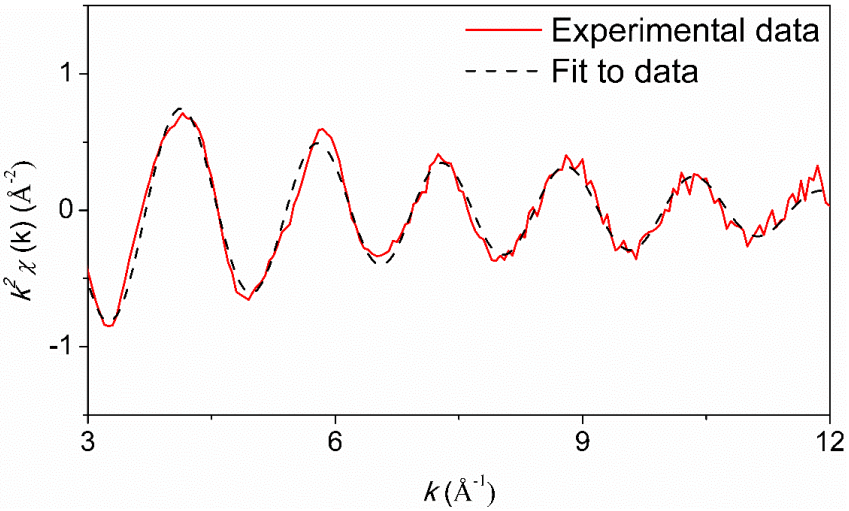


Figure S11. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and $AlMe_3$ (40 eq.) in toluene, frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

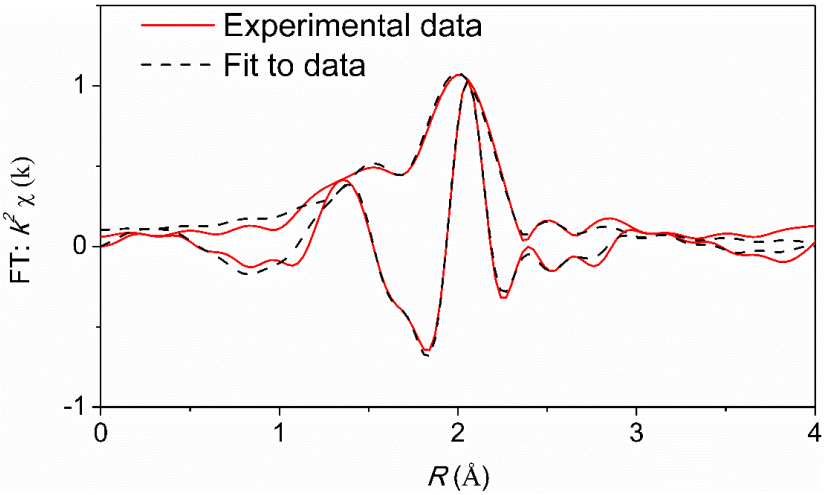


Figure S12. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and $AlMe_3$ (40 eq.) in toluene, frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

Table S4. Cr K-edge EXAFS data fitting results for the reaction complex 1 and $AlMe_3$ (40 eq.), frozen after 60 minutes. These parameters were used to obtain the fits shown in Figure Figure S11 and Figure S12.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–C	1.1(3)	0.002(3)	2.03(1)
Cr–Cl	1	0.0056(4)	2.440(5)
Cr–P	2	0.0056(4)	2.440(5)

General fitting parameters: S_0^2 = 0.84, E_0 = 1.0(6) eV, Δk = 2.70 – 12 Å^{-1}, ΔR = 1.16– 3.50 Å, R^2 = 0.011, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

2.2.2 X-Band EPR data

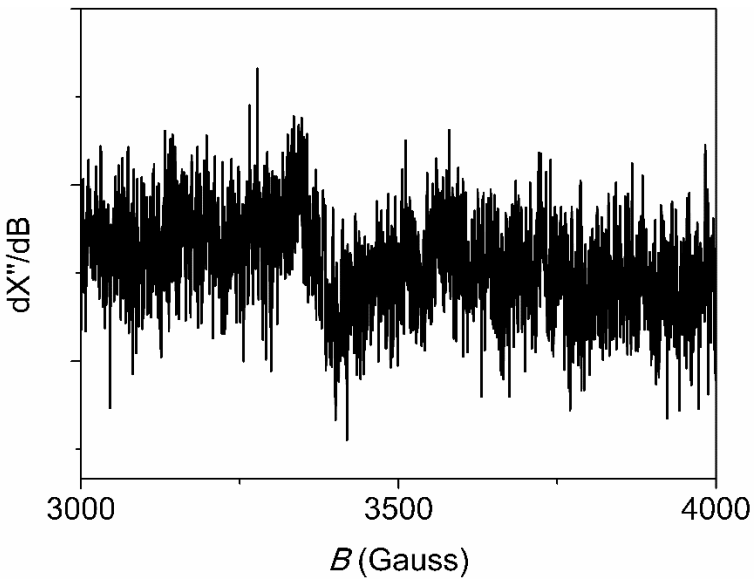


Figure S13. X-Band EPR spectrum for the reaction between 1 and $AlMe_3$ (40 eq.) in toluene, acquired at room temperature after a reaction time of 10 minutes. The final concentration in Cr after mixing was ~4.5 mM. The spectrometer was operating at a frequency of 9.4 GHz.

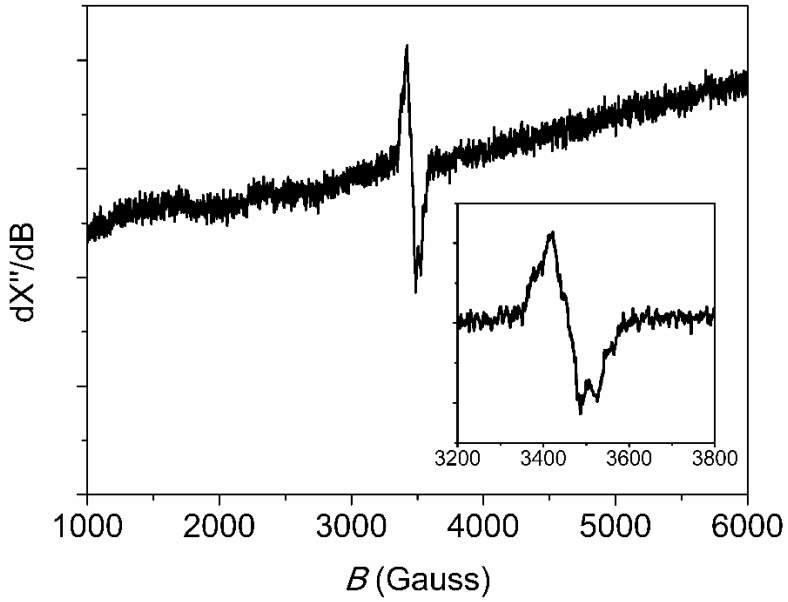


Figure S14. X-Band EPR spectrum for the reaction between 1 and $AlMe_3$ (40 eq.) in toluene, acquired at cryogenic temperatures after a reaction time of 10 minutes. The final concentration in Cr after mixing was ~4.5 mM. The spectrometer was operating at a frequency of 9.65 GHz.

2.2.3 UV–VIS data

In Figure S15, stopped-flow UV–VIS data for the reaction of complex **1** with $AlMe_3$ (30 eq.) in toluene is depicted. Complex **1** shows absorption peaks at λ = 502 nm and λ = 690 nm. After reaction with $AlMe_3$, the absorption peaks of complex **1** immediately (<5s) disappear and a novel absorption peak becomes visible at λ = 650 nm. Over time (~600s), the absorption peak shifts from λ = 650 nm to λ = 718 nm. The origin of this shift is unknown, as no X-Band EPR or Cr K-edge XAS data was acquired at shorter timescales (<120s).

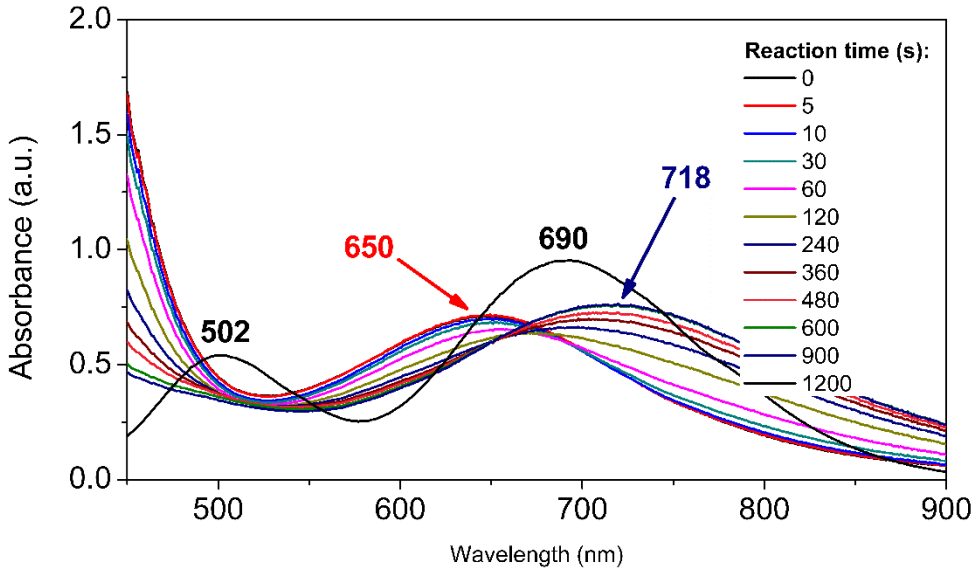


Figure S15. Stopped-flow UV–VIS spectra of the reaction of complex 1 with $AlMe_3$ (30 eq.) in toluene. The final concentration in Cr after mixing was ~3.0 mM.

2.3 Reaction of complex 1 with excess MMAO

2.3.1 Cr K-edge XAS data

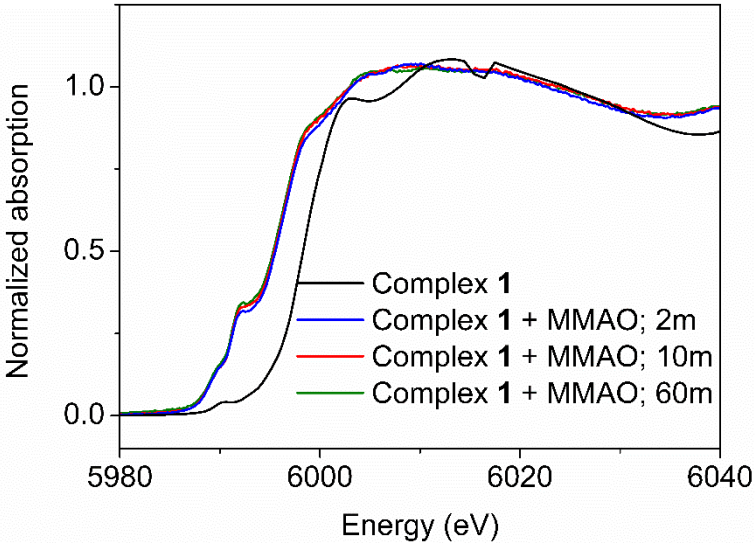


Figure S16. Cr K-edge XANES region for the reaction between complex 1 and MMAO (400 eq.) in toluene, frozen after reaction times of 2 minutes, 10 minutes and 60 minutes. The final concentration in Cr after mixing was ~5.0 mM.

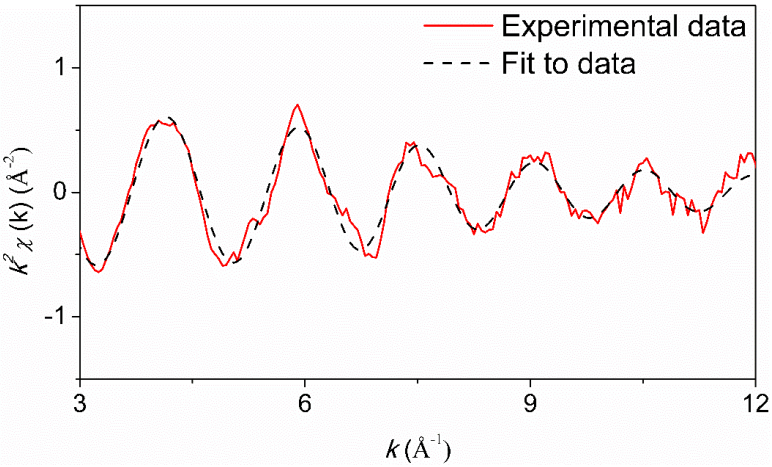


Figure S17. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, frozen after 2 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~5.0 mM.

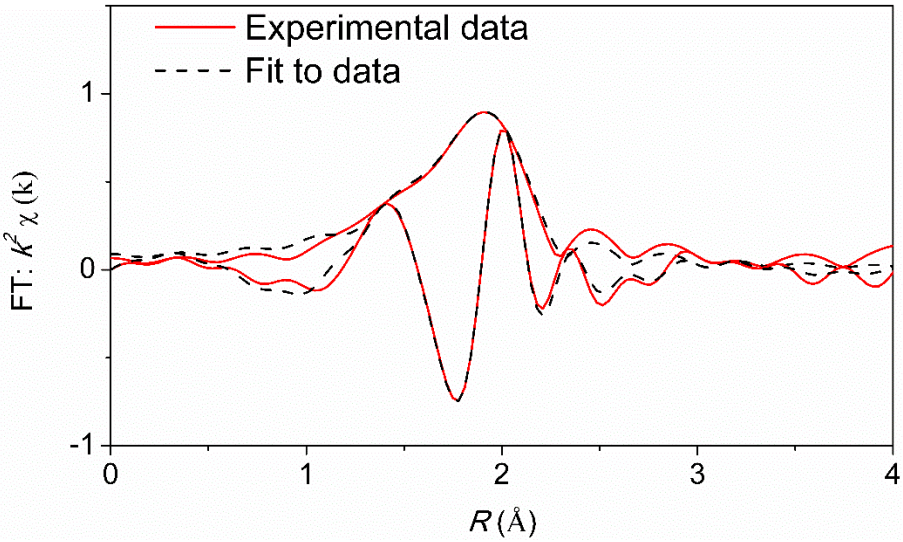


Figure S18. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, frozen after 2 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~5.0 mM.

Table S5. Cr K-edge EXAFS data fitting results for the reaction complex 1 and MMAO (400 eq.), frozen after 2 minutes. These parameters were used to obtain the fits shown in Figure S17 and Figure S18.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–C	1	0.003(3)	2.14(5)
Cr–P	2	0.0030(7)	2.41(1)

General fitting parameters: $S_0^2 = 0.84$, $E_0 = 0(2)$ eV, $\Delta k = 2.70 – 11.5$ Å^{-1}, $\Delta R = 1.16 – 3$ Å, $R^2 = 0.010$, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

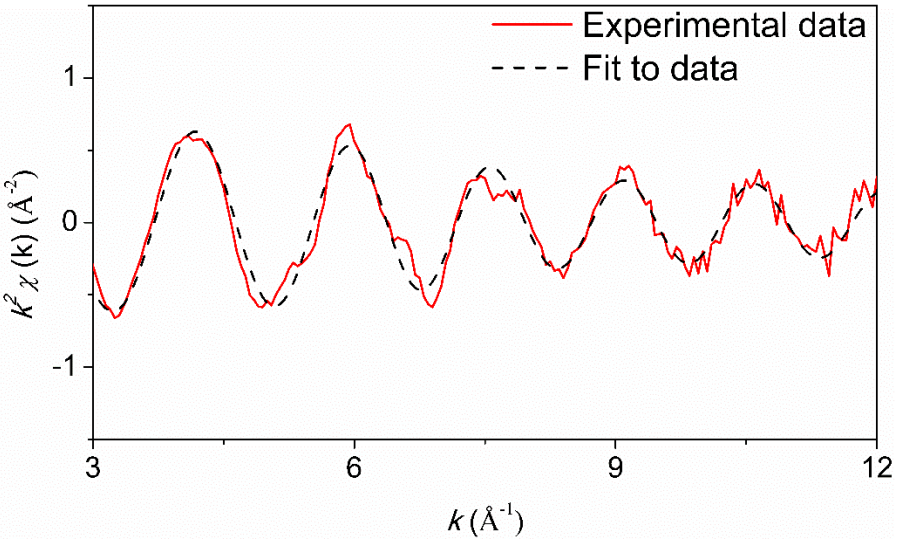


Figure S19. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, frozen after 10 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~5.0 mM.

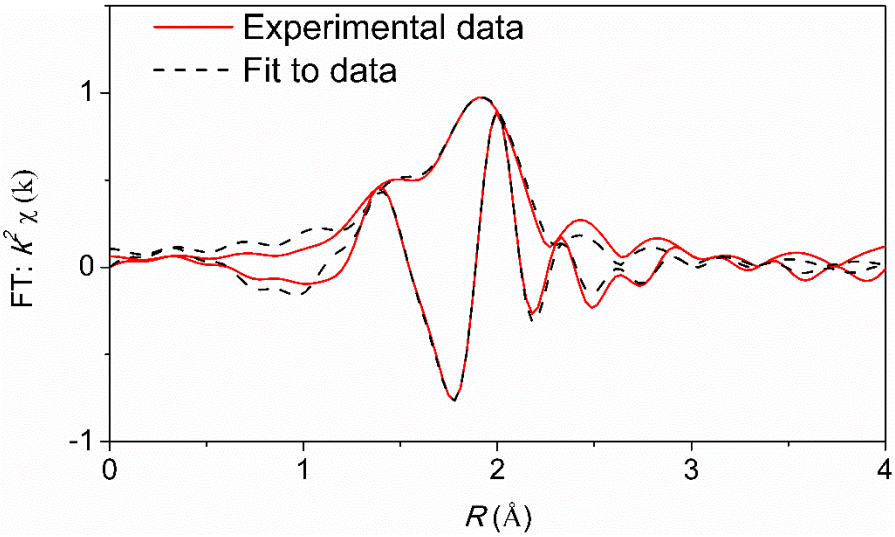


Figure S20. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, frozen after 10 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~5.0 mM.

Table S6. Cr K-edge EXAFS data fitting results for the reaction complex 1 and MMAO (400 eq.), frozen after 10 minutes. These parameters were used to obtain the fits shown in Figure S19 and Figure S20.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–C	1	0.003(4)	2.08(5)
Cr–P	2	0.0018(7)	2.39(1)

General fitting parameters: S_0^2 = 0.84, E_0 = -2(2) eV, Δk = 2.70 – 11.60 Å^{-1}, ΔR = 1.19– 3 Å, R^2 = 0.014, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

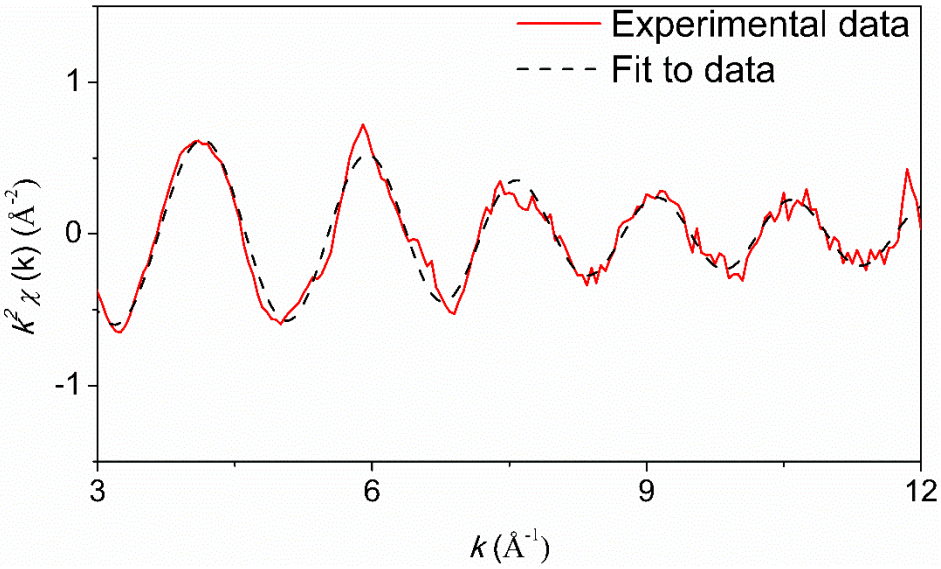


Figure S21. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~5.0 mM.

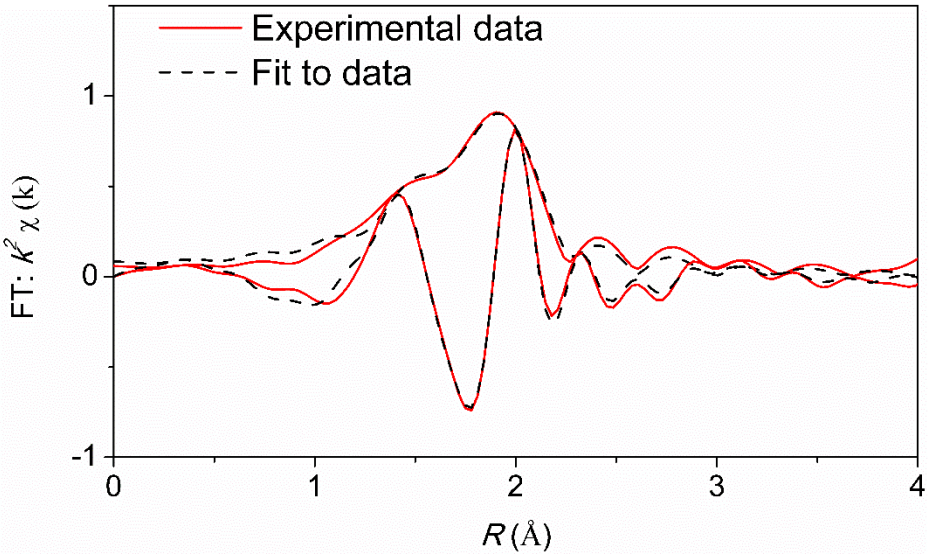


Figure S22. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~5.0 mM.

Table S7. Cr K-edge EXAFS data fitting results for the reaction complex 1 and MMAO (400 eq.), frozen after 60 minutes. These parameters were used to obtain the fits shown in Figure S21 and Figure S22

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–C	1	0.002(2)	2.08(3)
Cr–P	2	0.0023(5)	2.384(9)

General fitting parameters: S_0^2 = 0.84, E_0 = -3(1) eV, Δk = 2.80 – 12.00 Å^{-1}, ΔR = 1.19– 3 Å, R^2 = 0.009, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

2.3.2 X-Band EPR data

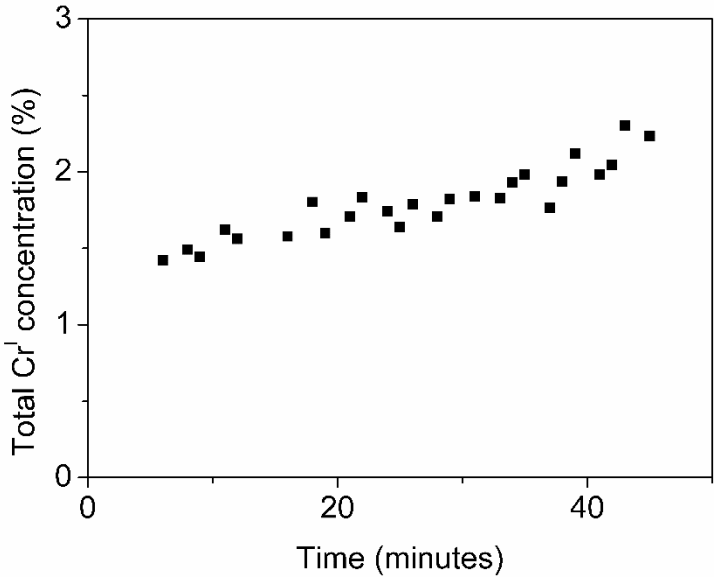


Figure S23. Concentration of bis(toluene)Cr^I as a function of time for the reaction between complex 1 and MMAO (~500 eq.). The concentration of Cr^I was determined by comparing the double integral to the double integral of a TEMPO solution in toluene with a known concentration. The concentration in Cr after mixing was ~2.5 mM. The spectrometer was operating at a frequency of 9.4 GHz.

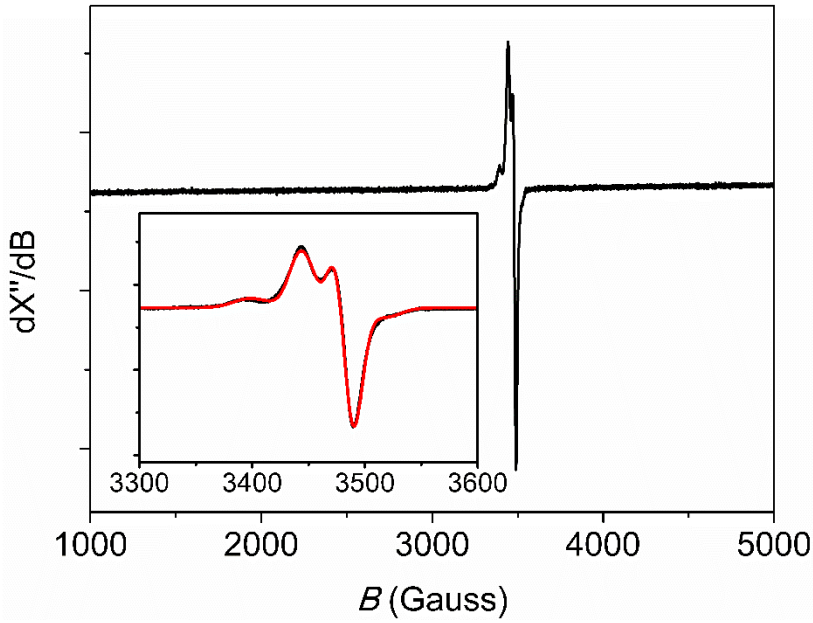


Figure S24. X-Band EPR spectrum for the reaction between 1 and MMAO (~500 eq.) in toluene, acquired at cryogenic temperatures after a reaction time of 10 minutes. The inset of the figure shows a fit (red) of the experimental spectrum (black) and was found to consist of two Cr^{I} complexes. For the first component (S=1/2) a fit was obtained using $g_{x,y}$ = 1.979 and g_z = 2.005, by applying Gaussian broadening (50 MHz) and a relative weighting of 1. For the second component (S=1/2) a fit was obtained using g_z = 2.032, g_y = 1.996 and g_x = 1.961, and by applying Gaussian broadening (88, 47 and 96 MHz respectively) and a relative weighting of 0.67. The concentration in Cr after mixing was ~2.5 mM. The spectrometer was operating at a frequency of 9.65 GHz.

2.3.3 UV–VIS data

In Figure S25, stopped-flow UV–VIS data for the reaction of complex **1** with MMAO (500 eq.) in toluene is depicted. The absorption peaks for complex **1** were already discussed in Section 2.2.3. After reaction with MMAO, the absorption peaks of complex **1** immediately (<1s) disappear and a novel absorption peak becomes visible at λ = 661 nm. In line with Cr K-edge XAS data (Section 2.3.1), no further time-dependent changes in the position of the absorption peak is observed.

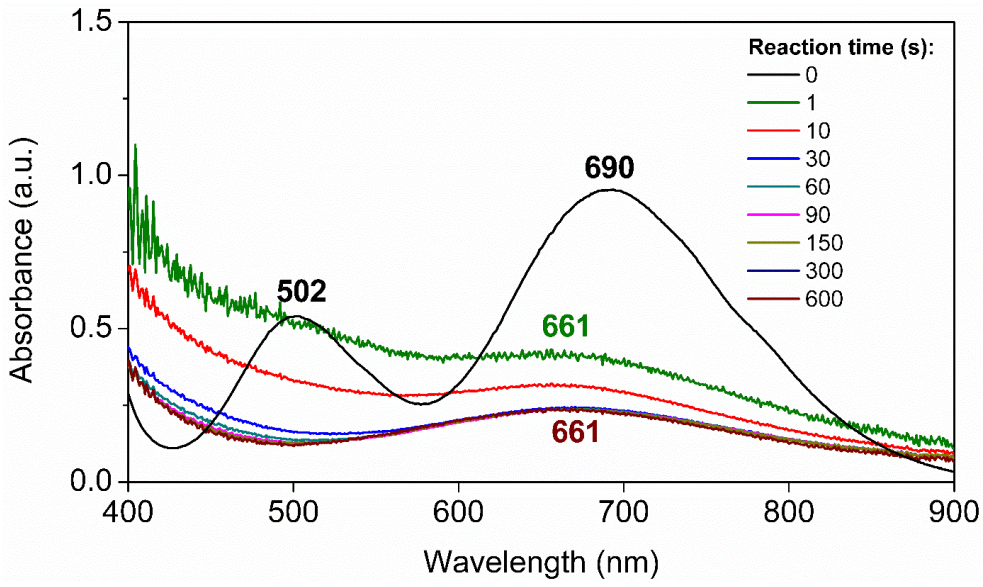


Figure S25. Stopped-flow UV–VIS spectra of the reaction of complex 1 with MMAO (~500 eq.) in toluene. The final concentration in Crafter mixing was ~2.5 mM.

2.4 Characterization of complex 2

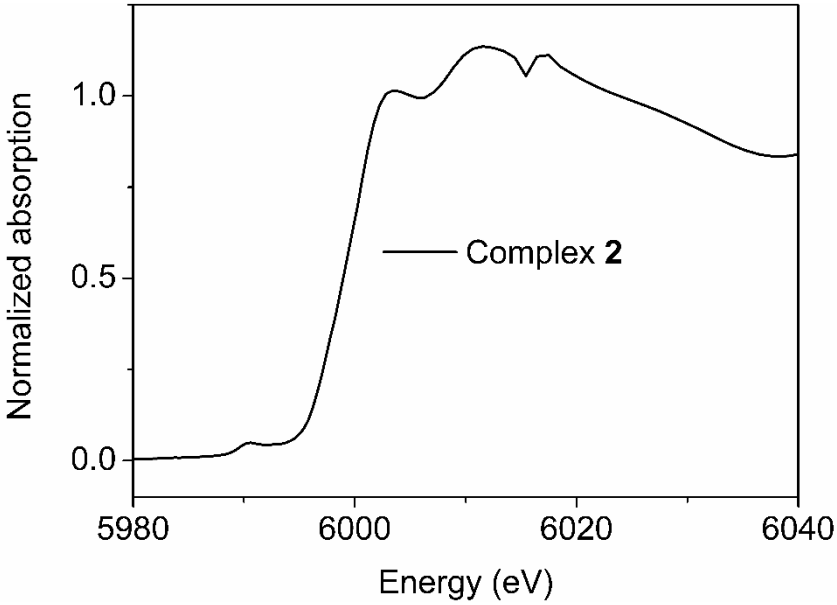


Figure S26. Cr K-edge XANES region of complex 2. The sample was measured as a pellet mixed with boron nitride.

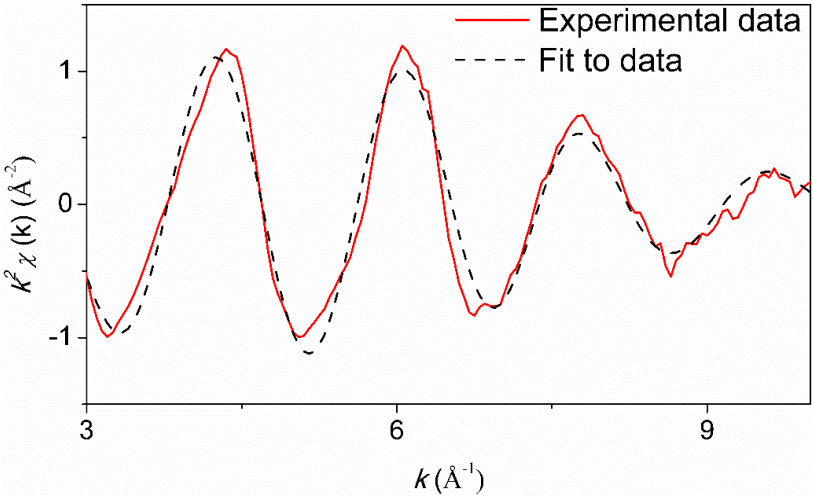


Figure S27. Cr K-edge k^2-weighted EXAFS data of complex 2. The sample was measured as a pellet mixed with boron nitride.

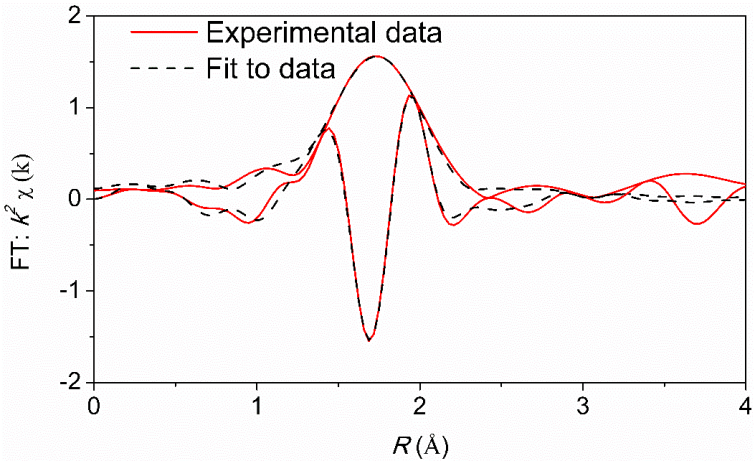


Figure S28. Fourier transform of the Cr K-edge k^2-weighted EXAFS data of complex 2. The sample was measured as a pellet mixed with boron nitride.

Table S8. Cr K-edge EXAFS data fitting results for complex 2. These parameters were used to obtain the fits shown in Figure S27 and Figure S28.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d* (Cr–X) (Å)**
Cr–O	1	0.0030	2.156
Cr–Cl	3	0.003(2)	2.24(2)
Cr–P	2	0.002(3)	2.43(3)

General fitting parameters: $S_0^2 = 0.90$, $E_0 = -1(2)$ eV, $\Delta k = 2.70 – 10$ Å^{-1}, $\Delta R = 1.28 – 3$ Å, $R^2 = 0.011$, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell. Parameters for the Cr–O shell were kept fixed.

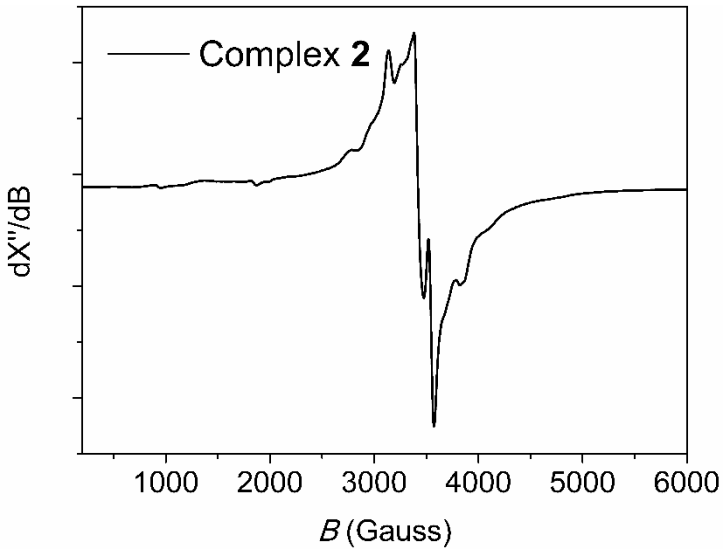


Figure S29. X-Band EPR spectrum of complex 2, measured in a 1:1 mixture of toluene and DCM, acquired at a temperature of 20K. The spectrometer was operating at a frequency of 9.4 GHz.

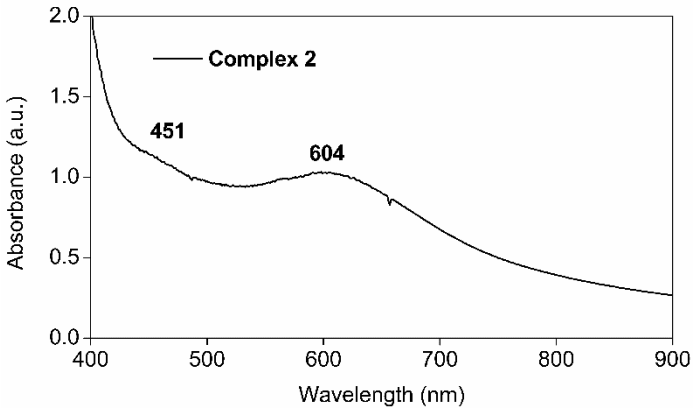


Figure S30. UV–VIS spectrum of complex 2, measured in DCM.

2.5 Reaction of complex 2 with excess $AlMe_3$

2.5.1 Cr K-edge XAS data

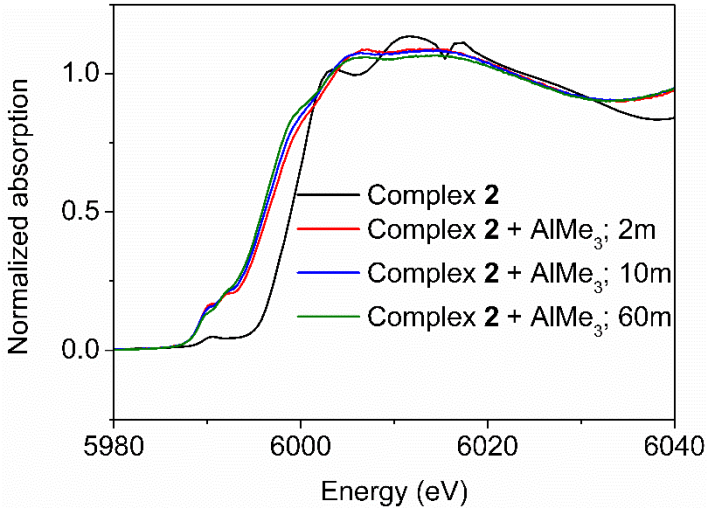


Figure S31. Cr K-edge XANES region for the reaction between complex 2 and $AlMe_3$ (40 eq.) in toluene, frozen after reaction times of 2 minutes, 10 minutes and 60 minutes. The final concentration in Cr after mixing was ~25.5 mM.

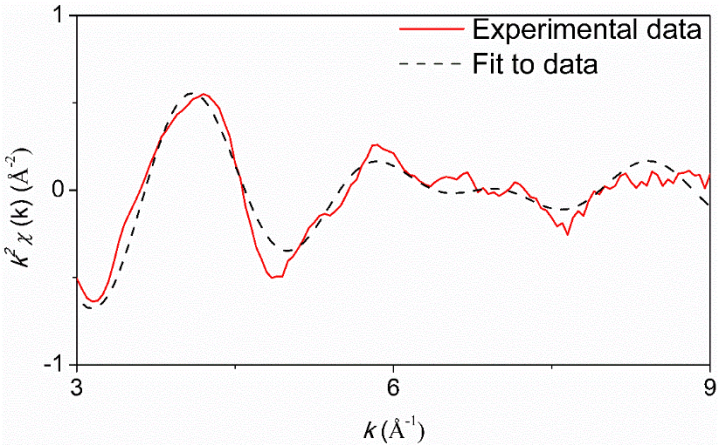


Figure S32. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 2 and $AlMe_3$ (40 eq.) in toluene, frozen after 2 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

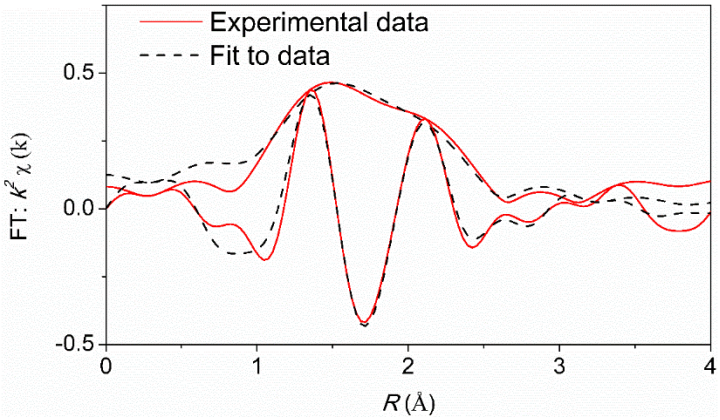


Figure S33. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 2 and $AlMe_3$ (40 eq.) in toluene, frozen after 2 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

Table S9. Cr K-edge EXAFS data fitting results for the reaction complex 2 and $AlMe_3$ (40 eq.), frozen after 2 minutes. These parameters were used to obtain the fits shown in Figure S32 and Figure S33.

Coordination shell	N	σ^2 (Å^{-2})	*d* (Cr–X) (Å)
Cr–C	2	0.002(2)	2.07(4)
Cr–P	2	0.010(3)	2.48(3)

General fitting parameters: S_0^2 = 0.84, E_0 = -1(3) eV, Δk = 2.70 – 8.00 Å^{-1}, ΔR = 1.19– 3.50 Å, R^2 = 0.018, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

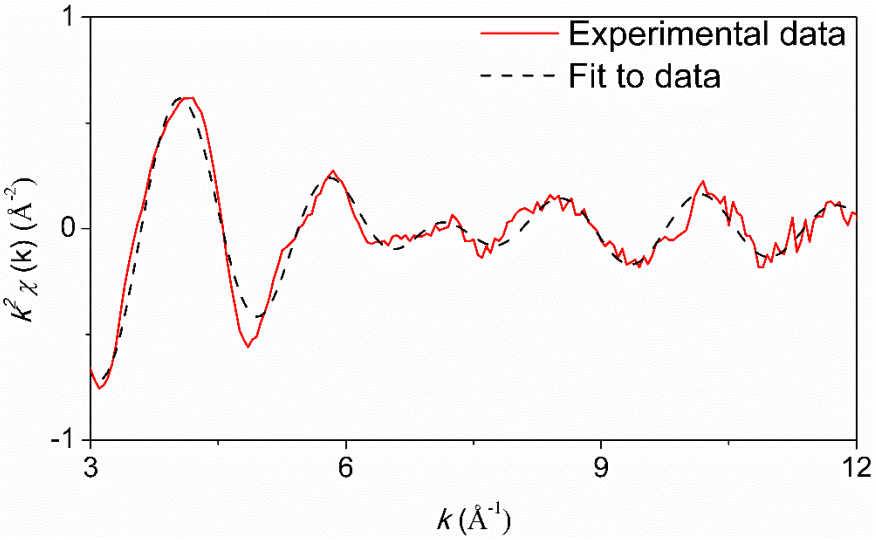


Figure S34. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 2 and $AlMe_3$ (40 eq.) in toluene, frozen after 10 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

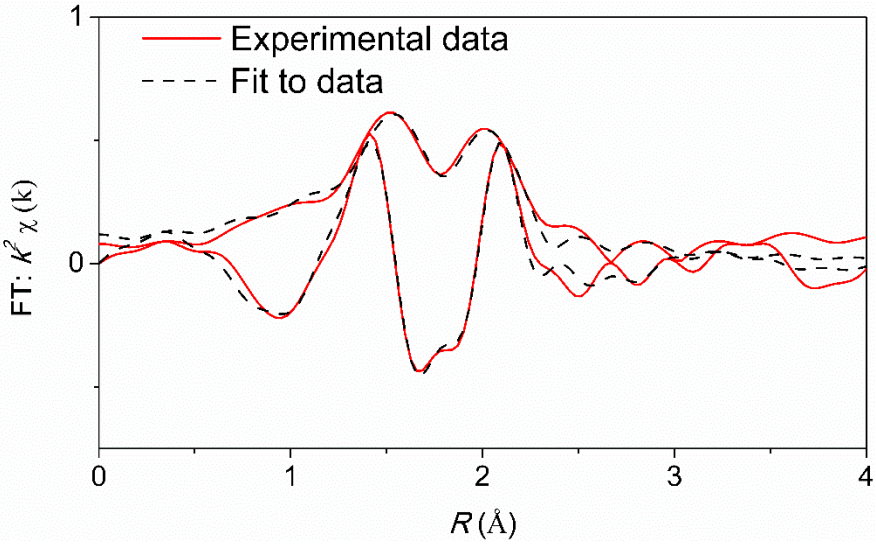


Figure S35. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 2 and $AlMe_3$ (40 eq.) in toluene, frozen after 10 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

Table S10. Cr K-edge EXAFS data fitting results for the reaction complex 2 and $AlMe_3$ (40 eq.), frozen after 10 minutes. These parameters were used to obtain the fits shown in Figure S34 and Figure S35.

Coordination shell	N	σ^2 (Å^{-2})	*d* (Cr–X) (Å)
Cr–C	2.3(4)	0.003(1)	2.07(2)
Cr–P	2	0.007(1)	2.46(1)

General fitting parameters: S_0^2 = 0.84, E_0 = -3(1) eV, Δk = 2.70 – 11.5 Å^{-1}, ΔR = 1.14– 3.00 Å, R^2 = 0.023, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

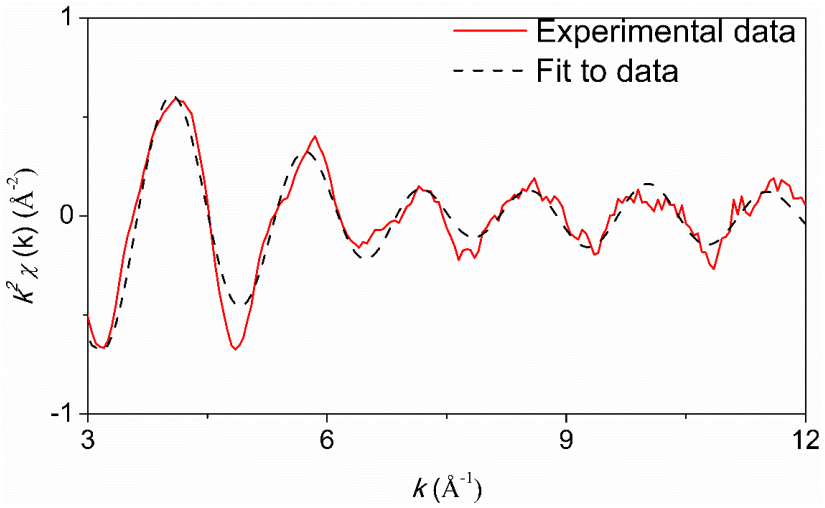


Figure S36. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 2 and $AlMe_3$ (40 eq.) in toluene, frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

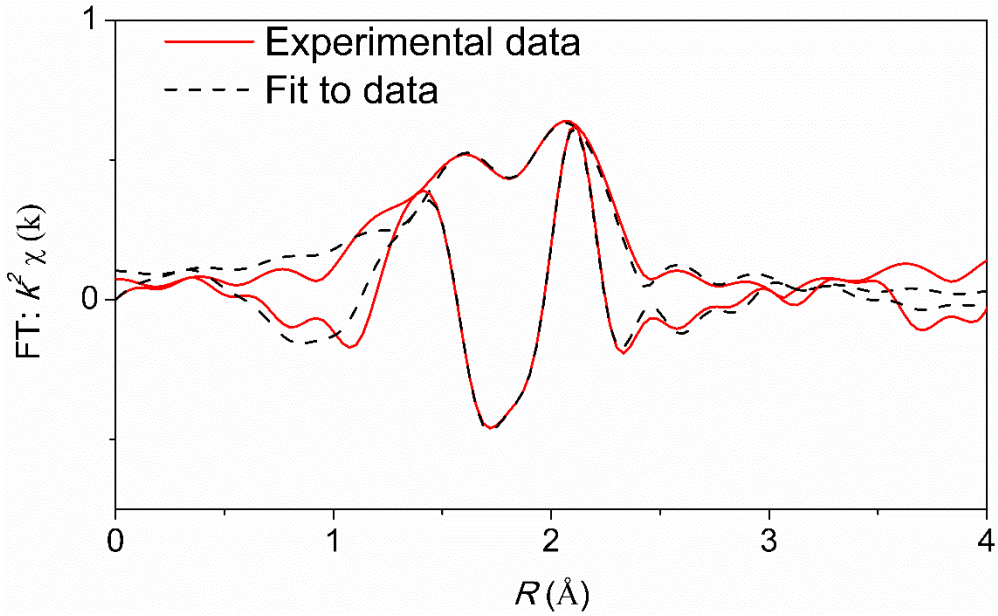


Figure S37. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 2 and $AlMe_3$ (40 eq.) in toluene, frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~25.5 mM.

Table S11. Cr K-edge EXAFS data fitting results for the reaction complex 2 and $AlMe_3$ (40 eq.), frozen after 60 minutes. These parameters were used to obtain the fits shown in Figure S36 and Figure S37.

Coordination shell	N	σ^2 (Å^{-2})	*d* (Cr–X) (Å)
Cr–C	1.7(4)	0.003(3)	2.13(2)
Cr–P	2	0.0058(9)	2.51(1)

General fitting parameters: S_0^2 = 0.84, E_0 =2(1) eV, Δk = 2.70 – 11.4 Å^{-1}, ΔR = 1.21– 3.00 Å, R^2 = 0.013, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

2.5.2 X-Band EPR data

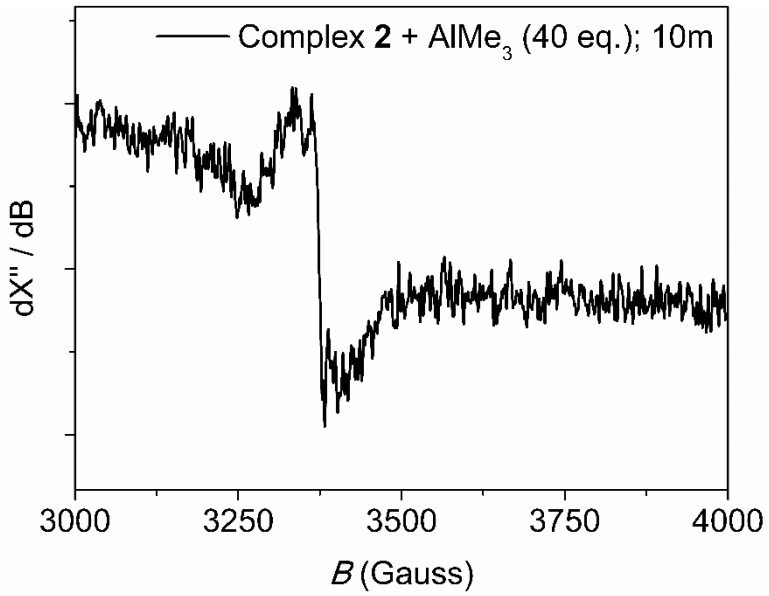


Figure S38. X-Band EPR spectrum for the reaction between 2 and $AlMe_3$ (40 eq.) in toluene, acquired at room temperature after a reaction time of 10 minutes. The final concentration after mixing was ~4.5 mM. The spectrometer was operating at a frequency of 9.4 GHz.

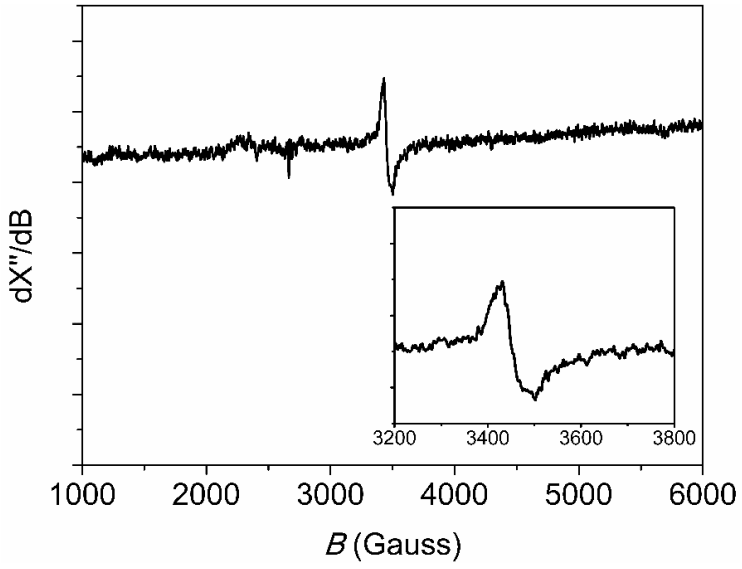


Figure S39. X-Band EPR spectrum for the reaction between 2 and $AlMe_3$ (40 eq.) in toluene, acquired at cryogenic temperatures (10K) after a reaction time of 10 minutes. The final concentration after mixing was ~4.5 mM. The spectrometer was operating at a frequency of 9.65 GHz.

2.5.3 UV–VIS data

Due to the poor solubility of complex **2** it was not possible to acquire stopped-flow data for the reaction between complex **2** and $AlMe_3$ (20 eq.). Instead, UV–VIS data was acquired in five minute intervals in a sealed cuvette; the results are depicted in Figure S40. Complex **2** shows absorption peaks at λ = 451 nm and λ = 604 nm. After reaction of complex **2** with $AlMe_3$ (20 eq.), a broad absorption peak ($\lambda \approx$ 550 nm) is observed in the UV–VIS data. In line with the Cr K-edge XAS data (Section 2.5.1), this feature does not change with time.

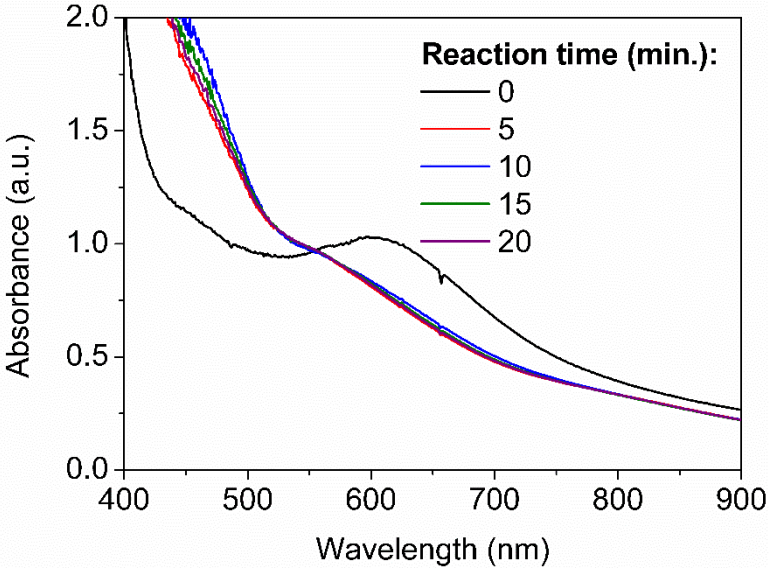


Figure S40. UV–VIS spectra of the reaction of complex 2 with $AlMe_3$ (20 eq.) in toluene. The final concentration in Cr after mixing was ~3.3 mM.

2.6 Reaction of complex 2 with excess MMAO

2.6.1 Cr K-edge XAS data

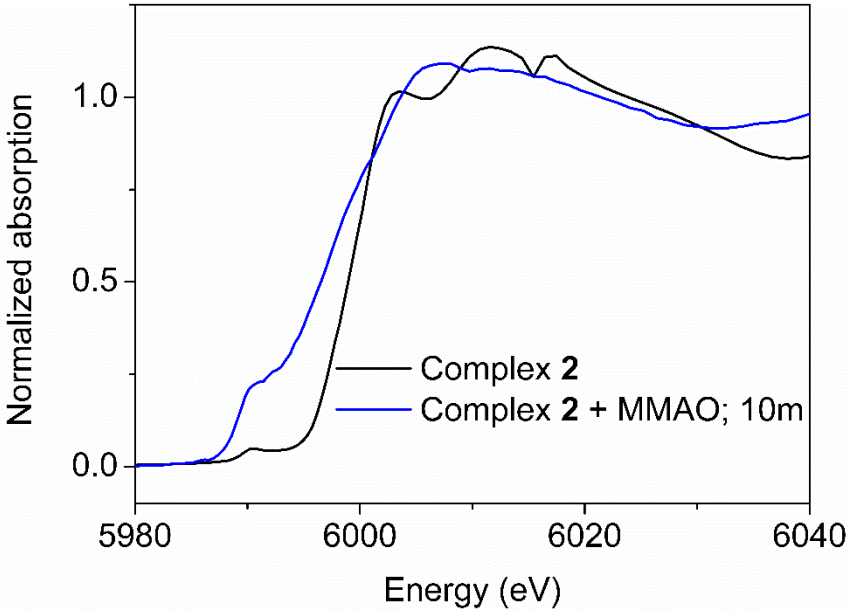


Figure S41. Cr K-edge XANES region for the reaction between complex 2 and MMAO (400 eq.) in toluene, frozen after a reaction time of 10 minutes. The final concentration of Cr in solution is unknown, due to the slow reactivity of the complex with MMAO.

2.6.2 X-band EPR results

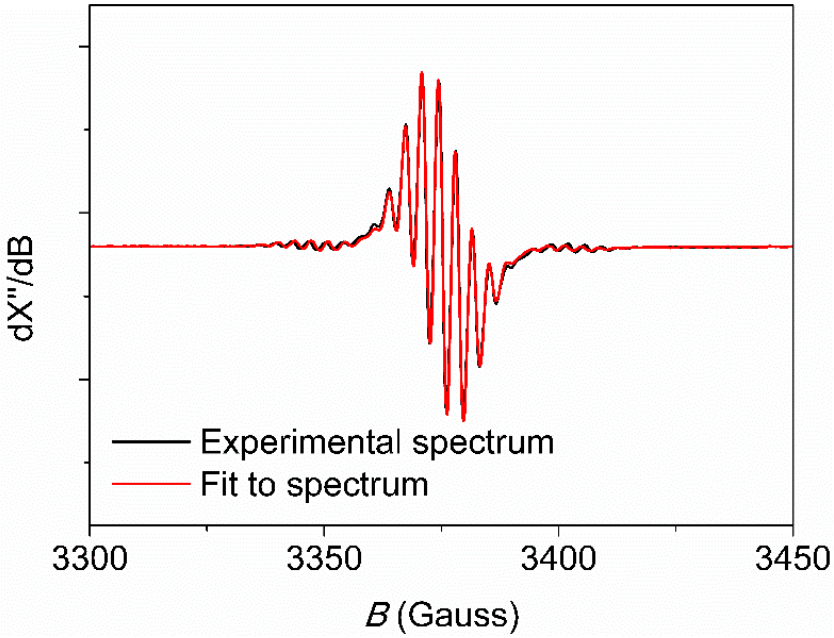


Figure S42. X-band EPR spectrum for the reaction between complex 2 and MMAO (400 eq.) in toluene, acquired in toluene after a reaction time of 10 minutes. The final concentration of Cr in solution is unknown, due to the slow reactivity of the complex with MMAO. The fit was obtained using g_{iso} = 1.987, by taking into account the (super)hyperfine interaction with 10 neighboring hydrogen atoms (A_H = 9.83 MHz) and 1 chromium atom (A_{Cr} = 51.2 MHz) and by applying Lorentzian broadening (0.3443 MHz). The spectrometer was operating at a frequency of 9.4 GHz.

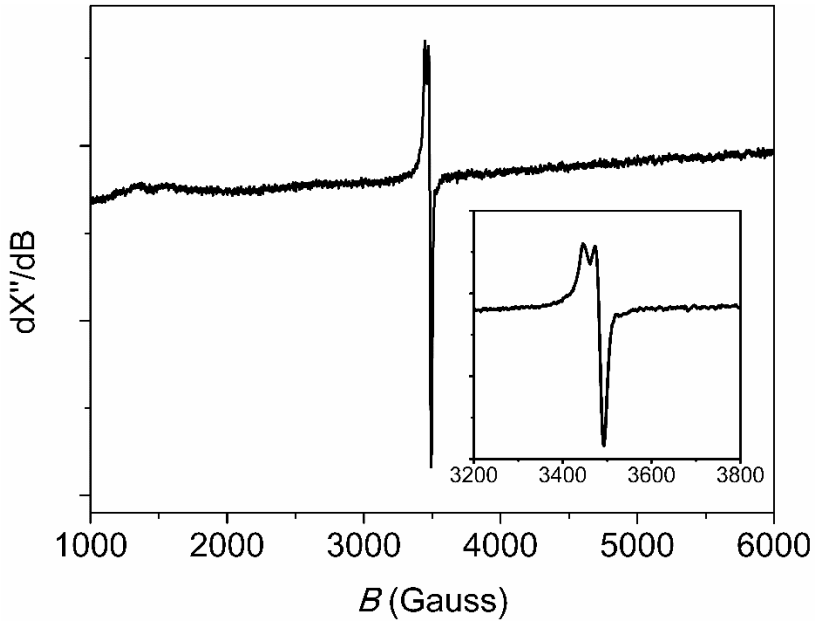


Figure S43. X-Band EPR spectrum for the reaction between 2 and MMAO (400 eq.) in toluene, acquired at cryogenic temperatures (10K) after a reaction time of 10 minutes. The final concentration of Cr in solution is unknown, due to the slow reactivity of the complex with MMAO. The spectrometer was operating at a frequency of 9.65 GHz.

3. DFT calculations of the activation pathway of complex 1 and complex 2

3.1 Benchmarking study of basis set and functional

DFT calculations were performed to assess the thermochemistry for the reaction of complex 1 and complex 2 with $AlMe_3$. Prior to performing these calculations, a small benchmarking study was performed. We had previously described that DFT-D3 calculations performed at the BP86/TZP level of theory can accurately model Cr-{SNS} and Cr-pyrrolyl complexes.[10]

In the current study we had evaluated whether this choice of basis set and functional is sufficient to model Cr-{PNP} complexes. In another study, the crystal structure of the Cr-{PNP} complex, $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$, was reported.[11] We had performed DFT calculations of $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$ with various functionals and basis sets and the calculated bond distances were compared to the experimental bond distances. The results are summarized in Table S12.

Table S12. Comparison of experimental and calculated bond lengths for the structure $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$.

Method	Cr–N distance (Å)	Mean Cr–Cl distance (Å)	Mean Cr–P distance (Å)
Experimental[a]	2.051	2.291	2.487
BP86-D3/TZP[b]	2.072	2.313	2.512
BP86-D3/TZ2P[b]	2.065	2.304	2.507
BP86-D3/TZ2P[c]	2.029	2.289	2.482
BP86-D3/TZ2P[d]	2.025	2.291	2.485
M06L/TZP[d]	2.098	2.292	2.530

Reported bond parameters are for the chromium complex in the quartet spin state. The doublet spin state was also evaluated and was found to be disfavored over the quartet spin state. [a] Bond distances for the crystal structure reported in reference 11. [b] Frozen core: large. [c] Frozen core: small. [d] Frozen core: none.

DFT-D3 calculations performed at the BP86/TZP level of theory are already capable of accurately predicting the bond lengths of $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$. The calculations could be improved by changing the basis set from TZP to TZ2P. In addition, performing the calculations without a frozen core approximation further improved the accuracy of the performed calculations and yields bond distances in excellent agreement with experimental bond distances.

We had also assessed whether this functional performs well in describing the thermochemistry of alkylaluminium compounds. Zurek and coworkers showed that the choice of basis set and functional is important to accurately describe the thermochemistry for the dimerization of trimethylaluminium. They had shown that GGA-type, with the inclusion of dispersion corrections (D3), can provide good estimates for the dimerization of trimethylaluminium (Table S13).[12] Building on these results, we had shown that DFT-D3 calculations performed at the BP86/TZP level of theory also provide good estimates for the dimerization of trimethylaluminium (Table S13).[10] Similarly, DFT-D3 calculations performed at the BP86/TZ2P level of theory can also accurately predict the energy for the dimerization of trimethylaluminium.

Table 13. Thermodynamic calculations performed on the dimerization of $AlMe_3$.

Method	*ΔE (kcal / mol)*	*ΔG (kcal/mol)*	*ΔH (kcal / mol)*
rev-PBE/TZP[a]	-10.1	6.9	-6.9
rev-PBE+D3/TZP[a]	-19.2	-4.1	-14.8
BP86 / TZP[b]	-12.6	5.1	-10.9
BP86+D3/TZP[b]	-20.9	-4.2	-17.9
BP86+D3/TZ2P[c]	-21.7	-4.0	-19.8
Experimental		-7.5	-20.4

[a]Calculations were performed in reference 12. [b]Calculations were performed in reference 10. [c]Calculations are performed in the current study. No frozen core approximation was applied.

3.2 Thermochemistry for the reaction of complex 1 with $AlMe_3$ and MMAO.

DFT calculations were performed to assess the thermochemistry for the reaction of complex **1** with either $AlMe_3$ or MMAO. All of these DFT calculations were performed at the BP86/TZ2P level of theory, with inclusion of dispersion corrections (D3) and no frozen core approximation.

In the reaction of complex **1** with $AlMe_3$, it is assumed that the complex only reacts with $AlMe_3$. MMAO is a complex mixture and consists of both trimethylaluminium and methylaluminoxane molecules.[13] In a DFT study, Van Rensburg *et al.* had compared the methylation aptitude of trimethylaluminium and methylaluminoxane and had shown that trimethylaluminium has a higher methylation aptitude compared to methylaluminoxane.[14] It is thus likely that methylation of complex **1** proceeds via reaction with free trimethylaluminium contained within MMAO. In calculations where we did take into consideration methylaluminoxane, we used the model $(AlOMe)_{10}.AlMe_3$, as described by Zurek and coworkers.[12]

First, the most favoured geometry of complex **1** was assessed. In our previous study we had shown that the meridional isomer was favoured over the facial isomer. Similar findings are obtained in this study (Table S14): the most favoured isomer was found to be the meridional isomer (Scheme S1). The most favoured spin state was found to be the quartet spin state, in line with EPR measurements (Figure S4).

Scheme S1. Most favored geometry of complex 1.

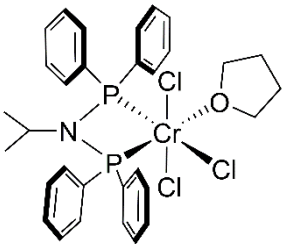


Table S14. Relative energies for the two spin states of complex 1.

Isomer	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
Meridional	Doublet	19.1	17.9	19.7
	Quartet	0	0	0
Facial	Doublet	25.4	25.7	25.6
	Quartet	7.1	6.1	7.9

In the first stages of the activation process, we envisioned the coordinated THF molecule to be abstracted from the metal center. This can occur either via reaction with $AlMe_3$ or MMAO; the reaction is summarized in Scheme S2 and the thermodynamic quantities are given in Table S15. In line with the enhanced Lewis acidity of methylaluminoxane with respect to $AlMe_3$, the reaction with methylaluminoxane (ΔG = -6.3 kcal mol^{-1}) is expected to be more exergonic compared to reaction with $AlMe_3$ (ΔG = -0.5 kcal mol^{-1}).

Scheme S2. Reaction of complex 1 with $AlMe_3$ or with methylaluminoxane, to abstract THF from the metal center.

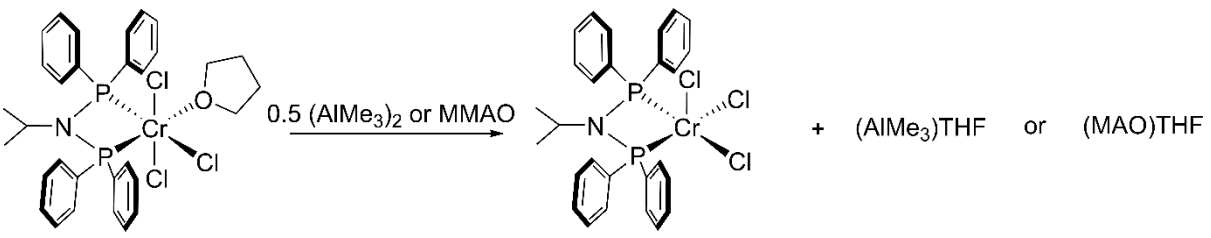


Table S15. Thermodynamic quantities for the reaction given in Scheme S2. Energies are reported with respect to the most favoured spin state of the depicted structure.

Alkylaluminium reagent	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
$AlMe_3$	Doublet	23.6	12.3	23.1
	Quartet	9.4	-0.5	8.4
Methylaluminoxane	Doublet	6.6	6.5	7.9
	Quartet	-7.6	-6.3	-6.9

In the next stages of the activation process, the metal is alkylated through the reaction with $AlMe_3$. The metal can either be monomethylated, dimethylated or trimethylated as shown in Scheme S3. The corresponding thermodynamic quantities are given in Table S16. Based on these calculations, monomethylation is expected to be slightly exergonic (ΔG = -6.7 kcal mol^{-1}) and di- and trimethylation are expected to be slightly endergonic (ΔG = 1.2 kcal mol^{-1} and 4.8 kcal mol^{-1} respectively).

Scheme S3. Stepwise methylation of the five-coordinate Cr^{III} complex through reaction with $AlMe_3$. The corresponding thermodynamic quantities are given in Table S16.

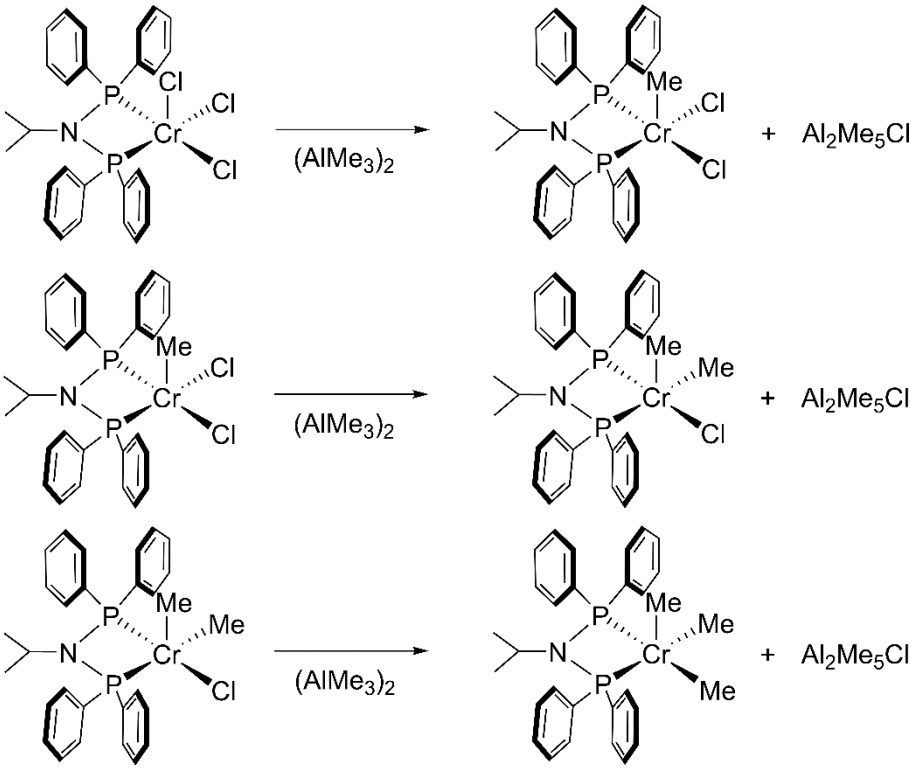


Table S16. Thermodynamic quantities for the reaction given in Scheme S3. Energies are reported with respect to the most favoured spin state of the depicted structure.

Methylation step	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
First	Doublet	10.5	9.8	10.1
	Quartet	-6.0	-6.7	-6.2
Second	Doublet	19.5	18.5	18.6
	Quartet	2.3	1.2	1.7
Third	Doublet	16.5	14.4	15.9
	Quartet	6.9	4.8	5.7

After alkylation of the metal, we envisioned the metal is capable of undergoing reduction to the divalent oxidation state. This is schematically depicted in Scheme S4 and the corresponding thermodynamic

quantities are given in Table S17. Based on these calculations, reduction to the divalent oxidation state is expected to be thermodynamically favoured (ΔG = -9.9 kcal mol^{-1}).

Scheme S4. Reduction of the five-coordinate Cr^{III} complex to form a square-planar Cr^{II} complex. The corresponding thermodynamic quantities are given in Table S17.

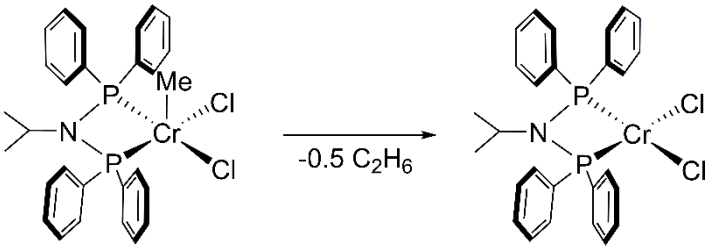


Table S17. Thermodynamic quantities for the reaction given in Scheme S4. Energies are reported with respect to the most favoured spin state of the depicted structure.

Spin state	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
Singlet	10.5	6.7	11.4
Triplet	1.9	-2.0	2.7
Quintet	-4.2	-9.9	-3.3

Further methylation of the metal, similar to what was shown in Scheme S3, could occur. This is schematically depicted in Scheme S5 and the corresponding thermodynamic quantities are reported in Table S18. Based on these calculations, the first methylation step is only slightly disfavoured (ΔG = 2.7 kcal mol^{-1}) whereas the second step becomes significantly more disfavoured (ΔG = 5.6 kcal mol^{-1}).

Scheme S5. Stepwise methylation of the square-planar Cr^{II} complex through reaction with $AlMe_3$. The corresponding thermodynamic quantities are given in Table S18.

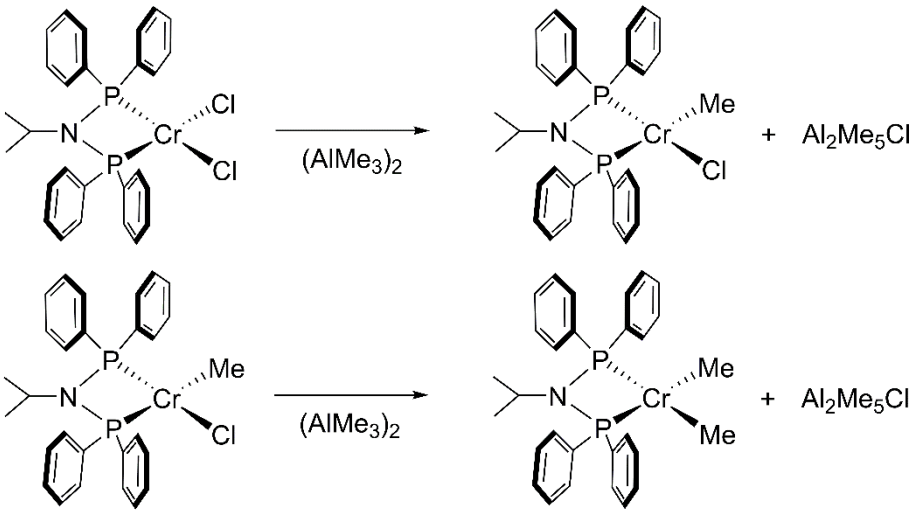


Table S18. Thermodynamic quantities for the reaction given in Scheme S5. Energies are reported with respect to the most favoured spin state of the depicted structure.

Methylation step	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
First	Singlet	18.8	19.4	18.0
	Triplet	10.2	10.7	9.4
	Quintet	3.7	2.7	3.2
Second	Singlet	23.9	24.6	23.0
	Triplet	17.4	16.6	15.8
	Quintet	7.7	5.6	6.8

Finally, we had considered the reduction from the divalent oxidation state to the monovalent oxidation state. Our envisioned reaction pathway is depicted in Scheme S6 and the corresponding thermodynamic quantities are given in Table S19. Based on these calculations, reduction to the monovalent oxidation state is expected to be disfavoured (ΔG = 4.5 kcal mol^{-1}).

Scheme S6. Reduction of the square-planar Cr^{II} complex to form a trigonal planar Cr^{I} complex. The corresponding thermodynamic quantities are given in Table S19.

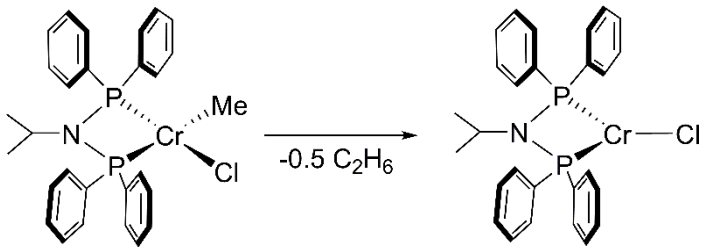


Table S19. Thermodynamic quantities for the reaction given in Scheme S6. Energies are reported with respect to the most favoured spin state of the depicted structure.

Spin state	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
Doublet	25.9	24.1	26.3
Quartet	8.1	4.5	8.9
Sextet	9.2	7.3	10.9

Further methylation of the metal was also taken into consideration (Scheme S7 and Table S20), but this was found to be highly disfavoured.

Scheme S7. Methylation of the trigonal planar Cr^{I} complex to form the monomethylated trigonal planar Cr^{I} complex. The corresponding thermodynamic quantities are given in Table S20.

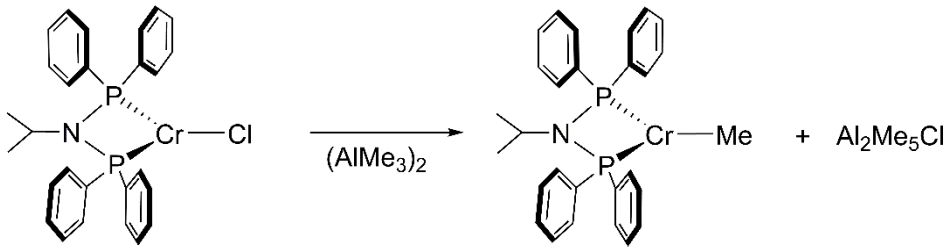


Table S20. Thermodynamic quantities for the reaction given in Scheme S6. Energies are reported with respect to the most favoured spin state of the depicted structure.

Spin state	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
Doublet	32.0	29.0	31.5
Quartet	12.5	9.4	11.9
Sextet	12.3	12.5	12.4

For the structures [$((C_6H_5)_2P)_2N^{iPr}CrCl_2$] and [$((C_6H_5)_2P)_2N^{iPr}CrClMe$] we also considered interaction of $AlMe_3$ with the chloride and methide moiety. Interaction of one or two molecules of $AlMe_3$ were considered (Scheme S8 and Table S21). In all cases, the formation of adducts was found to be exergonic; coordination of two $AlMe_3$ molecules was favored over the coordination of one molecule of $AlMe_3$ to the complexes.

Coordination of $AlMe_3$ in all cases lead to changes in the coordination geometry of the complex: the complexes became five-coordinate instead of remaining square-planar. Experimentally, this is not observed in the Cr K-edge EXAFS data: either a four-coordinate or a three-coordinate complex is

observed upon reaction with $AlMe_3$ or MMAO respectively. In these DFT calculations we did not include either an implicit or an explicit solvent model. Inclusion of a solvent model in the performed calculations might give a better agreement between the calculated geometry and the experimentally observed coordination numbers.

Scheme S8. Considered structures for the formation of adducts between square-planar Cr^{II} complexes and $AlMe_3$. The corresponding thermodynamic quantities are given in Table S21.

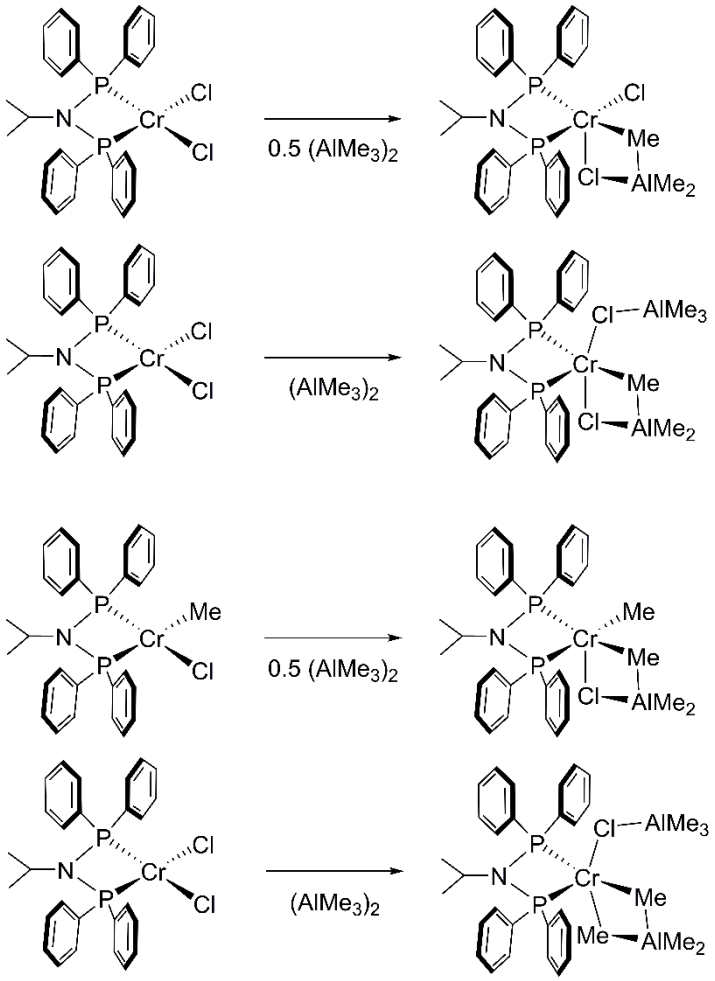


Table S21. Thermodynamic quantities for the reaction given in Scheme S8. Energies are reported with respect to the most favoured spin state of the depicted structure.

Complex	*Adduct*	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
$[((C_6H_5)_2P)_2N^{iPr}CrCl_2]$	$AlMe_3$	Singlet	4.1	13.9	4.6
		Triplet	-5.1	4.3	-4.7
		Quintet	-17.9	-8.3	-18.1
	2 $AlMe_3$	Singlet	-10.5	6.6	-9.7
		Triplet	-11.2	4.5	-10.5
		Quintet	-28.6	-14.0	-27.8
$[((C_6H_5)_2P)_2N^{iPr}CrClMe]$	$AlMe_3$	Singlet	2.8	14.1	3.5
		Triplet	-6.0	4.8	-6.2
		Quintet	-19.0	-9.3	-19.3
	2 $AlMe_3$	Singlet	-10.0	12.9	-6.6
		Triplet	-20.2	0.9	-16.5
		Quintet	-30.0	-14.5	-29.0

3.3 Thermochemistry for the reaction of complex 2 with $AlMe_3$

In a similar fashion to section 3.2, we had assessed the thermochemistry for the reaction of complex **2** with $AlMe_3$.

First, the most favoured geometry of complex **2** was assessed. The structure of complex **2** is depicted in Scheme S9 and the relative energies of the doublet and quartet spin state are given in Table S22. In line with EPR measurements (Figure S29), the quartet spin state was found to be most favoured.

Interestingly, a large discrepancy is observed between the Cr–O distance in the reported crystal structure of complex **2** (2.156 Å) and the DFT-optimized structure of complex **2** (2.446 Å).[15] This discrepancy is not caused by a small basis set and a poor choice of functional, as this level of theory was found to very accurately predict bond distances of another Cr-{PNP} complexes (Table S12). Additionaly, a very smilar distance was found using other functionals (B3LYP and S12G). Possibly, crystal packing effects could have a significant influence on the Cr–O distance.

Scheme S9. Most favored geometry of complex 2.

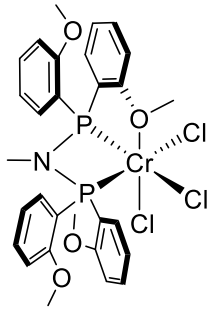


Table S22. Relative energies for the two spin states of complex 2.

Spin state	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
Doublet	17.9	17.9	17.9
Quartet	0	0	0

Next, similar to section 3.2, we investigated the stepwise methylation and reduction of complex **2** through the reaction with $AlMe_3$. The stepwise methylation of complex **2** is schematically depicted in Scheme S10 and the corresponding thermodynamic quantities are given in Table S23. Based on these calculations, the first methylation step is exergonic (ΔG = -9.1 kcal mol^{-1}) whereas the second (ΔG = 3.5 kcal mol^{-1}) and third (ΔG =1.8 kcal mol^{-1}) methylation steps are slightly endergonic.

Scheme S10. Stepwise methylation of complex 2 through reaction with $AlMe_3$. The corresponding thermodynamic quantities are given in Table S23.

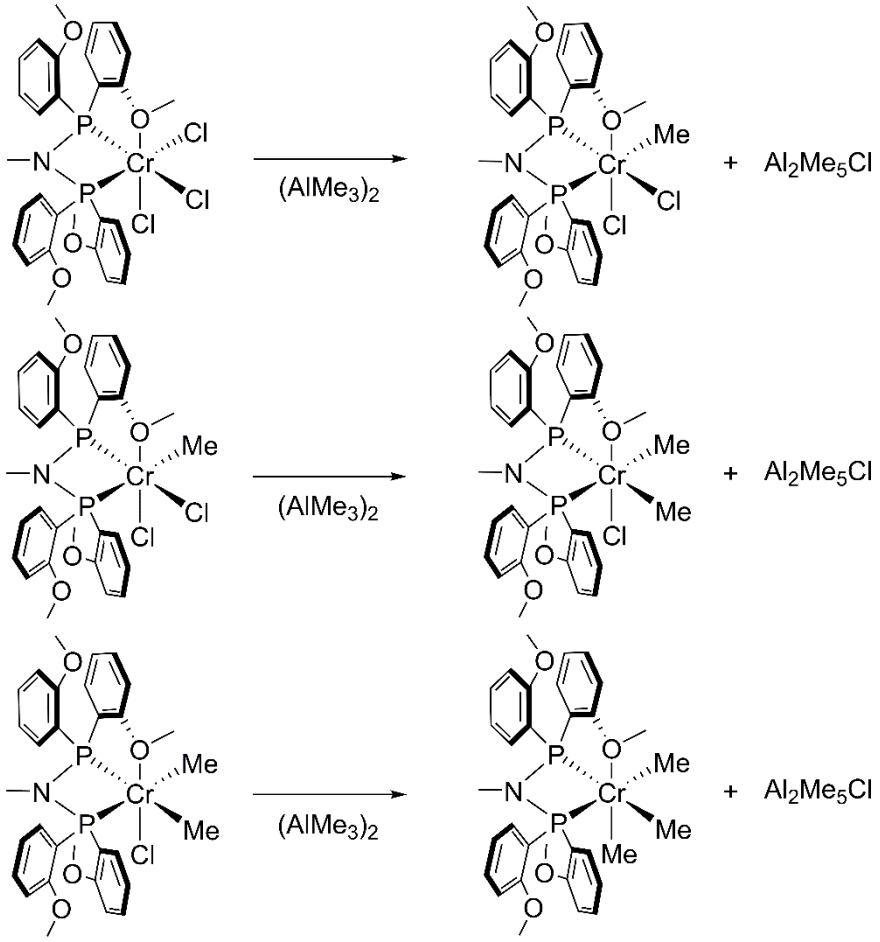


Table S23. Thermodynamic quantities for the reaction given in Scheme S10. Energies are reported with respect to the most favoured spin state of the depicted structure.

Methylation step	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
First	Doublet	11.7	11.3	11.5
	Quartet	-7.4	-9.1	7.0
Second	Doublet			
	Quartet	3.4	3.5	2.2
Third	Doublet	21.4	20.1	20.5
	Quartet	5.1	1.8	4.9

Subsequently, the monomethylated Cr^{III} complex can be reduced in a binuclear fashion through release of ethane. This is schematically depicted in Scheme S11 and the corresponding thermodynamic quantities are given in Table S24. Based on these calculations, reduction to the divalent oxidation state is expected to be favoured (ΔG = -6.5 kcal mol^{-1}).

Scheme S11. Reduction of complex to form a Cr^{II} complex. The corresponding thermodynamic quantities are given in Table S24.

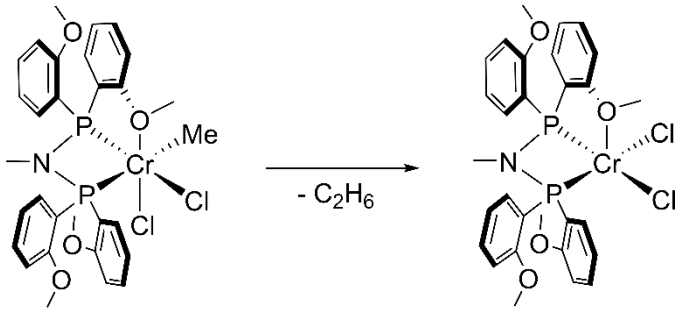


Table S24. Thermodynamic quantities for the reaction given in Scheme S11. Energies are reported with respect to the most favoured spin state of the depicted structure.

Spin state	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
Singlet	30.2	24.2	30.8
Triplet	21.3	16.8	21.1
Quintet	-1.3	-6.5	-1.3

This Cr^{II} complex can subsequently be alkylated through reaction with $AlMe_3$. This is schematically depicted in Scheme S12 and the thermodynamic quantities are given in Table S25. Based on these calculations, monoalkylation (ΔG = 0.2 kcal mol^{-1}) is slightly disfavoured and dialkylation is disfavoured (ΔG = 9.4 kcal mol^{-1}).

Scheme S12. Stepwise methylation of the Cr^{II} complex through reaction with $AlMe_3$. The corresponding thermodynamic quantities are given in Table S25.

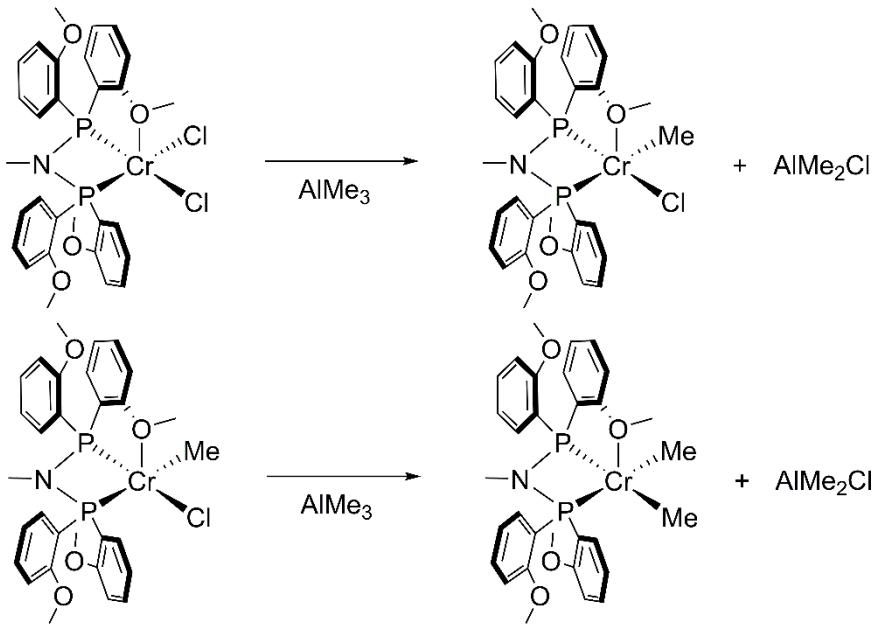


Table S25. Thermodynamic quantities for the reaction given in Scheme S11. Energies are reported with respect to the most favoured spin state of the depicted structure.

Methylation step	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
First	Singlet	23.3	24.8	23.6
	Triplet	22.6	22.6	22.0
	Quintet	2.9	0.2	2.3
Second	Singlet	31.2	34.2	31.1
	Triplet	21.1	24.0	20.9
	Quintet	10.8	9.4	10.5

Finally, we assessed the thermochemistry for the reduction of the divalent to the monovalent oxidation state. This is schematically depicted in Scheme S13 and the corresponding thermodynamic quantities are given in Table S26. Based on these calculations, reduction to the monovalent oxidation state is expected to be disfavoured (ΔG = 9.3 kcal mol^{-1}).

Scheme S13. Reduction of the square-planar Cr^{II} complex to form a trigonal planar Cr^{I} complex. The corresponding thermodynamic quantities are given in Table S25.

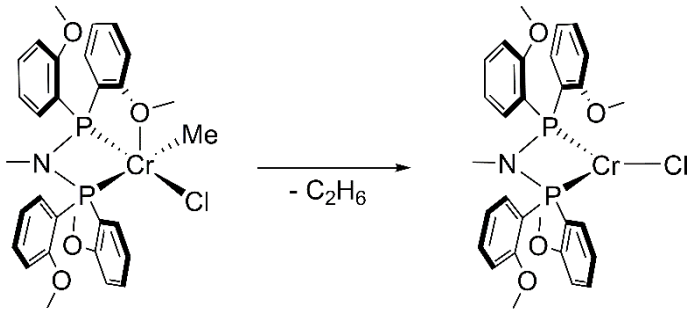


Table S26. Thermodynamic quantities for the reaction given in Scheme S13. Energies are reported with respect to the most favoured spin state of the depicted structure.

Spin state	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
Doublet	17.3	16.6	18.2
Quartet	12.0	10.0	12.1
Sextet	9.6	9.3	11.6

For the structures [((*o*-$C_6H_4OMe)_2P)_2N^{Me}CrCl_2$] and [((*o*-$C_6H_4OMe)_2P)_2N^{Me}CrClMe$] we also considered interaction of $AlMe_3$ with the chloride and methide moiety. Interaction of one or two molecules of $AlMe_3$ were considered (Scheme S14 and Table S27). In all cases, the formation of adducts was found to be exergonic; coordination of two $AlMe_3$ molecules was favored over the coordination of one molecule of $AlMe_3$ to the complexes.

In most cases, coordination of $AlMe_3$ leads to no changes in the coordination environment of chromium and all complexes are expected to be five-coordinate. This is not observed in the Cr K-edge EXAFS data: a four-coordinate chromium complex is observed; two of the bound ligands consist of low-Z scatterers. An interpretation for the experimental Cr K-edge EXAFS data is given in the article.

Scheme S14. Considered structures for the formation of adducts between square-planar Cr^{II} complexes and $AlMe_3$. The corresponding thermodynamic quantities are given in Table S27.

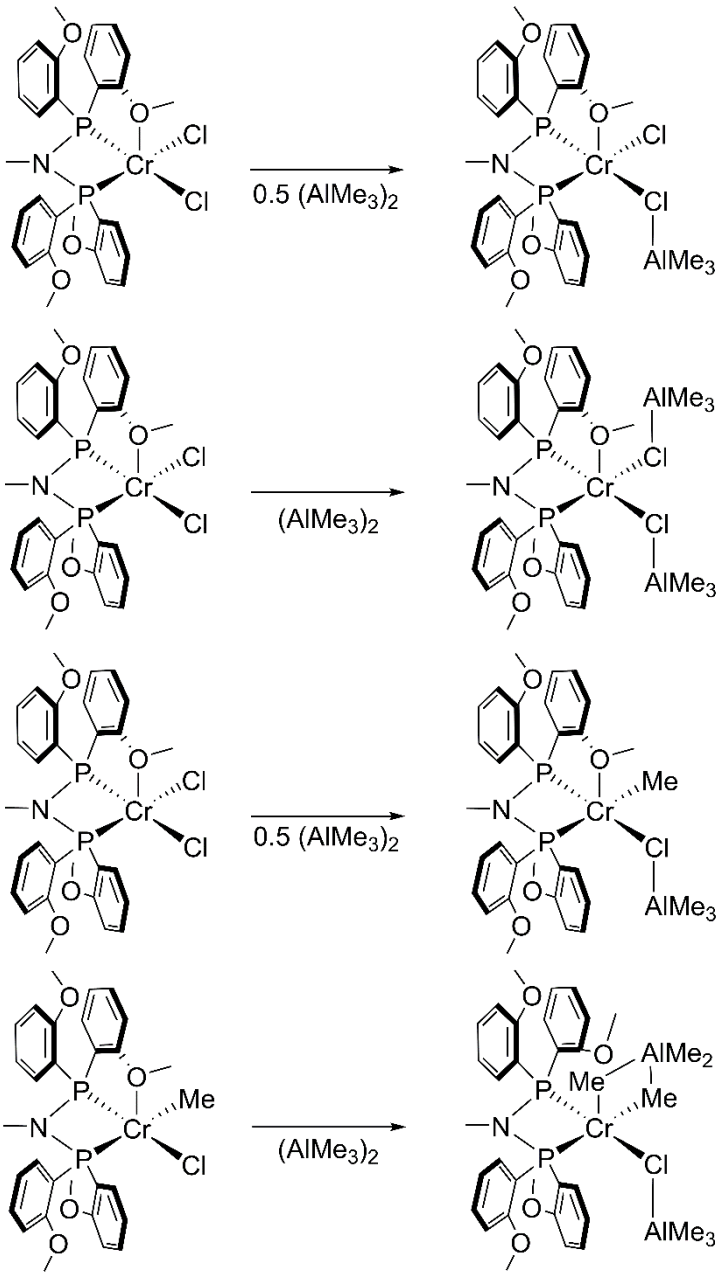


Table S27. Thermodynamic quantities for the reaction given in Scheme S14. Energies are reported with respect to the most favoured spin state of the depicted structure.

Complex	*Adduct*	*Spin state*	*ΔE (kcal mol^{-1})*	*ΔG (kcal mol^{-1})*	*ΔH (kcal mol^{-1})*
[((*o*-$C_6H_4OMe)_2P)_2N^{iPr}CrCl_2$]	$AlMe_3$	Singlet	3.4	14.1	3.9
		Triplet	6.4	15.9	8.0
		Quintet	-18.6	-12.1	-17.4
	2 $AlMe_3$	Singlet	-8.8	7.0	-7.2
		Triplet	-19.1	-2.8	-17.4
		Quintet	-32.7	-18.0	-31.0
[((*o*-$C_6H_4OMe)_2P)_2N^{iPr}CrClMe$]	$AlMe_3$	Singlet	11.6	24.5	11.8
		Triplet	-3.6	7.9	-2.1
		Quintet	-17.8	-10.5	-17.4
	2 $AlMe_3$	Singlet	-6.9	16.2	-4.0
		Triplet	-5.1	16.0	-3.3
		Quintet	-29.3	-9.2	-27.4

4. Spectroscopic results for activation experiments performed in the presence of substrates

4.1 Activation experiments for complex 2 in the presence of substrates

For complex **2**, we had performed activation experiments with $AlMe_3$ (40 eq.) and introduced various substrates (dienes and alkynes). The experiments were performed by first activating the metal. After 10 minutes, the substrate was injected into the solution and the solution was allowed to age for 50 minutes, after which the UV–VIS spectrum was acquired. Introduction of these substrates lead to no changes in the UV–VIS spectrum (Figure S44). Additionally, we had also studied the activation of complex **2** in the presence of isoprene (40 eq.) using Cr K-edge XANES (Figure S45). Also here, no changes are observed, making it likely that these substrates do not coordinate to the metal center.

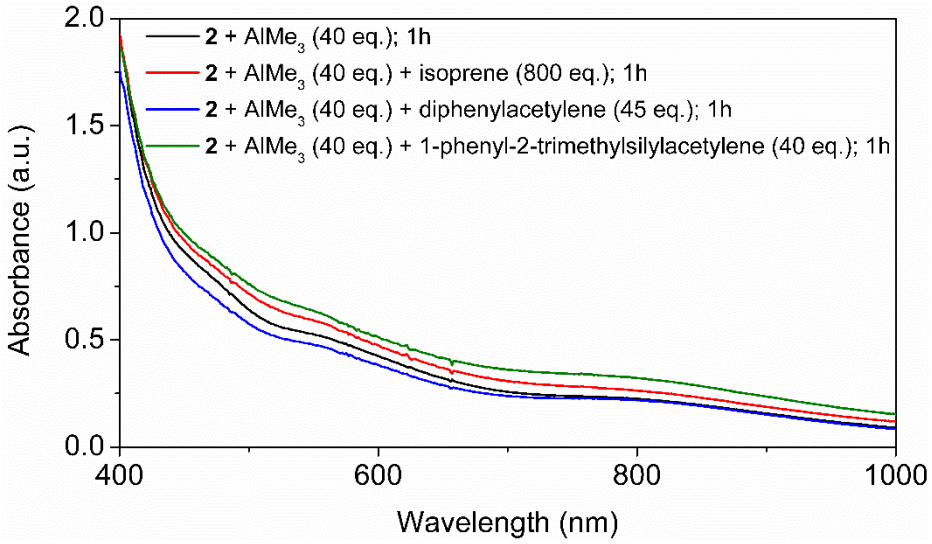


Figure S44. UV–VIS spectra for the reaction between complex 2 and $AlMe_3$ (40 eq.) in the presence of various substrates.

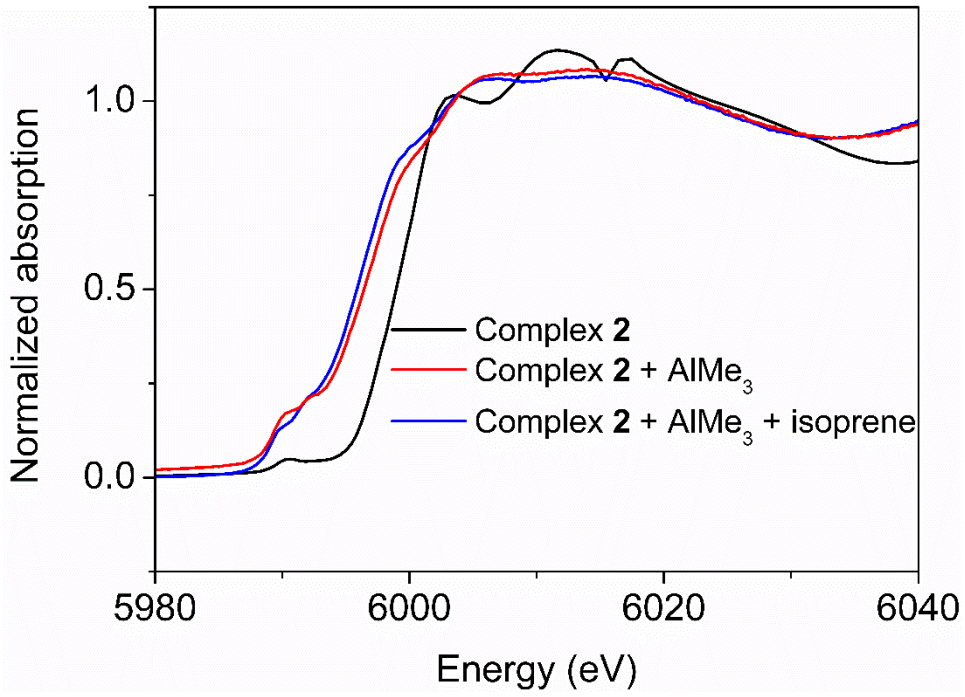


Figure S45. Cr K-edge spectra for the reaction between complex 2 and $AlMe_3$ (40 eq.) in the presence of various substrates. The spectra were acquired after a reaction time of 60 minutes.

``4.2 Activation experiments for complex 1 in the presence of substrates

In a similar fashion, for complex **1**, we had performed activation experiments with MMAO (400 eq.) in the presence of various substrates. Again, the complex was activated and allowed to react for 10 minutes, after which the substrate was introduced. After 50 minutes, either a UV–VIS spectrum was acquired or a Cr K-edge XAS spectrum was acquired. Now, clear changes in the UV–VIS spectra are observed after introduction of dienes or alkynes (Figure S46).

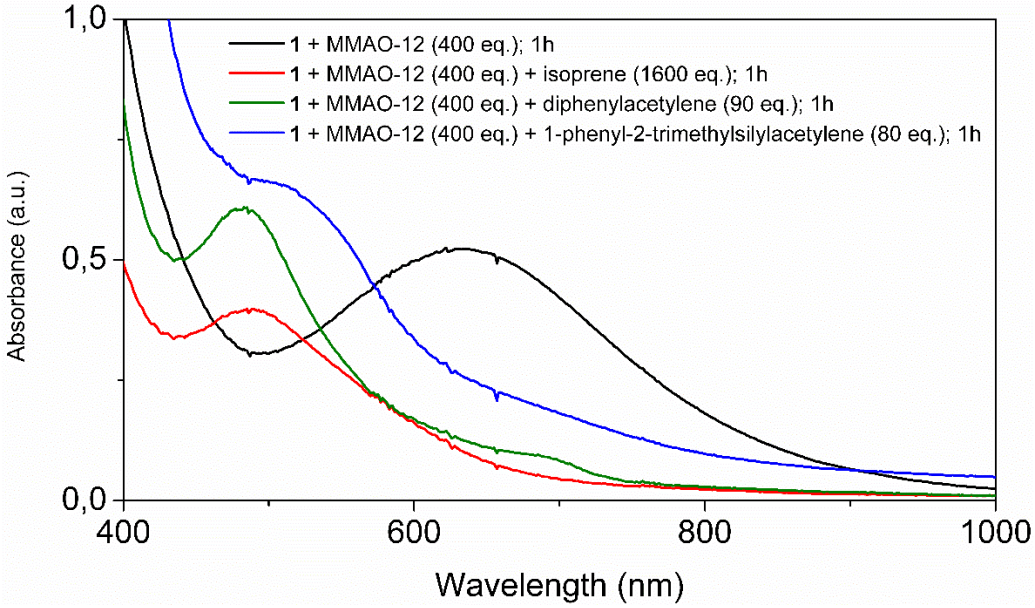


Figure S46. UV–VIS spectra for the reaction between complex 1 and $AlMe_3$ (40 eq.) in the presence of various substrates.

All following spectroscopic experiments were performed using solely isoprene due to closer resemblance of ethene and isoprene. First, the reaction was investigated using X-Band EPR spectroscopy. The results are presented in Figure S46.

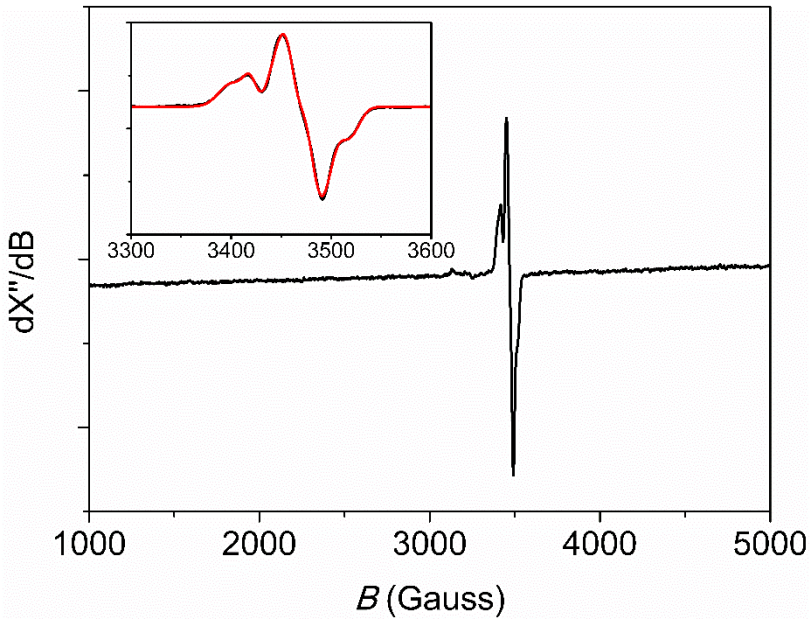


Figure S47. X-Band EPR spectrum for the reaction between 1, MMAO (~500 eq.) and isoprene in toluene, acquired at cryogenic temperatures (10K) after a reaction time of 60 minutes. The inset of the figure shows a fit (red) of the experimental spectrum (black) and was found to consist of three Cr^{I} complexes. For the first component (S=1/2) a fit was obtained using $g_{x,y}$ = 1.979 and g_z = 2.000, by applying Gaussian broadening (62 MHz) and a relative weighting of 1. For the second component (S=1/2) a fit was obtained using g_z = 2.029, g_y = 1.993 and g_x = 1.960, and by applying

Gaussian broadening (61, 48 and 82 MHz respectively) and a relative weighting of 1.62. For the third component (*S=1/2*) a fit was obtained using $g_{x,y}$ = 2.016 and g_z = 1.987, by applying Gaussian broadening (42 MHz) and a relative weighting of 0.15 The concentration in Cr after mixing was ~2.4 mM. The spectrometer was operating at a frequency of 9.65 GHz.

Additionally, the reaction was investigated using Cr K-edge XAS. The Cr K-edge XANES region is reported in the article (Figure 4). The results obtained using Cr K-edge EXAFS are reported below.

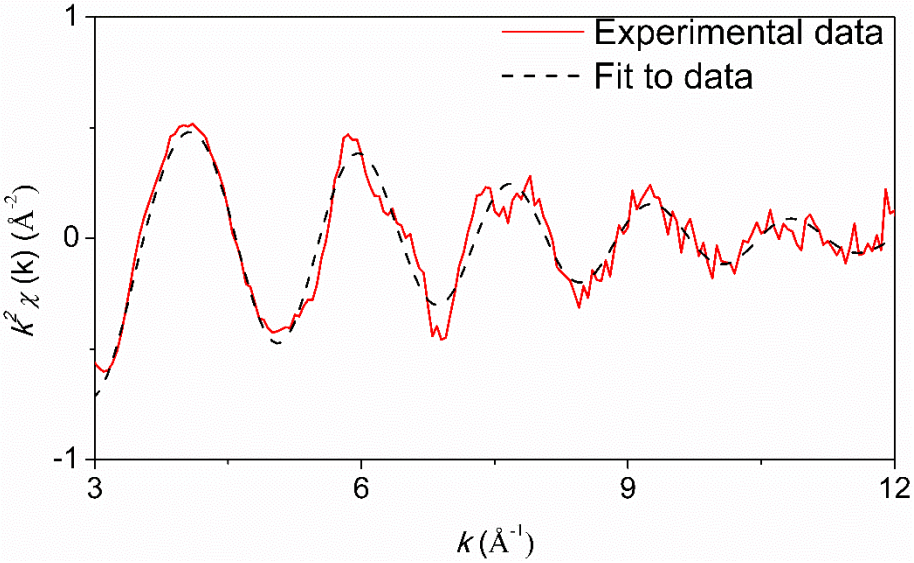


Figure S48. Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, in the presence of isoprene (40 eq.), frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~4.9 mM.

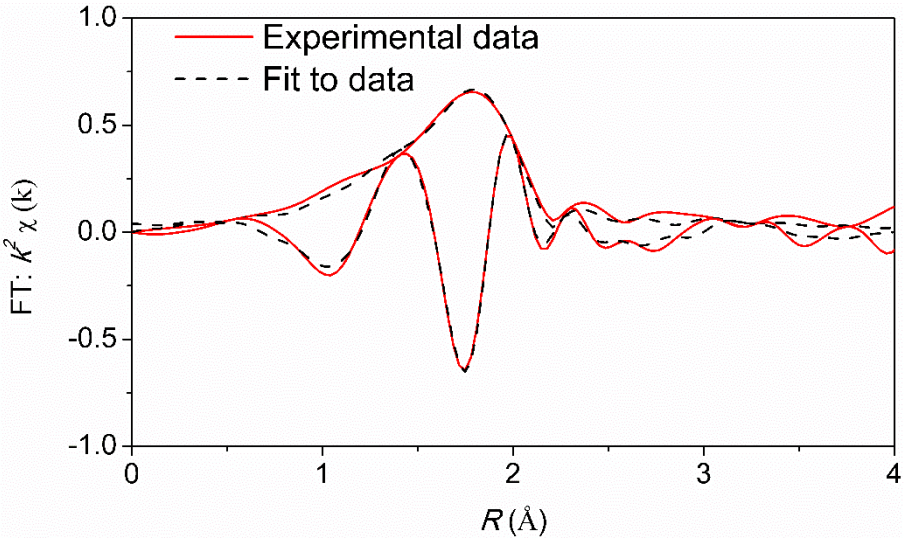


Figure S49. Fourier transform of the Cr K-edge k^2-weighted EXAFS data for the reaction of complex 1 and MMAO (400 eq.) in toluene, in the presence of isoprene (40 eq.), frozen after 60 minutes. The sample was measured as a frozen toluene solution. The final concentration in Cr after mixing was ~4.9 mM.

Table S28. Cr K-edge EXAFS data fitting results for the reaction complex 1 and MMAO (400 eq.), in the presence of isoprene (40 eq.), frozen after 60 minutes. These parameters were used to obtain the fits shown in Figure S48 and Figure S49.

Coordination shell	**N**	**σ^2 (Å^{-2})**	***d*** **(Cr–X) (Å)**
Cr–C	5.1(5)	0.006(3)	2.28(5)
Cr–P	2	0.008(5)	2.31(5)

General fitting parameters: S_0^2 = 0.84, E_0 =3(3) eV, Δk = 3 – 12.0 Å^{-1}, ΔR = 1.00– 3.00 Å, R^2 = 0.012, fitting was performed in R-space with a *k*-weighting of k^1-k^3. Parameters without parentheses were kept fixed. Similar parameters were used for the Cr–P and Cr–Cl shell.

5. DFT calculations of the mechanism of selective ethene oligomerization

5.1 Mechanism for the selective ethene oligomerization catalyzed by monocationic chromium PNP (PNP = $((C_6H_5)_2P)_2N^{iPr}$) complexes

Depicted below, in Scheme S15, are the intermediates considered for a catalytic cycle proceeding via monocationic Cr^{II}/Cr^{IV} intermediates, ligated by $((C_6H_5)_2P)_2N^{iPr}$. Additionally, the energies of the various spin states are reported in Table S29.

The starting point of the calculations, is the monocationic complex **A1**. Coordination of one (ΔG = -10.0 kcal mol^{-1}) and two molecules of ethene (ΔG = -15.4 kcal mol^{-1}) is exergonic. Subsequent oxidative coupling of these two ethene molecules to yield chromacyclopentane **A4** ($\Delta\Delta G$ = 3.6 kcal mol^{-1}) proceeds with a moderate barrier (**TSA1**, $\Delta\Delta G$ = 16.3 kcal mol^{-1}). Elimination of 1-butene from chromacyclopentane **A4** proceeds with a high barrier (**TSA4**, $\Delta\Delta G$ = 26.4 kcal mol^{-1}).

Alternatively, ethene can coordinate to **A4** to yield chromacycopentane **A5** ($\Delta\Delta G$ = 3.4 kcal mol^{-1}). This ethene molecule can subsequently insert into the chromacyclopentane intermediate (**TSA2**, $\Delta\Delta G$ = 26.2 kcal mol^{-1}) to yield chromacycloheptane **A6** ($\Delta\Delta G$ = -18.7 kcal mol^{-1}). Finally, 3,7-H shift from chromacycloheptane **A6** (**TSA3**, $\Delta\Delta G$ = 14.0 kcal mol^{-1}) yields 1-hexene.

This model is incapable of correctly predicting the experimentally observed product selectivity. Firstly, chromacycloheptane **A6** is not capable of coordinating ethene, presumably due to the steric hindrance imposed by the ligand and the methide. This hampers the formation of 1-octene. Additionaly, formation of 1-butene is expected to proceed with a lower barrier compared to the formation of chromacycloheptane **A6** (difference **TSA4** and **TSA2**, $\Delta\Delta G$ = 3.2 kcal mol^{-1})

Scheme S15. DFT-D3 calculations for a mechanism proceeding via monocationic Cr^{II}/Cr^{IV} intermediates. Calculations were performed at the BP86/TZP level of theory, without inclusion of a solvent model. The singlet (not depicted), triplet (red) and quintet (blue) spin state were taken into consideration. Reported are the Gibbs free energies, and the electronic energies in parentheses, in kcal mol^{-1}. Parts of the ligand are removed for clarity of the image.

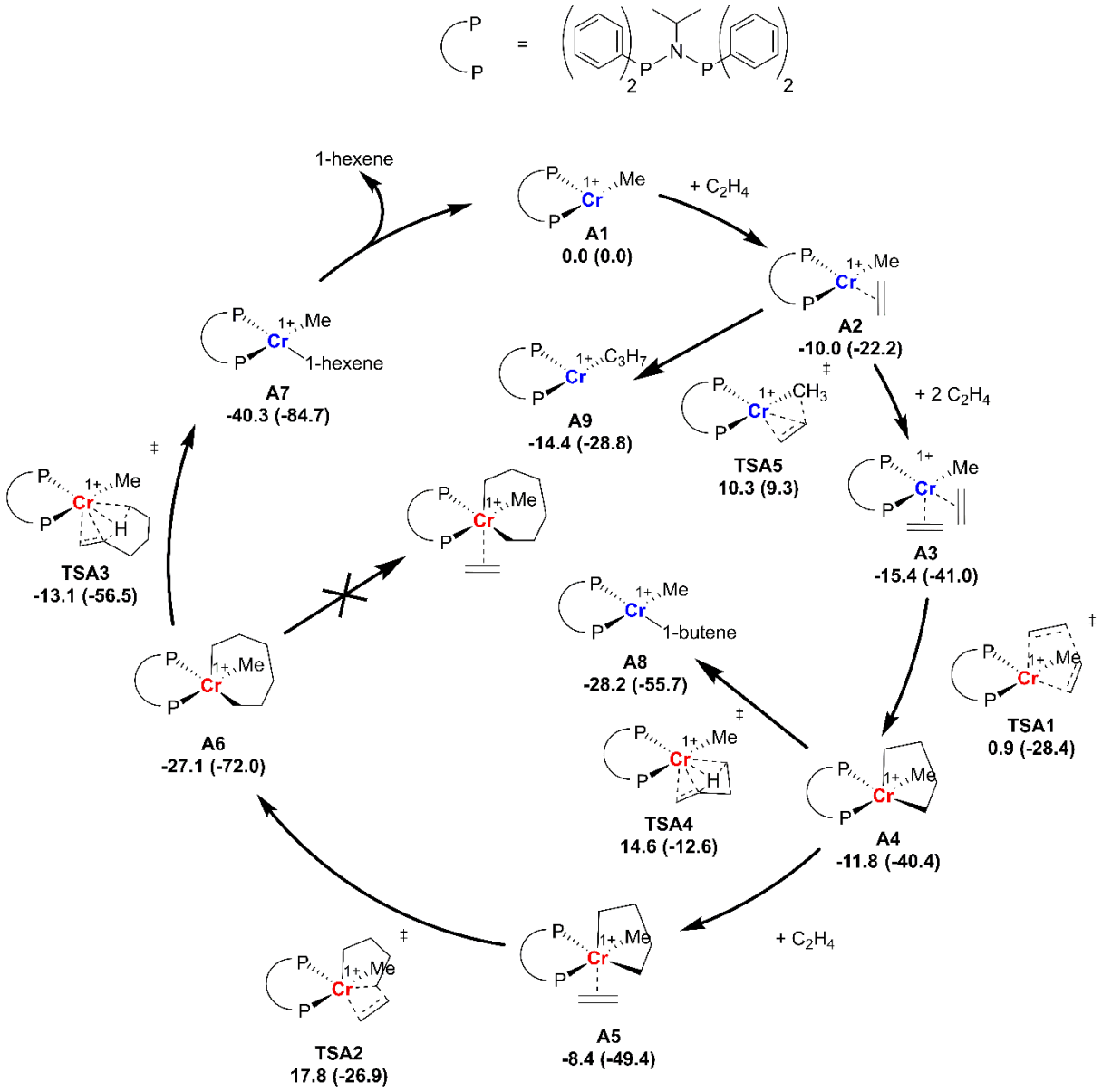
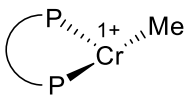
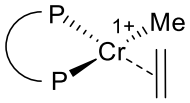
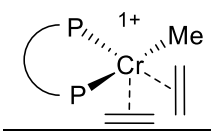
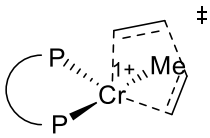
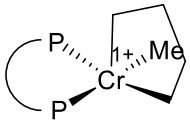
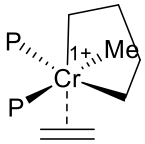
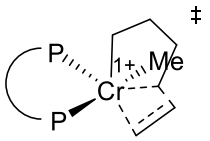
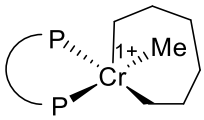
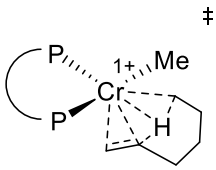
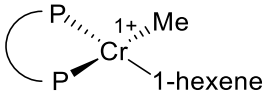
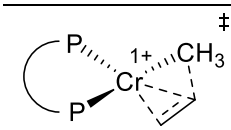
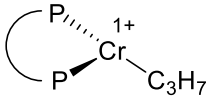
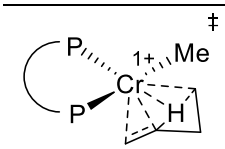
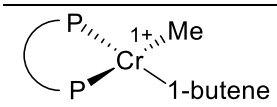


Table S29. Overview of the relative energies of the various spin states for the intermediates depicted in Scheme S15.

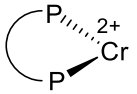
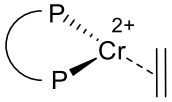
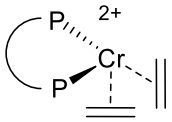
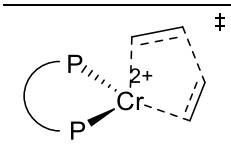
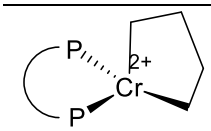
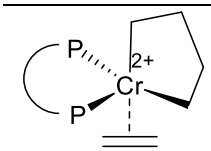
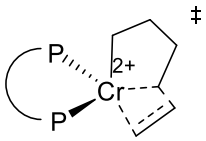
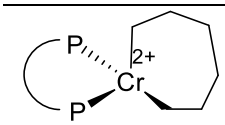
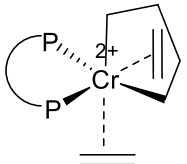
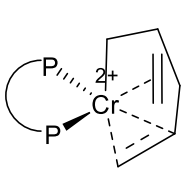
Structure	Spin state	*ΔE* (kcal mol^{-1})	*ΔG* (kcal mol^{-1})	*ΔH* (kcal mol^{-1})
	**Singlet** **Triplet** **Quintet**	28.7 27.2 0	29.4 28.8 0	28.4 26.6 0
	**Singlet** **Triplet** **Quintet**	-9.5 -19.7 -22.2	4.6 -5.3 -10.0	-21.5 -15.4 -30.3

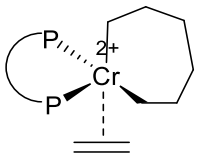
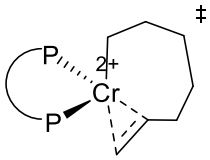
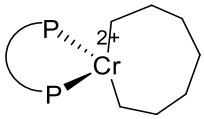
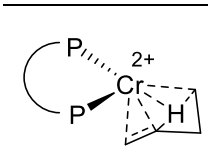
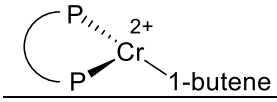
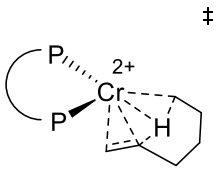
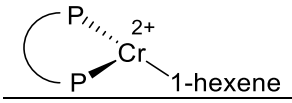
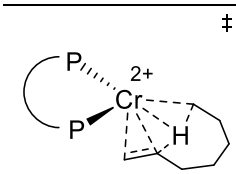
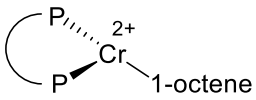
	**Singlet** **Triplet** **Quintet**	-18.9 -33.8 -41.0	9.9 -7.2 -15.4	-15.4 -30.3 -38.1
	**Triplet**	-28.4	0.9	-24.8
	**Singlet** **Triplet**	-29.9 -40.4	-0.7 -11.8	-26.9 -37.4
	**Singlet** **Triplet**	-27.2 -49.4	18.5 -8.4	-21.7 -43.7
	**Triplet**	-26.9	17.8	-21.5
	**Singlet** **Triplet**	-63.0 -72.0	-18.7 -27.1	-56.1 -65.8
	**Triplet**	-56.5	-13.1	-49.2
	**Singlet** **Triplet** **Quintet**	-60.6 -71.6 -84.7	-15.6 -26.7 -40.3	-54.6 -65.5 -78.8
	**Quintet**	9.3	10.3	9.8
	**Singlet** **Triplet** **Quintet**	-3.3 -14.1 -28.8	13.7 2.9 -14.4	-1.2 -12.1 -25.9
	**Triplet**	9.3	10.3	9.8
	**Singlet** **Triplet** **Quintet**	-30.7 -41.8 -55.7	-2.2 -13.1 -28.2	-27.0 -38.0 -52.2

5.2 Mechanism for the selective ethene oligomerization catalyzed by dicationic chromium PNP (PNP = $((C_6H_5)_2P)_2N^{iPr}$) complexes

The DFT calculations for a mechanism proceeding via dicationic Cr^{II}/Cr^{IV}, ligated by $((C_6H_5)_2P)_2N^{iPr}$, have been detailed in the main text of the article. Below, in Table S30, the relative energies of the various intermediates are reported.

Table S30. Overview of the relative energies of the various spin states for the intermediates depicted in Scheme 6 of the main text of the article.

Structure	Spin state	*ΔE* (kcal mol^{-1})	*ΔG* (kcal mol^{-1})	*ΔH* (kcal mol^{-1})
	**Singlet** **Triplet** **Quintet**	39.9 32.2 0	39.9 32.1 0	39.9 32.1 0
	**Singlet** **Triplet** **Quintet**	-3.8 -14.6 -30.4	4.5 -5.5 -20.0	-2.3 -13.7 -29.1
	**Singlet** **Triplet** **Quintet**	-37.4 -46.9 -57.6	-14.4 -22.8 -34.4	-34.1 -44.1 -54.7
	**Triplet**	-36.6	-13.8	-33.7
	**Singlet** **Triplet**	-31.6 -42.1	-6.3 -17.7	-28.6 -39.1
	**Singlet** **Triplet**	-56.8 -68.6	-18.1 -29.9	-52.3 -64.0
	**Triplet**	-53.4	-12.6	-49.4
	**Singlet** **Triplet**	-68.8 -80.2	-30.2 -42.8	-63.3 -74.1
	**Singlet** **Triplet**	-66.4 -79.8	-14.5 -28.1	-58.7 -72.0
	**Triplet**	-68.8	-12.5	-62.5

	**Singlet** **Triplet**	-82.1 -100.1	-28.8 -47.8	-74.7 -91.9
	**Triplet**	-88.9	-33.2	-81.0
	**Singlet** **Triplet**	-96.5 -108.3	-39.2 -54.8	-88.4 -99.1
	**Triplet**	-10.5	12.0	-10.8
	**Singlet** **Triplet** **Quintet**	-43.1 -52.5 -69.3	-18.3 -29.1 -44.3	-39.1 -48.0 -65.4
	**Triplet**	-70.6	-31.6	-66.6
	**Singlet** **Triplet** **Quintet**	-72.2 86.0 -101.0	-33.2 -45.7 -61.5	-65.4 -79.2 -93.6
	**Triplet**	-94.3	-37.0	-87.8
	**Singlet** **Triplet** **Quintet**	-104.3 -114.7 -128.8	-47.6 -58.2 -75.3	-95.0 -105.5 -118.5

5.3 Mechanism for the selective ethene oligomerization catalyzed by monocationic chromium PNP (PNP = ((*o*-C_6H_4OMe)P)$_2N^{Me}$) complexes

Depicted below, in Scheme S16, are the intermediates considered for a catalytic cycle proceeding via monocationic Cr^{II}/Cr^{IV} intermediates, ligated by ((*o*-C_6H_4OMe)P)$_2N^{Me}$. Additionally, the energies of the various spin states are reported in Table S31.

The starting point of the calculations is the dicationic Cr^{II} complex, **C1**. Coordination of the first (ΔG = -13.0 kcal mol^{-1}) and second (ΔG = -20.0 kcal mol^{-1}) ethene molecule to **C1** is exergonic. Oxidative coupling of the two ethene molecules to yield chromacyclopentane C**4** ($\Delta\Delta G$ = 8.4 kcal mol^{-1}) occurs with a moderate barrier (**TSC1**, $\Delta\Delta G$ = 19.1 kcal mol^{-1}). The oxidative coupling is accompanied by a spin crossover from the quintet to the triplet spin state. Subsequent elimination of 1-butene from chromocyclopentane C**4** is deemed unlikely due to the high barrier (**TSC7**, $\Delta\Delta G$ = 34.6 kcal mol^{-1}).

Subsequent coordination of ethene to **C4** to form **C5** is endergonic ($\Delta\Delta G$ = 4.0 kcal mol^{-1}). Either, this ethene molecule can insert into the metallacycle (**TSC2**, $\Delta\Delta G$ = 10.4 kcal mol^{-1}) to form chromacycloheptane intermediate **C6** ($\Delta\Delta G$ = -19.1 kcal mol^{-1}). Or a second ethene molecule can coordinate to **C5** ($\Delta\Delta G$ = 6.3 kcal mol^{-1}) and subsequently insert into the metallacycle (**TSC4**, $\Delta\Delta G$ = 16.0 kcal mol^{-1}) to form the chromacycloheptane intermediate **C8** ($\Delta\Delta G$ = -14.5 kcal mol^{-1}). Here, the mono-ethene insertion pathway is favored over the bis-ethene insertion pathway (difference **TSC4** and **TSC2**, $\Delta\Delta G$ = 11.9 kcal mol^{-1})

1-hexene is formed through a concerted 3,7-H shift from **C6** (**TSC3**, $\Delta\Delta G$ = 9.0 kcal mol^{-1}). 1-octene is formed through insertion of ethene into the chromacycloheptane intermediate C**8** (**TSC5**, $\Delta\Delta G$ = 3.7 kcal mol^{-1}) to form chromacyclononane intermediate **C9** ($\Delta\Delta G$ = 24.0 kcal mol^{-1}). Chromacyclononane intermediate **C9** can subsequently undergo a 3,7-H shift to form 1-octene (**TSC6**, $\Delta\Delta G$ = 10.4 kcal mol^{-1}). This DFT model correctly explains that the formation of 1-hexene is favored over 1-octene (difference **TSC3** and **TSC5**, $\Delta\Delta G$ = 5.6 kcal mol^{-1}).

Scheme S16. DFT-D3 calculations for a mechanism proceeding via dicationic Cr^{II}/Cr^{IV} intermediates. Calculations were performed at the BP86/TZP level of theory, without inclusion of a solvent model. The singlet (not depicted), triplet (red) and quintet (blue) spin state were taken into consideration. Reported are the Gibbs free energies, and the electronic energies in parentheses, in kcal mol^{-1}. Depicted are the catalytic cycles for the formation of 1-butene (green), 1-hexene (blue) and 1-octene (red). Parts of the ligand are removed for clarity of the image.

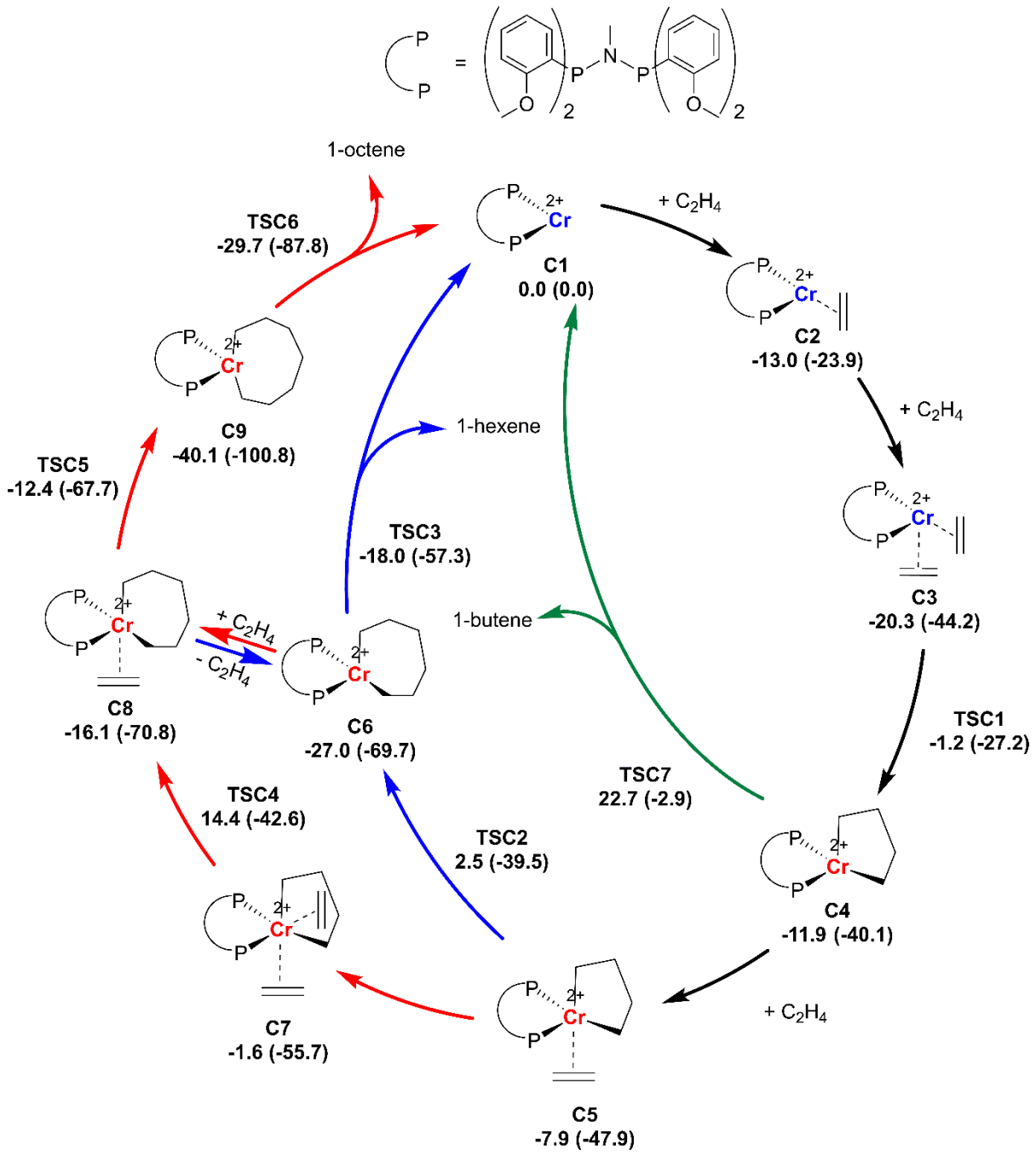
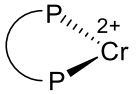
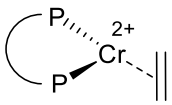
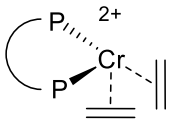
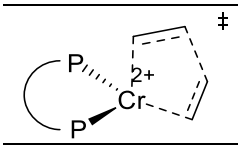
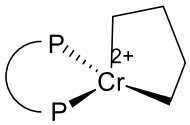
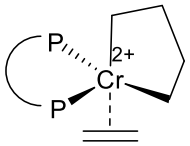
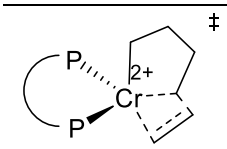
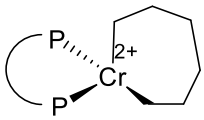
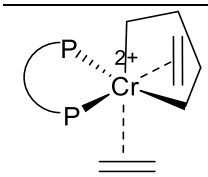
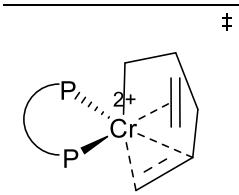
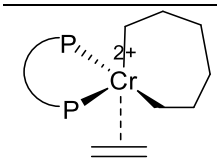
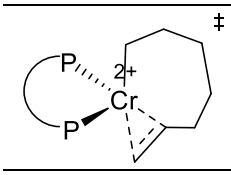
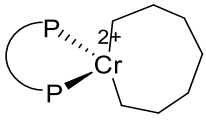
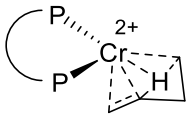
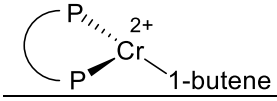
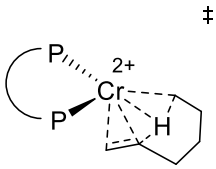
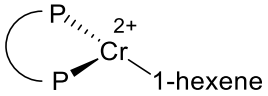
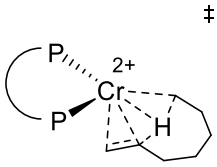
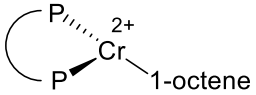


Table S31. Overview of the relative energies of the various spin states for the intermediates depicted in Scheme S16

Structure	Spin state	*ΔE* (kcal mol^{-1})	*ΔG* (kcal mol^{-1})	*ΔH* (kcal mol^{-1})
	**Singlet**	35.4	34.3	35.9
	Triplet	25.5	25.0	26.0
	Quintet	0	0	0

	**Singlet** **Triplet** **Quintet**	-4.0 -23.2 -23.9	8.9 -8.7 -13.0	-2.1 -22.0 -22.1
	**Singlet** **Triplet** **Quintet**	-25.4 -37.6 -44.2	0.6 -10.9 -20.3	-21.6 -33.8 -40.7
	**Triplet**	-27.2	-1.2	-24.2
	**Singlet** **Triplet**	-27.2 -40.1	1.1 -11.9	-23.5 -36.4
	**Singlet** **Triplet**	-32.9 -47.9	11.8 -7.9	-27.2 -42.5
	**Triplet**	-39.5	2.5	-36.1
	**Singlet** **Triplet**	-57.4 -69.7	-14.5 -27.0	-50.6 -63.0
	**Singlet** **Triplet**	-42.8 -55.7	11.8 -1.6	-35.3 -48.3
	**Triplet**	-42.6	14.4	-36.2
	**Singlet** **Triplet**	-59.9 -70.8	-1.8 -16.1	-49.0 -62.6
	**Triplet**	-67.7	-12.4	-60.4
	**Singlet** **Triplet**	-88.5 -100.8	-27.2 -40.1	-76.8 -89.5

‡ 	**Triplet**	-2.9	22.7	-3.4
	**Singlet** **Triplet** **Quintet**	-32.7 -44.5 -54.9	-5.1 -15.1 -30.1	-29.2 -39.3 -50.1
‡ 	**Triplet**	-54.3	-8.2	-48.3
	**Singlet** **Triplet** **Quintet**	-65.2 -76.5 -88.6	-21.6 -32.8 -45.5	-57.8 -69.1 -81.5
‡ 	**Triplet**	-87.8	-29.7	-78.7
	**Singlet** **Triplet** **Quintet**	-96.9 -104.0 -113.3	-34.3 -44.5 -56.2	-83.8 -94.3 -103.4

6. DFT coordinates

6.1 Benchmarking

Structure: $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$
BP86-D3/TZP (Large frozen core)
Spin state: Quartet

E = -10461.39 kcal mol-1
H = -10077.87 kcal mol-1
TS = -72.92 kcal mol-1
G (298.15 K) = -10150.79 kcal mol-1

Cr 5.124225 8.407324 3.354603
Cl 6.692659 8.606039 5.050835
Cl 4.223437 10.512384 3.622842
Cl 6.654246 8.526378 1.621054
P 3.512575 7.344366 4.975940
P 5.266103 5.911584 3.486090
N 4.156375 5.746238 4.809904
N 3.668427 8.046314 1.924366
C 4.114827 4.566692 5.722512
H 4.461424 3.715409 5.112120
C 5.101531 4.725901 6.891010
H 4.788489 5.584533 7.502617
H 6.098684 4.958484 6.493574
C 5.131715 3.458200 7.753888
H 5.518433 2.616752 7.152404
H 5.832752 3.593726 8.590548
C 3.728523 3.114552 8.272110
H 3.751003 2.192086 8.871425
H 3.383050 3.922258 8.940059
C 2.738664 2.966459 7.108331
H 1.726047 2.755801 7.483591
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H 1.715956 8.013108 -0.577554
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C 1.186372 8.642779 4.245980
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C 8.998383 3.358582 4.505758
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H 7.811519 1.648263 3.911954
C 6.723462 3.496709 3.692473
H 5.837080 3.004719 3.289540
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C 3.475491 4.084226 2.200063
H 3.068801 3.857093 3.185713
C 2.938776 3.464983 1.066596
H 2.115816 2.756395 1.173651
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H 3.043587 3.265044 -1.083749
C 4.520290 4.656049 -0.329247
H 4.926260 4.886244 -1.315489
C 5.057251 5.277655 0.799736
H 5.855721 6.017828 0.699370

Structure: $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$
BP86-D3/TZ2P (Large frozen core)
Spin state: Quartet

E = -10505.61 kcal mol-1
H = -10121.45 kcal mol-1
TS = -73.22 kcal mol-1
G (298.15 K) = -10194.67 kcal mol-1

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Cl 6.524943 8.612969 1.497846
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P 5.306005 5.886673 3.494272
N 4.232516 5.760012 4.841110
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C 4.873418 4.804342 7.069701
H 4.391180 5.623589 7.619756
H 5.901689 5.120358 6.856740
C 4.852100 3.533620 7.926845
H 5.402023 2.730954 7.406975
H 5.381642 3.715654 8.872515
C 3.412788 3.077058 8.193023
H 3.403294 2.152668 8.788192
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H 3.116822 2.030618 6.323968

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C 1.126304 8.538950 4.466097
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C 1.287079 6.264083 3.654274
H 1.860027 5.350298 3.521339
C 3.378013 7.800075 6.726301
C 2.202932 7.498823 7.434784
H 1.360731 7.033112 6.924580
C 2.106365 7.803058 8.791044
H 1.194145 7.559806 9.335784
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H 3.095954 8.662630 10.507059
C 4.330032 8.753162 8.736917
H 5.155280 9.258342 9.238388
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H 5.335793 8.704282 6.820194
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H 6.349334 3.272011 2.499662
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C 4.363504 4.738620 -0.310793
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H 5.629155 6.192569 0.675881

Structure: $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$
BP86-D3/TZ2P (Small frozen core)
Spin state: Quartet

E = -10519.62 kcal mol-1
H = -10134.77 kcal mol-1
TS = -74.81 kcal mol-1
G (298.15 K) = -10209.58 kcal mol-1

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Cl 4.183840 10.433956 3.676662
Cl 6.517789 8.605197 1.525020
P 3.570057 7.351429 4.960674
P 5.301523 5.896442 3.490965
N 4.231957 5.767647 4.837823
N 3.640094 8.046495 1.953002
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H 4.662070 3.779043 5.208839
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H 5.896106 5.138473 6.861794
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C 1.842497 7.337782 4.364772
C 1.127425 8.544121 4.460516
H 1.577619 9.401965 4.960818
C -0.138462 8.653550 3.888343
H -0.684000 9.593979 3.965810
C -0.704117 7.566785 3.214072
H -1.698709 7.652961 2.775869
C 0.013758 6.374330 3.097279
H -0.414367 5.525794 2.562293
C 1.287763 6.266136 3.657863
H 1.860827 5.352019 3.527404
C 3.379320 7.807739 6.717762
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H 7.451297 6.281416 5.395886
C 8.725066 4.539809 5.289265
H 9.395666 4.895405 6.071432
C 8.971852 3.321154 4.652658

H 9.832871 2.717661 4.941165
C 8.119749 2.883387 3.637543
H 8.311606 1.937908 3.129893
C 7.017172 3.653764 3.265873
H 6.361062 3.302005 2.471505
C 4.556649 4.970069 2.094989
C 3.631574 3.931369 2.262640
H 3.355531 3.601152 3.263199
C 3.063413 3.306398 1.151468
H 2.342686 2.500444 1.292262
C 3.426528 3.705972 -0.136847
H 2.986104 3.214548 -1.004812
C 4.361128 4.731126 -0.309802
H 4.652174 5.043689 -1.313114
C 4.922684 5.365960 0.798893
H 5.626162 6.191838 0.667150

Structure: $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$
BP86-D3/TZ2P (No frozen core)
Spin state: Quartet

E = -10516.42 kcal mol-1
H = -10132.03 kcal mol-1
TS = -72.61 kcal mol-1
G (298.15 K) = -10204.64 kcal mol-1

Cr 5.122887 8.372956 3.330442
Cl 6.779302 8.566275 4.904811
Cl 4.204321 10.432915 3.714039
Cl 6.536163 8.604223 1.540669
P 3.569626 7.341380 4.956669
P 5.301423 5.889064 3.487642
N 4.236509 5.759190 4.838532
N 3.655843 8.067997 1.968760
C 4.144713 4.581832 5.748737
H 4.685645 3.775879 5.223080
C 4.877340 4.828735 7.078602
H 4.378776 5.645679 7.618741
H 5.902029 5.159874 6.869392
C 4.870604 3.564078 7.946487
H 5.436610 2.765900 7.436043
H 5.392379 3.761570 8.893775
C 3.436582 3.085873 8.208215
H 3.438497 2.165743 8.810709
H 2.902815 3.851367 8.796430
C 2.690523 2.853820 6.887717
H 1.650792 2.548892 7.076319
H 3.168510 2.020336 6.344477
C 2.707695 4.105798 5.996800
H 2.201870 3.897439 5.044518
H 2.140685 4.913760 6.483153
C 2.830310 7.870796 1.183629
C 1.807670 7.582755 0.205227
H 2.053831 6.637063 -0.298998
H 1.753694 8.390367 -0.536462
H 0.838663 7.482078 0.712730
C 1.843760 7.317227 4.352547
C 1.124701 8.523267 4.433248
H 1.573633 9.389135 4.921561
C -0.143139 8.620885 3.861287
H -0.692534 9.560361 3.927925
C -0.706868 7.522806 3.202080
H -1.703357 7.599356 2.765490
C 0.015655 6.331217 3.098636
H -0.410306 5.474193 2.574897
C 1.291550 6.234525 3.659179
H 1.867126 5.320086 3.540386
C 3.363107 7.816274 6.707152
C 2.191471 7.496655 7.415329
H 1.366293 6.994506 6.910734
C 2.075463 7.831400 8.763470
H 1.166276 7.574476 9.308096
C 3.118408 8.502197 9.409693
H 3.024653 8.766959 10.463608
C 4.270387 8.849008 8.700008
H 5.075787 9.393307 9.193769
C 4.396921 8.512411 7.351753
H 5.291937 8.783587 6.790785
C 6.755155 4.857402 3.895971
C 7.632410 5.292118 4.904952
H 7.456782 6.252867 5.388487
C 8.733982 4.513605 5.255774
H 9.409345 4.862356 6.037453
C 8.979883 3.302592 4.602821
H 9.844849 2.698052 4.878291
C 8.121970 2.874214 3.587664
H 8.313276 1.935214 3.067111
C 7.014323 3.646209 3.232111
H 6.354566 3.302632 2.436684
C 4.545135 4.972369 2.090099
C 3.634005 3.920479 2.259213
H 3.376686 3.575561 3.260280
C 3.056093 3.301494 1.148892
H 2.346148 2.485730 1.290869
C 3.396048 3.720028 -0.140529
H 2.947905 3.233542 -1.007819
C 4.317569 4.757525 -0.315342
H 4.590895 5.083988 -1.319600
C 4.888650 5.386771 0.792837
H 5.583128 6.220783 0.661007

Structure: $[Ph_2PN(Cy)PPh_2]CrCl_3(CH_3CN)$
M06L/TZP (No frozen core)
Spin state: Quartet

E = - -11117.18 kcal mol-1

Cr 5.140698 8.390483 3.296443
Cl 6.802847 8.495749999999999 4.874729
Cl 4.244709 10.461033 3.700315
Cl 6.511903 8.606782000000003 1.472427
P 3.577731 7.342306 4.967588
P 5.312852 5.860307 3.501695
N 4.274737 5.777971 4.867313
N 3.582675 8.118164 1.917071
C 4.130087 4.597203 5.763983
H 4.686844 3.794964 5.263625
C 4.787322 4.82503 7.122762
H 4.280828 5.643567 7.635714
H 5.820432 5.13723 6.978247

C 4.704471 3.571114 7.980389
H 5.269857 2.763453 7.503429
H 5.180094 3.75001 8.944611999999999
C 3.257854 3.138348000000001
8.165043000000001
H 3.197956 2.234486 8.771663
H 2.718749 3.91764 8.713585
C 2.587057 2.916773 6.818091
H 1.541043 2.637182 6.946453
H 3.069597 2.07356 6.312578
C 2.684979 4.147737 5.925849
H 2.241011 3.943654 4.951450999999999
H 2.106468 4.968715 6.360314
C 2.735611 8.086767999999999 1.140846
C 1.679614 8.052580000000001 0.167001
H 1.786074 7.171452 -0.462507
H 1.723425 8.943398999999999 -0.455132
H 0.716813 8.013439 0.67284
C 1.859279 7.265801 4.374484
C 1.048978 8.391431000000001 4.553266
H 1.411051 9.229448 5.136651
C -0.208983 8.447906 3.972473
H -0.826503 9.324071999999999 4.121088
C -0.675865 7.386656 3.205962
H -1.664323 7.427658 2.766354
C 0.134363 6.276675999999999 3.001765
H -0.21449 5.448816 2.396526000000001
C 1.398875 6.223929 3.571262
H 2.039409 5.372596 3.381658
C 3.384151 7.837759 6.705942
C 2.244387 7.494894 7.440689
H 1.42522 6.975498 6.959259
C 2.156763 7.817745 8.785318999999999
H 1.276038 7.539046 9.349164
C 3.196838 8.500621000000001
9.404151000000001
H 3.128895 8.750795999999999 10.455195
C 4.313306 8.875845 8.671283000000001
H 5.113479 9.428770999999999
9.145379999999999
C 4.41134 8.551271 7.326008999999999
H 5.280904 8.840479999999999 6.749202
C 6.763915 4.847821 3.92222
C 7.549832 5.210001 5.021025
H 7.295495 6.09812 5.583745
C 8.661390000000001 4.457699 5.362854
H 9.260332 4.749544 6.215484
C 9.015696 3.34776 4.607073
H 9.887874999999999 2.765102 4.874232
C 8.255578999999999 2.994547 3.501904
H 8.532339 2.136903 2.902758
C 7.135472 3.737845 3.158424
H 6.551737 3.450013 2.294712
C 4.55012 4.916093 2.141031
C 3.767525 3.775449 2.33026
H 3.597641 3.392767 3.329937
C 3.20118 3.125239 1.243508
H 2.591549 2.244431 1.399123
C 3.427421 3.597101 -0.044175
H 2.989902 3.084144 -0.891215
C 4.221452 4.719119 -0.241964
H 4.40794 5.084337 -1.244091
C 4.77727 5.382138 0.844596
H 5.382364 6.273685 0.6998450000000001

Structure: $AlMe_3$
BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -1450.04 kcal mol-1
H = -1379.61 kcal mol-1
TS = -26.66 kcal mol-1
G (298.15 K) = -1406.28 kcal mol-1

Al -4.372094 -0.970056 -0.053940
C -3.727826 0.851396 0.315193
C -3.172826 -2.507452 0.205432
C -6.210728 -1.252177 -0.693285
H -2.677283 0.888903 0.637375
H -4.334153 1.330856 1.101411
H -3.827428 1.494174 -0.574871
H -2.270419 -2.412950 -0.420932
H -3.640723 -3.474168 -0.029685
H -2.812268 -2.555735 1.246139
H -6.210286 -1.719050 -1.692243
H -6.798937 -0.325784 -0.761400
H -6.757019 -1.948607 -0.036424

Structure: $AlMe_3$(THF)
BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -3116.66 kcal mol-1
H = -2969.89 kcal mol-1
TS = -34.79 kcal mol-1
G (298.15 K) = -3004.68 kcal mol-1

Al -4.744445 2.253660 -0.094496
C -2.780837 2.221793 0.185886
C -5.377438 2.254201 -1.984164
C -5.895800 1.360533 1.250401
H -5.660830 1.684340 2.277689
H -5.754402 0.267410 1.229550
H -6.972828 1.533894 1.091865
H -2.209473 2.727882 -0.609496
H -2.403146 1.186596 0.223465
H -2.493720 2.690568 1.141569
H -4.833250 2.978315 -2.614619
H -6.451847 2.480928 -2.088656
H -5.227434 1.269305 -2.456514
O -5.126335 4.174932 0.369944
C -4.394052 5.211008 -0.379903
C -5.476571 6.025388 -1.072386
H -3.703015 4.699185 -1.058522
H -3.822366 5.802105 0.349716
C -6.609789 6.001427 -0.032778
H -5.790348 5.520654 -1.996502
H -5.139458 7.038909 -1.320283
C -6.544191 4.570154 0.493894
H -7.592555 6.230650 -0.461589

H -6.408457 6.721834 0.772462
H -7.136128 3.876351 -0.118818
H -6.821048 4.454590 1.547403

Structure: $(AlMe_3)_2$
BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -2921.81 kcal mol-1
H = -2779.03 kcal mol-1
TS = -37.57 kcal mol-1
G (298.15 K) = -2816.60 kcal mol-1

Al 0.173039 0.595908 0.534518
C 1.764048 0.907267 -0.577869
C 0.012688 -0.875428 1.824885
C -1.543562 0.378775 -0.736833
H 2.662844 1.078393 0.035219
H 1.649973 1.782774 -1.234973
H 1.983561 0.044024 -1.225696
H 0.114074 -1.856965 1.336675
H -0.960544 -0.865713 2.338785
H 0.792030 -0.822847 2.600681
H -2.068741 0.872946 -1.574693
H -2.272924 -0.268958 -0.232168
H -0.846290 -0.279390 -1.286971
Al -1.691402 2.351904 0.096648
C -3.425293 2.364168 1.018169
C -0.244228 2.361264 1.682596
C -1.168076 3.670877 -1.264345
H -3.511328 1.538572 1.740872
H -4.262769 2.266806 0.310191
H -3.584140 3.301701 1.573076
H -0.377991 3.453255 1.574420
H 0.844970 2.301230 1.861753
H -0.744377 2.062600 2.613575
H -1.178128 4.696494 -0.862913
H -1.854773 3.662622 -2.125397
H -0.156165 3.487870 -1.656642

Structure: MAO (Based on reference 12)
BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -9234.64 kcal mol-1
H = -8879.60 kcal mol-1
TS = -86.60 kcal mol-1
G (298.15 K) = -8966.21 kcal mol-1

Al -0.924910 2.267782 1.762690
Al -1.310663 4.177019 -0.033882
Al -3.557468 2.774297 0.017077
Al -4.010623 4.934433 1.466850
Al -1.164589 5.216728 3.028491
Al -1.054764 2.489471 4.745576
Al -3.838293 2.145433 3.139776
Al -4.000610 4.986357 4.452842
Al -3.806649 2.483312 6.274116
Al -1.468904 4.668748 6.175041
Al -3.674032 7.207059 6.190710
O -3.059886 4.611437 -0.031755
O -3.031552 5.270315 2.950338
O -0.761615 4.306714 4.523711
O -1.991094 2.086621 3.225551
O -4.207171 3.214518 4.563403
O -2.926716 5.637356 5.759399
O -1.815831 2.357339 0.189325
O -2.031571 2.942019 6.215024
O -4.241193 3.111439 1.666706
O -0.717929 4.117877 1.677769
C -0.403527 5.465229 7.589593
H 0.492222 4.869857 7.818897
H -0.978132 5.557496 8.524110
H -0.057070 6.474460 7.316898
C -3.902321 0.519544 6.234929
H -4.878684 0.123725 5.920014
H -3.721428 0.154556 7.259752
H -3.142674 0.037859 5.599121
C -5.634833 6.065618 4.754849
H -6.181472 5.706254 5.639350
H -5.576028 7.170636 4.821705
H -6.302755 5.922419 3.892039
C -4.652307 0.383561 2.947403
H -4.125957 -0.412162 3.489307
H -5.696301 0.380605 3.296306
H -4.678897 0.096512 1.882961
C 0.464984 1.334254 5.126319
H 0.508380 1.128098 6.206360
H 0.411653 0.368948 4.604429
H 1.419460 1.802350 4.844676
C -0.432118 7.017148 2.901585
H -0.647010 7.609484 3.803641
H -0.849455 7.580043 2.051737
H 0.660826 7.001815 2.774720
C -5.592845 6.048511 1.227918
H -5.736581 6.260900 0.157594
H -5.521673 7.015203 1.747024
H -6.509666 5.552155 1.579682
C -4.665684 1.941179 -1.335029
H -4.882046 0.892384 -1.081868
H -4.180868 1.945750 -2.322029
H -5.631949 2.457330 -1.433802
C -0.144809 4.797774 -1.449433
H 0.068504 5.872767 -1.349972
H -0.593998 4.644517 -2.441531
H 0.820932 4.271676 -1.434338
C 0.696588 1.199009 1.708280
H 0.502676 0.141252 1.939139
H 1.127701 1.240006 0.696132
H 1.466723 1.546907 2.409800
C -4.483677 7.326459 7.954421
H -3.733661 7.131017 8.737493
H -5.281486 6.582553 8.090448
H -4.907613 8.322663 8.147131
C -3.158570 8.663590 5.000861
H -2.188481 9.096494 5.292941
H -3.889371 9.486051 5.008504
H -3.051068 8.311655 3.964231
C -4.781518 3.519793 7.638423
H -4.250600 4.427470 7.961354

H -4.945874 2.912386 8.542333
H -5.777794 3.838975 7.292318

Structure: MAO.THF
BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -10907.31 kcal mol-1
H = -10475.25 kcal mol-1
TS = -93.13 kcal mol-1
G (298.15 K) = -10568.39 kcal mol-1

Al 0.440748 1.332685 3.071303
Al 0.610305 3.837978 2.237647
Al -1.626107 2.899376 1.189963
Al -2.365877 4.332784 3.286077
Al -0.051433 3.508882 5.384038
Al -0.498828 0.342725 5.736530
Al -2.741896 1.101743 3.562183
Al -3.208158 3.139133 5.902295
Al -3.545151 0.080203 6.428929
Al -1.225761 1.780996 7.817730
Al -2.998724 4.235671 8.912687
O -1.052129 4.494831 2.045563
O -1.813648 3.879210 4.950255
O -0.112416 2.033704 6.383981
O -0.983394 0.726769 4.011694
O -3.399210 1.489544 5.193543
O -2.499249 3.069516 7.592935
O -0.008658 2.186414 1.538741
O -1.813520 0.274053 6.994246
O -2.718325 2.649494 2.620380
O 0.727177 3.011004 3.843975
C -0.307564 1.502347 9.505878
H 0.400916 0.674311 9.342317
H -0.965841 1.208133 10.333691
H 0.277735 2.369525 9.839451
C -3.688402 -1.664346 5.527846
H -4.548955 -1.741997 4.847558
H -3.815917 -2.441992 6.298998
H -2.796420 -1.949651 4.947501
C -4.918518 4.053258 5.697738
H -5.635913 3.617259 6.408007
H -4.936476 5.141403 5.828703
H -5.307654 3.840710 4.690428
C -3.531075 -0.269470 2.422075
H -3.231377 -1.291782 2.684881
H -4.630693 -0.232440 2.453613
H -3.243718 -0.102232 1.370571
C 0.840366 -1.060483 5.912387
H 0.603363 -1.682281 6.788558
H 0.886708 -1.721780 5.036325
H 1.850347 -0.653169 6.064655
C 0.734460 5.084158 6.235025
H 0.213570 5.303016 7.179559
H 0.655656 5.983114 5.603117
H 1.799593 4.947447 6.471345
C -3.642755 5.804124 3.170305
H -3.380239 6.453951 2.322295
H -3.647567 6.428578 4.076140
H -4.676388 5.463816 3.019796
C -2.371534 2.851772 -0.597270
H -2.713967 1.838260 -0.854858
H -1.638258 3.152965 -1.359137
H -3.240911 3.519695 -0.685044
C 2.136254 4.797977 1.525964
H 2.348626 5.706037 2.110202
H 1.966527 5.112450 0.485888
H 3.045344 4.179384 1.544362
C 1.997000 0.177648 2.930859
H 1.726041 -0.852699 2.658771
H 2.669665 0.558518 2.147310
H 2.572861 0.124005 3.864589
C -2.120965 3.985665 10.651320
H -1.027909 4.094800 10.658249
H -2.341101 2.997385 11.080280
H -2.532522 4.723650 11.360189
C -4.905881 4.695650 8.961290
H -5.264873 5.349019 8.155138
H -5.110798 5.209728 9.914766
H -5.547289 3.801217 8.943372
C -4.850239 0.589950 7.817016
H -4.720315 1.605150 8.221807
H -4.805708 -0.100162 8.674696
H -5.878603 0.538364 7.425060
C -2.496232 6.548877 7.005511
C -1.706303 7.848103 7.029406
C -1.614362 8.160233 8.531251
C -1.372675 6.787659 9.140823
O -2.115278 5.855044 8.260632
H -2.235563 5.881043 6.178241
H -3.581698 6.708920 7.038433
H -2.208048 8.635773 6.455649
H -0.704970 7.690279 6.608120
H -2.560034 8.581678 8.899041
H -0.805084 8.858617 8.774702
H -1.757651 6.664238 10.157552
H -0.315936 6.490478 9.106254

Structure: $AlMe_2Cl$
BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -1081.74 kcal mol-1
H = -1032.28 kcal mol-1
TS = -26.57 kcal mol-1
G (298.15 K) = -1058.84 kcal mol-1

Al -4.451704 0.032273 -0.006380
Cl -2.916191 1.501377 0.010092
C -3.892752 -1.835814 0.054091
H -2.961715 -1.998583 -0.506555
H -4.663627 -2.511832 -0.342656
H -3.696452 -2.140765 1.094120
C -6.294544 0.668395 -0.082290
H -6.414126 1.635082 0.425861
H -6.997394 -0.050972 0.362381
H -6.603325 0.815605 -1.129574

Structure: Al_2Me_5Cl

BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -2556.14 kcal mol-1
H = -2434.63 kcal mol-1
TS = -37.19 kcal mol-1
G (298.15 K) = -2471.82 kcal mol-1

Al 0.267316 0.533053 0.458322
C 1.869131 0.999871 -0.562971
C 0.089236 -0.958817 1.708355
H -0.066287 3.643344 -1.553817
H 2.743340 1.135513 0.093931
H 1.738347 1.933469 -1.130635
H 2.130354 0.214003 -1.287955
H 0.305487 -1.923772 1.225391
H -0.927572 -1.022226 2.124302
H 0.785948 -0.858743 2.555846
H -0.916393 1.841803 2.491452
H -1.092434 4.847785 -0.752204
H -1.718364 3.922698 -2.125831
Al -1.760837 2.479834 0.004432
C -3.494454 2.488959 0.908752
C -0.367680 2.221231 1.619197
C -1.094603 3.850896 -1.221779
H -3.633266 1.595436 1.535781
H -4.328254 2.517494 0.190995
H -3.601019 3.369418 1.562414
H -0.500103 3.320807 1.606966
H 0.710860 2.173655 1.866868
Cl -1.495422 0.432278 -1.044136

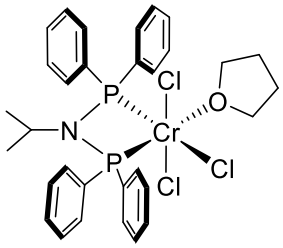
Structure: C_2H_6
BP86-D3/TZ2P (No frozen core)
Spin state: Singlet

E = -924.47 kcal mol-1
H = -876.19 kcal mol-1
TS = -16.25 kcal mol-1
G (298.15 K) = -892.44 kcal mol-1

C -0.000000 -0.000000 0.766131
C -0.000000 0.000000 -0.766131
H 0.886272 -0.511689 1.166286
H -0.886272 -0.511689 1.166286
H 0.000000 1.023379 1.166286
H 0.886272 0.511689 -1.166286
H -0.886272 0.511689 -1.166286
H 0.000000 -1.023379 -1.166286

6.2 Activation of complex 1

Structure (Meridonial):



Spin state: doublet

E = -10343.62 kcal mol-1
H = -9955.53 kcal mol-1
TS = -72.99 kcal mol-1
G (298.15 K) = -10028.52 kcal mol-1

H -1.904291 7.770322 13.844899
C -0.611012 2.424451 9.032885
C -0.820405 7.799328 13.729944
C 1.270044 9.010751 13.839076
Cl 4.548019 4.087761 10.145652
C 1.252095 6.682464 13.154781
C -0.138496 6.658917 13.303722
H -0.653556 9.871146 14.319052
H -1.044933 2.289376 14.714636
H -1.457044 4.513663 11.584249
H -0.870284 1.998902 12.973396
C -0.770131 2.757414 13.760027
H 5.955812 4.143948 16.662594
C 0.666164 3.274274 13.846884
H 3.039432 7.895810 13.311823
H 0.684968 4.105597 14.568860
C 1.714891 1.522308 11.125779
C -0.488285 3.143537 10.233467
C -1.574012 3.890804 10.701884
C 2.586189 -1.091106 11.647566
H 2.924876 -2.107494 11.851203
C -2.787075 3.875449 10.015127
Cr 2.457991 5.062089 10.024989
C 1.954180 7.868213 13.424223
C -0.119114 8.977894 13.994704
H -1.486387 3.560262 13.553626
C 4.634661 4.354436 13.524777
Cl 2.145363 4.301622 7.911281
P 1.176113 3.265938 10.963320
Cl 0.502647 6.290650 9.970967
H 4.569747 -0.236912 11.739227
C 5.540758 4.054531 14.543510
H 3.811038 5.290450 17.206430
C 4.044215 5.025299 16.174677
H 4.865028 4.103800 12.488936
C 1.616861 2.180314 14.355533
H -3.860783 3.133177 8.293894
C -2.915330 3.135691 8.837191
H 2.661028 2.508489 14.320550
H 1.822261 9.928634 14.042891
H 1.366015 1.941449 15.398002
H 1.522309 1.263129 13.762799
N 1.121599 3.897462 12.563148

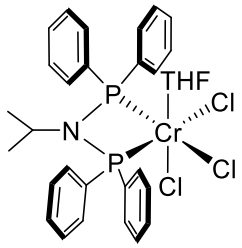
P 2.182359 5.256823 12.490180
C 3.420431 4.990283 13.826070
C 5.247022 4.382072 15.868655
H -0.685337 5.747579 13.070391
H 6.482860 3.564272 14.295942
H -1.907614 1.861973 7.409883
C -1.822958 2.418078 8.343626
H 0.504660 -1.650150 11.472690
C 1.228853 -0.835802 11.434581
C 3.137631 5.333265 15.160866
H 2.208010 5.844786 15.409449
C 3.507609 -0.042667 11.587816
H -0.267849 0.652086 11.010904
C 0.792561 0.463283 11.173640
H 3.798349 2.073033 11.267666
C 3.077817 1.258019 11.328248
O 3.559680 6.854936 9.653769
C 4.222681 6.965125 8.349558
C 3.238421 7.781240 7.516522
C 2.573326 8.733061 8.549954
C 3.053661 8.202523 9.911360
H 4.407737 5.950053 7.989415
H 5.179633 7.487025 8.512420
H 2.491144 7.102581 7.088129
H 3.739110 8.317493 6.701074
H 1.481634 8.671573 8.484249
H 2.877419 9.778277 8.410114
H -3.627101 4.461338 10.389087
H 0.247127 1.889187 8.626921
H 2.265005 8.122981 10.663995
H 3.899468 8.785548 10.309982

Spin state: quartet

E = -10362.67 kcal mol-1
H = -9975.18 kcal mol-1
TS = -71.24 kcal mol-1
G (298.15 K) = -10046.42 kcal mol-1

H -1.918596 7.762249 13.856587
C -0.609470 2.425024 9.032004
C -0.834606 7.794188 13.743622
C 1.251876 9.012588 13.853413
Cl 4.559721 4.074754 10.145778
C 1.241970 6.683226 13.173619
C -0.148760 6.655382 13.319687
H -0.674955 9.867383 14.329681
H -1.042487 2.286729 14.712693
H -1.462120 4.509471 11.585724
H -0.868445 1.997570 12.971396
C -0.768349 2.755693 13.758357
H 5.960754 4.141821 16.669895
C 0.667596 3.272907 13.846214
H 3.025651 7.902681 13.330374
H 0.685628 4.103392 14.569108
C 1.709627 1.516473 11.129246
C -0.490721 3.141374 10.234627
C -1.577440 3.887335 10.702675
C 2.580489 -1.096455 11.649109
H 2.919124 -2.113028 11.851981
C -2.788944 3.872242 10.013354
Cr 2.470101 5.071605 10.011365
C 1.940338 7.871507 13.441664
C -0.137237 8.975289 14.007592
H -1.485181 3.558188 13.552857
C 4.629031 4.360468 13.537324
Cl 2.148167 4.318292 7.882997
P 1.171922 3.258880 10.966066
Cl 0.497539 6.294732 9.982832
H 4.564991 -0.243816 11.734665
C 5.538932 4.058561 14.552089
H 3.816309 5.282521 17.225736
C 4.045805 5.021174 16.192204
H 4.855793 4.114297 12.499140
C 1.618557 2.179066 14.354455
H -3.858106 3.133168 8.288005
C -2.913832 3.135073 8.833362
H 2.662883 2.506444 14.317703
H 1.800766 9.932779 14.055719
H 1.368884 1.942121 15.397642
H 1.522583 1.260930 13.763530
N 1.124544 3.899090 12.562800
P 2.179584 5.263739 12.511089
C 3.414790 4.992798 13.846264
C 5.248649 4.381130 15.879261
H -0.692652 5.742679 13.084881
H 6.481283 3.571159 14.299934
H -1.901904 1.866544 7.404448
C -1.819965 2.419713 8.340132
H 0.498341 -1.655006 11.478694
C 1.222625 -0.840829 11.439194
C 3.135132 5.331087 15.182686
H 2.205362 5.840550 15.435237
C 3.502538 -0.048757 11.586637
H -0.274118 0.647891 11.017472
C 0.786367 0.458293 11.178891
H 3.793702 2.067246 11.263418
C 3.073115 1.252233 11.327828
O 3.575479 6.857837 9.633506
C 4.238337 6.962655 8.328677
C 3.257286 7.777956 7.489810
C 2.571741 8.719322 8.520448
C 3.062697 8.204737 9.883180
H 4.420487 5.945623 7.972055
H 5.196283 7.482411 8.491695
H 2.520639 7.096963 7.047302
H 3.765042 8.323441 6.684962
H 1.481731 8.631739 8.456095
H 2.851151 9.770877 8.376965
H -3.630151 4.456941 10.386462
H 0.250504 1.892844 8.625962
H 2.278773 8.126632 10.641352
H 3.907904 8.795603 10.271555

Structure (Facial):



Spin state: doublet

E = -10337.31 kcal mol-1
H = -9949.59 kcal mol-1
TS = -71.16 kcal mol-1
G (298.15 K) = -10020.75 kcal mol-1

H -1.873087 7.456521 14.394236
C -0.344918 2.490951 8.924959
C -0.871026 7.599696 13.988603
C 0.921362 9.066052 13.289419
O 4.648726 4.182671 10.358181
C 1.174511 6.665744 13.089594
C -0.109122 6.489602 13.617743
H -0.953428 9.753628 14.115554
H -0.948766 2.157303 14.546641
H 0.514774 1.960853 8.514998
H -1.198833 4.550765 11.501327
H -0.715469 1.938301 12.799978
C -0.633908 2.660420 13.622836
H 6.175369 4.597925 16.605736
C 0.807956 3.147574 13.773560
H 2.657634 8.101416 12.439097
H 0.841249 3.928631 14.549240
C 2.000332 1.575571 11.007151
C -0.233502 3.180112 10.143797
C -1.315852 3.936002 10.611600
C 2.982495 -1.020761 11.443952
H 3.360898 -2.028563 11.617231
C -2.520095 3.941397 9.909763
Cr 2.687489 5.253553 10.096400
H -3.357878 4.532254 10.280545
C 1.684205 7.962277 12.912015
C -0.354924 8.887742 13.831172
H -1.333227 3.478733 13.419684
C 4.413211 4.087053 13.736925
Cl 2.610165 4.439642 7.983191
P 1.411777 3.314495 10.902393
Cl 0.708092 6.345349 9.907851
H 4.903056 -0.072471 11.736553
C 5.383857 3.901245 14.718175
H 4.483846 6.410944 16.838176
C 4.467098 5.755713 15.966743
H 4.393455 3.436740 12.864022
C 1.713467 1.998413 14.240567
H -3.580179 3.237589 8.163843
C -2.641294 3.222110 8.718057
H 2.761473 2.307923 14.292467
H 1.317115 10.070551 13.138276
H 1.399993 1.686197 15.246320
H 1.637141 1.128986 13.578139
N 1.302737 3.838227 12.538520
P 2.217354 5.290210 12.509738
C 3.451071 5.103886 13.859395
C 5.414694 4.738928 15.837466
H -0.529064 5.491479 13.724698
H 6.118642 3.102525 14.610775
H -1.626877 1.971611 7.274996
C -1.548847 2.507028 8.221327
H 0.951263 -1.671181 11.099006
C 1.631038 -0.820227 11.151631
C 3.488266 5.938847 14.986115
H 2.750887 6.732359 15.100038
C 3.846462 0.075526 11.510104
H 0.082012 0.612970 10.720346
C 1.140040 0.468544 10.934742
H 4.025588 2.217945 11.354426
C 3.357620 1.361879 11.290881
Cl 3.891520 7.178310 10.099464
C 6.461361 2.708348 9.946190
H 6.167300 5.604106 10.159499
H 6.264068 1.713097 10.364455
C 5.836498 4.852737 10.890175
C 6.843405 3.717637 11.065145
C 5.191076 3.300144 9.320134
H 5.544319 5.365578 11.809645
H 6.735603 3.260123 12.057187
H 7.874094 4.081561 10.977236
H 7.251268 2.599343 9.193513
H 4.415068 2.573127 9.068825
H 5.398972 3.908879 8.429527

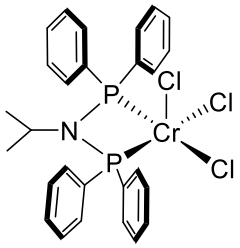
Spin state: quartet

E = -10355.57 kcal mol-1
H = -9967.24 kcal mol-1
TS = -73.10 kcal mol-1
G (298.15 K) = -10040.34 kcal mol-1

H -1.790036 7.495049 14.534721
C -0.346478 2.483483 8.919308
C -0.809205 7.625949 14.076499
C 0.948503 9.071693 13.255231
O 4.617199 4.199540 10.386683
C 1.187384 6.666979 13.099579
C -0.067882 6.505162 13.695915
H -0.881960 9.782473 14.157733
H -0.943242 2.183268 14.562037
H 0.517338 1.964411 8.503576
H -1.212498 4.515438 11.513773
H -0.740577 1.971034 12.810661
C -0.631322 2.685780 13.636792
H 6.143264 4.579360 16.657118
C 0.822217 3.141027 13.770267
H 2.637066 8.081942 12.337223
H 0.882683 3.917615 14.548461
C 1.988067 1.552019 11.010777
C -0.239658 3.163326 10.143853
C -1.326631 3.906834 10.619377
C 2.966329 -1.045813 11.444956
H 3.343235 -2.054393 11.616824

C -2.531464 3.909411 9.918558
Cr 2.701423 5.261252 10.066120
H -3.373269 4.490910 10.294990
C 1.689472 7.957502 12.864988
C -0.299473 8.908854 13.863786
H -1.315680 3.520411 13.449945
C 4.398242 4.065485 13.778401
Cl 2.647183 4.496150 7.919210
P 1.408324 3.291965 10.896138
Cl 0.697214 6.316208 9.924133
H 4.885882 -0.099747 11.752075
C 5.360329 3.878125 14.767648
H 4.464444 6.407011 16.866716
C 4.448668 5.746644 15.999149
H 4.381689 3.411584 12.907830
C 1.706741 1.971003 14.225299
H -3.587430 3.213717 8.166969
C -2.648062 3.200035 8.720405
H 2.763046 2.253208 14.256567
H 1.337301 10.071297 13.060336
H 1.403728 1.672829 15.238490
H 1.595807 1.100040 13.569993
N 1.320116 3.828735 12.531702
P 2.227469 5.289447 12.524363
C 3.441979 5.089593 13.888720
C 5.389118 4.721675 15.882704
H -0.483043 5.510992 13.849474
H 6.090326 3.073793 14.669794
H -1.625277 1.971144 7.264763
C -1.550902 2.497463 8.216447
H 0.936970 -1.694148 11.085725
C 1.616747 -0.843638 11.145173
C 3.478479 5.931699 15.010377
H 2.747250 6.732537 15.113053
C 3.830617 0.049747 11.520526
H 0.071002 0.592325 10.708773
C 1.127680 0.445938 10.928736
H 4.012002 2.192303 11.373569
C 3.343678 1.336879 11.302518
Cl 3.889139 7.211129 9.972223
C 6.445032 2.740803 9.998315
H 6.115023 5.643035 10.196191
H 6.247735 1.750753 10.428784
C 5.794706 4.887269 10.926210
C 6.816081 3.765945 11.107086
C 5.178933 3.319178 9.354061
H 5.488709 5.395557 11.843863
H 6.720424 3.315737 12.103548
H 7.840701 4.144234 11.010312
H 7.240640 2.624146 9.252914
H 4.410092 2.587346 9.094433
H 5.391056 3.930505 8.466706

Structure:



Spin state: doublet

E = -8683.38 kcal mol-1
H = -8371.66 kcal mol-1
TS = -66.06 kcal mol-1
G (298.15 K) = -8437.72 kcal mol-1

H -1.797418 8.020455 13.823755
C -0.859798 2.046717 9.380148
C -0.716633 7.964464 13.690894
C 1.457972 9.025275 13.709777
Cl 4.590293 5.131618 10.298757
C 1.260120 6.677088 13.141625
C -0.127292 6.758102 13.309339
H -0.389423 10.041358 14.182286
H -1.497294 2.587230 14.655326
H -1.274179 4.922369 11.166353
H -1.169526 2.091751 12.982573
C -1.091386 2.925096 13.692895
H 5.793517 3.527876 16.513179
C 0.362580 3.361322 13.875560
H 3.130690 7.769232 13.183715
H 0.379287 4.222992 14.562516
C 1.786464 1.574651 11.107972
C -0.580287 3.068941 10.300126
C -1.525021 4.083737 10.518990
C 2.996914 -0.933911 11.390496
H 3.468560 -1.910669 11.502734
C -2.758190 4.040586 9.874081
Cr 2.379611 4.926049 10.099871
C 2.051164 7.821103 13.334556
C 0.073573 9.098014 13.891783
H -1.718902 3.740582 13.315214
C 4.341161 3.869708 13.449268
Cl 2.269482 3.769190 8.191317
P 1.077488 3.256980 11.020173
Cl 0.848878 6.512706 9.809618
H 4.817854 0.051008 10.770252
C 5.220620 3.418528 14.432271
H 4.017022 5.173365 17.095244
C 4.109968 4.806979 16.072344
H 4.434372 3.508635 12.427110
C 1.214645 2.246688 14.496955
H -4.011774 2.973109 8.474726
C -3.048714 3.000785 8.985251
H 2.253848 2.563241 14.632297
H 2.077233 9.910694 13.854660
H 0.804421 1.984244 15.481860
H 1.208048 1.345349 13.873984
N 0.929821 3.901915 12.603545
P 2.072649 5.181223 12.500474

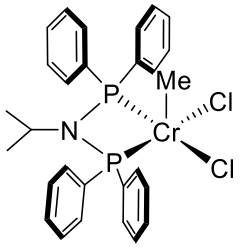
C 3.331584 4.790466 13.773401
C 5.105393 3.883069 15.745405
H -0.747379 5.880099 13.134079
H 6.000775 2.703317 14.170828
H -2.307273 1.215377 8.019427
C -2.095228 2.012496 8.732249
H 1.031531 -1.647180 11.944820
C 1.628736 -0.787425 11.639775
C 3.226390 5.261512 15.092162
H 2.447046 5.975784 15.356331
C 3.755361 0.166414 10.985098
H -0.044386 0.567900 11.683968
C 1.024045 0.460852 11.496200
H 3.739950 2.271120 10.494943
C 3.153745 1.417299 10.838843
H -3.487715 4.831537 10.049092
H -0.109718 1.289333 9.157707

Spin state: quartet

E = -8697.59 kcal mol-1
H = -8386.44 kcal mol-1
TS = -64.08 kcal mol-1
G (298.15 K) = -8450.52 kcal mol-1

H -1.847845 7.967371 13.814861
C -0.848375 2.094704 9.356979
C -0.763925 7.936642 13.701495
C 1.386489 9.042522 13.775656
Cl 4.669163 4.842193 10.211691
C 1.249273 6.699478 13.168312
C -0.141946 6.748992 13.313520
H -0.490283 10.012984 14.227632
H -1.433813 2.586515 14.657122
H -1.295368 4.915038 11.221778
H -1.129882 2.111787 12.974434
C -1.042409 2.936836 13.693097
H 5.779802 3.621487 16.608916
C 0.412979 3.372346 13.864021
H 3.095108 7.830644 13.264177
H 0.435612 4.227739 14.558197
C 1.786582 1.586269 11.082414
C -0.579262 3.097403 10.301300
C -1.537622 4.089476 10.555733
C 2.969469 -0.935960 11.344991
H 3.430196 -1.918901 11.447546
C -2.775569 4.041982 9.919979
Cr 2.423771 4.948325 10.075886
C 2.011809 7.856964 13.393079
C -0.002222 9.083750 13.932926
H -1.677848 3.755170 13.336128
C 4.378798 3.953220 13.519605
Cl 2.216876 3.797290 8.140449
P 1.083139 3.268051 11.007766
Cl 0.777749 6.450637 9.802486
H 4.802473 0.037320 10.741053
C 5.251982 3.518319 14.515901
H 3.944186 5.207331 17.172606
C 4.067913 4.855184 16.147971
H 4.506049 3.610134 12.494345
C 1.269696 2.251566 14.467023
H -4.022440 2.991363 8.502833
C -3.055888 3.021477 9.006536
H 2.311336 2.563952 14.591638
H 1.984026 9.938554 13.944646
H 0.870711 1.984974 15.455279
H 1.252111 1.353966 13.838944
N 0.977672 3.923763 12.591350
P 2.107545 5.226687 12.532175
C 3.337038 4.841495 13.834032
C 5.096718 3.964404 15.831167
H -0.739379 5.860960 13.114515
H 6.058757 2.830548 14.261980
H -2.292247 1.275759 7.986173
C -2.088571 2.056293 8.719355
H 0.993890 -1.634908 11.882311
C 1.601746 -0.778248 11.589878
C 3.191440 5.295218 15.155410
H 2.387540 5.985034 15.410837
C 3.740619 0.160730 10.954358
H -0.058479 0.592192 11.639273
C 1.009821 0.476976 11.456491
H 3.752623 2.268783 10.484270
C 3.153622 1.419801 10.817663
H -3.515999 4.816308 10.120998
H -0.085994 1.358994 9.106089

Geometry:



Spin state: doublet

E = -9052.75 kcal mol-1
H = -8720.79 kcal mol-1
TS = -64.74 kcal mol-1
G (298.15 K) = -8785.53 kcal mol-1

H -1.908451 7.717068 14.026727
C -0.680283 2.124712 9.289002
C -0.828933 7.717621 13.872172
C 1.288370 8.886231 13.856681
C 4.297947 5.615199 10.712191
C 1.200360 6.532073 13.277101
C -0.185787 6.544199 13.474305
H -0.599029 9.807383 14.366834
H -1.404039 2.275087 14.667066
H 0.073798 1.377074 9.045486
H -1.151288 4.876221 11.247097
H -1.033234 1.855251 12.982588
C -0.993886 2.662636 13.725336
H 5.912213 3.502790 16.516859
C 0.443118 3.140165 13.941631

H 3.011285 7.720451 13.292164
H 0.424885 3.971575 14.665241
C 1.852665 1.504088 11.113478
C -0.429385 3.081985 10.284017
C -1.381274 4.082219 10.537819
C 2.987169 -1.052109 11.298798
H 3.428284 -2.046536 11.373753
C -2.592819 4.085766 9.851800
Cr 2.424158 4.984017 10.276737
H -3.327375 4.865232 10.055607
C 1.933618 7.715287 13.463411
C -0.094499 8.889602 14.063806
H -1.640106 3.472403 13.366029
C 4.385087 3.846726 13.491529
Cl 2.786608 3.899948 8.362909
P 1.201367 3.217484 11.087242
Cl 1.011368 6.669843 9.915586
H 4.852171 -0.089428 10.783939
C 5.302127 3.409016 14.445025
H 4.084896 5.065071 17.164536
C 4.171158 4.722376 16.132740
H 4.457924 3.500978 12.460501
C 1.337510 2.034450 14.517548
H -3.799190 3.119077 8.340674
C -2.853872 3.109716 8.884176
H 2.360378 2.393341 14.674698
H 1.864498 9.801673 13.994305
H 0.935051 1.705916 15.485918
H 1.375636 1.165466 13.850890
N 0.985171 3.754187 12.699446
P 2.062600 5.084088 12.583486
C 3.346863 4.721133 13.849512
C 5.195193 3.844594 15.769618
H -0.764989 5.636375 13.310495
H 6.102563 2.727617 14.155395
H -2.081595 1.390874 7.826369
C -1.892780 2.138236 8.597549
H 0.985459 -1.736031 11.750042
C 1.615585 -0.878827 11.510973
C 3.250982 5.161451 15.178109
H 2.450603 5.841512 15.469634
C 3.787092 0.045742 10.974386
H -0.021992 0.518027 11.569407
C 1.049491 0.391803 11.414052
H 3.832930 2.173802 10.588317
C 3.221275 1.318026 10.876448
H 4.323291 6.399059 9.931679
H 4.970070 4.796553 10.412779
H 4.625203 6.032412 11.670858

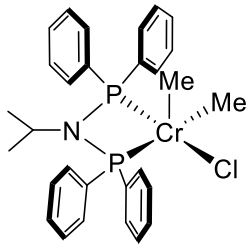
Spin state: quartet

E = -9069.24 kcal mol-1
H = -8737.00 kcal mol-1
TS = -65.02 kcal mol-1
G (298.15 K) = -8802.01 kcal mol-1

H -1.304526 6.974616 15.792724
C -0.761269 2.727736 9.270335
C -0.886507 6.985151 14.785662
C -0.898340 7.832359 12.516990
C 4.455323 4.017267 11.019785
C 0.752142 6.185349 13.183828
C 0.213318 6.184080 14.482068
H -2.305903 8.433587 14.040437
H -0.847893 2.157055 15.050143
H -0.047980 2.102291 8.733997
H -1.059759 4.570340 12.127940
H -0.984415 2.115491 13.278156
C -0.561266 2.673505 14.123848
H 6.096075 5.610678 16.701015
C 0.963410 2.745309 14.019112
H 0.633179 7.050567 11.205772
H 1.340595 3.382252 14.834154
C 1.607253 1.264466 10.842176
C -0.419714 3.265444 10.524647
C -1.323538 4.116942 11.175781
C 2.165406 -1.441748 10.406677
H 2.382770 -2.496966 10.238203
C -2.563737 4.398550 10.601573
Cr 2.704882 4.845868 10.341925
H -3.258464 5.059232 11.120825
C 0.196907 7.023839 12.205212
C -1.447248 7.805718 13.800292
H -1.009026 3.673784 14.134636
C 4.072521 4.078597 14.428070
Cl 2.517781 4.120052 8.213218
P 1.299003 3.043100 11.105750
Cl 3.186037 7.037840 10.103367
H 4.146370 -0.782351 9.849443
C 5.069975 4.233696 15.389901
H 4.750332 7.576522 15.972497
C 4.557169 6.592353 15.545108
H 3.897534 3.103342 13.978164
C 1.601532 1.361134 14.187766
H -3.874191 4.069151 8.915623
C -2.906834 3.845225 9.366031
H 2.680072 1.388822 13.994919
H -1.321474 8.483775 11.752215
H 1.441661 1.010096 15.216030
H 1.158436 0.626534 13.506606
N 1.430911 3.430850 12.779282
P 2.081558 5.027370 12.684567
C 3.293275 5.176839 14.033308
C 5.313504 5.489845 15.951590
H 0.661024 5.562692 15.258326
H 5.662736 3.371773 15.697343
H -2.255736 2.592633 7.728176
C -2.000853 3.013482 8.701036
H 0.106476 -1.797661 10.966066
C 0.886353 -1.050364 10.816703
C 3.550669 6.440468 14.591610
H 2.965022 7.304535 14.277893
C 3.156896 -0.481673 10.194235
H -0.397941 0.604782 11.327154
C 0.604476 0.298022 11.027074
H 3.639148 1.625222 10.208724
C 2.879671 0.870518 10.405435
H 4.387015 3.155597 11.697667
H 5.028599 4.817659 11.506418

H 4.955397 3.715174 10.087778

Geometry:



Spin state: doublet

E = -9415.39 kcal mol-1
H = -9062.81 kcal mol-1
TS = -65.44 kcal mol-1
G (298.15 K) = -9128.26 kcal mol-1

H -0.101243 7.851790 15.974674
C -1.018559 4.374355 10.296076
C 0.107298 7.657618 14.921982
C -0.207699 8.205916 12.585413
C 4.208793 6.373581 10.858625
C 1.234858 6.356359 13.212361
C 0.969407 6.620350 14.565592
H -1.158455 9.259311 14.214595
H -1.642755 3.776585 14.646177
H -0.373305 5.251283 10.320400
H -0.913006 0.998911 10.772851
H -1.683798 3.359861 12.919489
C -1.094528 3.858822 13.697298
H 6.237968 4.430247 16.721328
C 0.289661 3.210280 13.853260
H 0.885446 6.978289 11.178992
H 0.767142 3.637273 14.750745
C 1.787497 1.327237 10.961093
C -0.469917 3.109975 10.566669
C -1.313851 1.987623 10.551533
C 2.894762 -1.223942 10.561744
H 3.321006 -2.215797 10.409450
C -2.675341 2.131133 10.280233
Cr 3.048183 4.722701 10.517775
H -3.321116 1.252168 10.280772
C 0.651807 7.166426 12.227535
C -0.487019 8.447619 13.932897
H -1.012271 4.920365 13.439930
C 3.694820 3.531004 14.639065
Cl 4.571733 3.172840 10.079623
P 1.296535 3.079816 11.080276
C 1.959049 5.435370 8.962348
H 3.939217 -0.882437 12.422820
C 4.688107 3.413027 15.612515
H 5.825873 6.625879 15.618448
C 5.226191 5.756601 15.347079
H 3.098885 2.663354 14.359254
C 0.175816 1.697328 14.046870
H -4.278066 3.505669 9.818007
C -3.213017 3.395765 10.024306
H 1.147482 1.237812 14.261935
H -0.654179 8.832195 11.812392
H -0.505891 1.481571 14.880281
H -0.230079 1.220273 13.145415
N 1.233042 3.540311 12.747254
P 2.242273 4.918549 12.659204
C 3.454650 4.764166 14.018960
C 5.457581 4.523973 15.965741
H 1.438256 6.012934 15.340479
H 4.863584 2.450134 16.093245
H -2.791574 5.507188 9.832668
C -2.379757 4.517335 10.031816
H 1.775189 -1.243478 8.712993
C 2.026185 -0.680325 9.612455
C 4.228765 5.879482 14.380880
H 4.049674 6.843119 13.903031
C 3.236050 -0.478640 11.693757
H 0.823270 1.010963 9.043616
C 1.481025 0.589706 9.804579
H 3.005789 1.389971 12.739799
C 2.697221 0.792088 11.884299
H 4.690082 6.537902 9.879834
H 4.994126 6.178172 11.603668
H 3.655926 7.282111 11.143404
H 2.749319 5.383825 8.188621
H 1.064990 4.922221 8.588181
H 1.727598 6.499673 9.133347

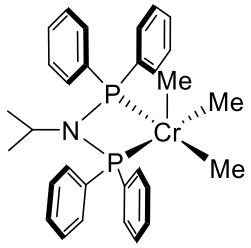
Spin state: quartet

E = -9432.64 kcal mol-1
H = -9079.71 kcal mol-1
TS = -65.91 kcal mol-1
G (298.15 K) = -9145.62 kcal mol-1

H -1.318797 8.429739 12.877114
C -1.239618 4.039536 10.089576
C -0.273882 8.208146 13.095871
C 1.908384 8.920235 13.857702
C 4.659547 5.804369 10.801684
C 1.562986 6.622504 13.157680
C 0.222110 6.923476 12.872383
H 0.179662 10.213255 13.760771
H -1.993663 3.637822 14.485083
H -0.705108 4.989732 10.076951
H -0.786816 0.758533 10.919573
H -1.650745 2.662127 13.042521
C -1.404402 3.596899 13.559151
H 5.551277 3.200988 16.995569
C 0.083773 3.667885 13.912098
H 3.456162 7.419028 13.847600
H 0.237105 4.575447 14.518384
C 1.800800 1.430884 11.366972
C -0.593091 2.885397 10.565078
C -1.276782 1.659784 10.551793
C 3.240976 -0.981754 11.373849
H 3.798253 -1.918748 11.376563
C -2.590963 1.595198 10.087094
Cr 2.990465 4.648708 10.432329
H -3.116709 0.639681 10.085380

C 2.407632 7.635868 13.641281
C 0.566964 9.208583 13.589972
H -1.713598 4.426962 12.914080
C 4.421918 3.690572 13.818987
Cl 3.800175 3.355858 8.792918
P 1.112316 3.109934 11.182427
C 1.741598 6.065521 9.645089
H 3.862039 -0.415269 13.364993
C 5.209827 3.204080 14.862677
H 3.660808 4.747833 17.478385
C 3.874094 4.449317 16.451562
H 4.637404 3.392731 12.791957
C 0.505037 2.457816 14.750060
H -4.263828 2.696427 9.276457
C -3.235884 2.750232 9.635922
H 1.549341 2.540311 15.074143
H 2.570538 9.700061 14.234585
H -0.125477 2.392623 15.647714
H 0.382893 1.528322 14.179183
N 0.957474 3.888642 12.718036
P 2.260515 5.009049 12.681175
C 3.347841 4.555145 14.084414
C 4.934695 3.579709 16.179949
H -0.428635 6.148716 12.467937
H 6.042526 2.535176 14.644864
H -3.051294 4.874052 9.275467
C -2.556799 3.972399 9.637912
H 2.497349 -1.242857 9.360607
C 2.506542 -0.605645 10.245112
C 3.084729 4.937266 15.409753
H 2.260737 5.617668 15.626133
C 3.275521 -0.140623 12.487543
H 1.267305 0.898540 9.332813
C 1.801171 0.595860 10.233944
H 2.627476 1.723146 13.342888
C 2.567751 1.062507 12.481593
H 5.072749 6.061288 9.814706
H 5.420469 5.226541 11.351802
H 4.452432 6.733108 11.355536
H 2.424910 6.830422 9.246117
H 1.203839 5.591132 8.810056
H 1.027426 6.554766 10.322785

Geometry:



Spin state: doublet

E = -9781.84 kcal mol-1
H = -9408.26 kcal mol-1
TS = -67.79 kcal mol-1
G (298.15 K) = -9476.05 kcal mol-1

H 0.292031 7.605440 16.315724
C -1.374589 4.490719 10.420550
C 0.341679 7.475201 15.233923
C -0.319904 8.155316 13.007263
C 1.205538 6.287074 13.301311
C 1.144515 6.471000 14.691330
H -1.020212 9.100995 14.819209
H -1.590810 3.694545 14.828264
H -0.736234 5.374160 10.394309
H -1.175739 1.111889 10.812167
H -1.773135 3.382325 13.087984
C -1.116558 3.825948 13.845479
H 6.689946 4.186678 15.881418
C 0.264570 3.151437 13.850662
H 0.550632 7.021898 11.383933
H 0.825153 3.529307 14.721900
C 1.476163 1.468194 10.665553
C -0.786612 3.234029 10.628326
C -1.611445 2.098472 10.654439
C 2.513225 -1.044099 9.940843
H 2.912342 -2.019719 9.662168
C -2.992935 2.222185 10.495837
Cr 2.561587 4.854165 10.279591
H -3.622638 1.331928 10.525010
C 0.480076 7.148180 12.466212
C -0.395379 8.315159 14.393392
H -1.034870 4.899815 13.644706
C 3.823052 3.412243 14.207070
C 3.731539 6.526061 10.489261
P 1.027353 3.211598 10.984325
C 4.088326 3.529789 10.085015
H 3.608145 -0.945702 11.801999
C 4.956633 3.240168 15.003234
H 6.156634 6.429685 14.934454
C 5.501586 5.581292 14.733272
H 3.166791 2.568189 13.997755
C 0.141561 1.632265 13.983076
H -4.648722 3.577815 10.190078
C -3.569001 3.482118 10.310114
H 1.120599 1.154360 14.106120
H -0.878939 8.820268 12.347836
H -0.481032 1.381944 14.852524
H -0.334566 1.204166 13.091296
N 1.118039 3.510291 12.686695
P 2.119113 4.890184 12.512716
C 3.515365 4.671182 13.673765
C 5.801012 4.322519 15.264855
H 1.726752 5.825040 15.349708
H 5.182412 2.257377 15.418920
H -3.196717 5.602702 10.118716
C -2.754697 4.617215 10.270374
H 1.333239 -0.832351 8.142144
C 1.626613 -0.378356 9.089541
C 4.364377 5.757551 13.946518
H 4.131129 6.742679 13.540467
C 2.899797 -0.443166 11.142282
H 0.431088 1.384520 8.767987
C 1.114893 0.870191 9.444897
H 2.731319 1.294393 12.407818

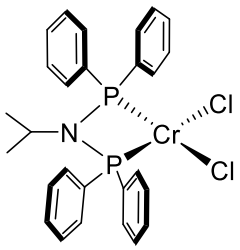
C 2.395042 0.808000 11.494106
H 4.597056 3.895259 9.171451
H 3.861629 2.462693 9.964482
H 4.782053 3.651810 10.931707
C 1.416561 5.084011 8.652562
H 1.075012 6.126726 8.811643
H 0.576443 4.482182 8.286696
H 2.225254 5.089735 7.894474
H 4.107494 6.668244 9.458885
H 4.601111 6.421289 11.153002
H 3.166796 7.424844 10.787164

Spin state: quartet

E = -9791.40 kcal mol-1
H = -9418.40 kcal mol-1
TS = -67.21 kcal mol-1
G (298.15 K) = -9485.61 kcal mol-1

H 0.543125 7.945289 16.324112
C -1.514376 4.332479 10.294718
C 0.475928 7.710174 15.261203
C -0.490129 8.114512 13.079440
C 1.190047 6.381735 13.359448
C 1.273560 6.697856 14.724591
H -1.032266 9.206139 14.864610
H -1.639202 3.752791 14.798288
H -0.903959 5.232036 10.214069
H -1.231081 0.993930 10.944409
H -1.818308 3.499787 13.048767
C -1.169186 3.928697 13.820669
H 6.517409 4.012935 16.084401
C 0.223894 3.282518 13.804537
H 0.254013 6.878091 11.475335
H 0.786689 3.687212 14.661277
C 1.512750 1.477695 10.796499
C -0.900373 3.109685 10.615390
C -1.690428 1.951787 10.700598
C 2.823757 -0.952914 10.265513
H 3.329488 -1.896825 10.060792
C -3.067455 2.021824 10.487329
Cr 2.725662 4.733965 10.120995
H -3.672308 1.117236 10.561437
C 0.307858 7.107060 12.539474
C -0.410335 8.416181 14.442606
H -1.105064 5.010410 13.659800
C 3.586108 3.434366 14.441301
C 4.591122 5.556556 10.331964
P 0.896558 3.188460 10.957567
C 3.120468 3.563974 8.488151
H 4.059897 -0.471561 11.972089
C 4.688082 3.203735 15.268945
H 6.279579 6.193310 14.898708
C 5.521465 5.418952 14.777802
H 2.837682 2.653810 14.316031
C 0.137171 1.763188 13.958066
H -4.749474 3.299416 10.029781
C -3.672368 3.247016 10.191017
H 1.127269 1.294519 14.004110
H -1.170473 8.670922 12.433937
H -0.409702 1.515773 14.877589
H -0.403920 1.315541 13.114944
N 1.032685 3.672625 12.608527
P 2.116063 5.012465 12.566377
C 3.439485 4.660832 13.778091
C 5.656344 4.194545 15.440776
H 1.961487 6.149116 15.368425
H 4.787936 2.245967 15.780984
H -3.356612 5.358416 9.850992
C -2.891696 4.402163 10.092651
H 1.470371 -1.128798 8.589603
C 1.778876 -0.523661 9.442778
C 4.425996 5.649084 13.947893
H 4.336814 6.598915 13.418686
C 3.229607 -0.155975 11.339291
H 0.339419 1.022024 9.030290
C 1.132981 0.686273 9.698024
H 2.932974 1.687822 12.412659
C 2.586637 1.054525 11.596738
H 3.761446 4.083363 7.760505
H 2.215186 3.201384 7.975163
H 3.668682 2.682116 8.871767
C 1.727554 6.291167 9.259897
H 1.770845 7.194307 9.888306
H 0.680569 6.052792 9.014040
H 2.263798 6.493122 8.320149
H 5.086550 5.686518 9.358365
H 5.192171 4.855170 10.941287
H 4.572647 6.527233 10.853142

Geometry:



Spin state: singlet

E = -8596.49 kcal mol-1
H = -8287.53 kcal mol-1
TS = -61.61 kcal mol-1
G (298.15 K) = -8349.14 kcal mol-1

H -1.115694 8.588815 12.861753
C -1.312689 3.645104 9.878600
C -0.135993 8.244909 13.194902
C 1.900489 8.605595 14.449075
C 1.607445 6.556018 13.183106
C 0.348185 7.013270 12.759874
H 0.259303 10.008683 14.380654
H -2.103697 3.988607 14.332484
H -0.851070 4.603297 9.635528
H -0.577625 0.660884 11.368053
H -1.886615 3.098121 12.812035
C -1.498530 3.924815 13.417705

H 6.007660 2.832419 16.213995
C -0.028464 3.708774 13.797687
H 3.374665 7.036389 14.340254
H 0.248846 4.517587 14.491925
C 1.947152 1.490780 11.342458
C -0.565529 2.669155 10.555842
C -1.152154 1.426823 10.847291
C 3.465019 -0.862368 11.482095
H 4.056270 -1.777033 11.535928
C -2.475500 1.174646 10.483195
Cr 2.483172 4.666424 10.268387
H -2.926275 0.209361 10.716587
C 2.387110 7.369010 14.020406
C 0.637558 9.043206 14.043390
H -1.628130 4.854571 12.852783
C 3.183694 4.356627 15.068791
Cl 4.328960 3.611478 9.714307
P 1.121687 3.108663 11.121679
H 4.041854 -0.179694 13.450626
C 4.081991 3.781822 15.967324
H 6.585264 2.986847 13.793829
C 5.630812 3.370237 14.155313
H 2.237589 4.754798 15.435668
C 0.181199 2.363086 14.495322
H -4.255888 1.958176 9.543716
C -3.221473 2.156905 9.825886
H 1.203102 2.269833 14.881598
H 2.511988 9.228444 15.102834
H -0.518195 2.258685 15.336339
H 0.000156 1.535027 13.796658
N 0.897769 3.892002 12.645234
P 2.236338 4.986109 12.482865
C 3.495761 4.428404 13.698791
C 5.306686 3.283520 15.510733
H -0.237496 6.406611 12.070375
H 3.827138 3.724642 17.026144
H -3.212004 4.154097 8.998630
C -2.636634 3.389762 9.521804
H 2.735159 -1.263727 9.486477
C 2.722621 -0.575648 10.332199
C 4.730091 3.937145 13.251133
H 4.971733 3.971884 12.189040
C 3.455717 0.030793 12.555550
H 1.405917 0.822329 9.353914
C 1.971757 0.596267 10.258829
H 2.722959 1.906571 13.315982
C 2.704944 1.205203 12.485050
Cl 1.204628 6.265968 9.455410

Spin state: triplet

E = -8605.13 kcal mol-1
H = -8296.22 kcal mol-1
TS = -61.55 kcal mol-1
G (298.15 K) = -8357.77 kcal mol-1

H -0.940254 8.742944 12.853556
C -1.347264 3.607574 9.897910
C 0.017244 8.349461 13.196160
C 2.045044 8.594906 14.491526
C 1.685019 6.585753 13.178156
C 0.453843 7.106403 12.743682
H 0.468352 10.070350 14.424744
H -2.122362 4.215243 14.293170
H -0.882163 4.555144 9.621448
H -0.619465 0.671830 11.485992
H -1.934102 3.271847 12.800447
C -1.513880 4.097591 13.385959
H 6.080172 2.734777 16.063843
C -0.057602 3.827240 13.783703
H 3.451452 6.965980 14.373695
H 0.248465 4.635934 14.465927
C 1.911463 1.487358 11.411709
C -0.603275 2.652714 10.608818
C -1.192974 1.422444 10.942156
C 3.402553 -0.875994 11.625349
H 3.984205 -1.794736 11.707680
C -2.517327 1.162211 10.587126
Cr 2.456601 4.638073 10.231040
H -2.970820 0.206561 10.852775
C 2.484702 7.347290 14.045285
C 0.809792 9.095993 14.073872
H -1.596279 5.015526 12.793431
C 3.234985 4.281544 15.004880
Cl 4.290339 3.573868 9.633771
P 1.090589 3.099029 11.142122
H 3.953202 -0.158671 13.589201
C 4.146241 3.679809 15.872253
H 6.631807 2.982023 13.645179
C 5.679199 3.346344 14.030396
H 2.288929 4.657060 15.395041
C 0.089754 2.485578 14.504050
H -4.295578 1.918960 9.622054
C -3.260535 2.124056 9.897350
H 1.104687 2.351899 14.896787
H 2.672039 9.176800 15.167916
H -0.617580 2.426402 15.342827
H -0.125755 1.654807 13.818533
N 0.886413 3.950310 12.635031
P 2.259275 5.004935 12.460339
C 3.533809 4.406901 13.635549
C 5.369228 3.207111 15.384928
H -0.145937 6.541259 12.031366
H 3.902637 3.581046 16.930684
H -3.244724 4.091557 9.001314
C -2.671750 3.344016 9.550721
H 2.701565 -1.312496 9.626492
C 2.681605 -0.606930 10.457541
C 4.766074 3.940553 13.156882
H 4.996431 4.014475 12.094113
C 3.384084 0.038645 12.680250
H 1.393113 0.782390 9.429749
C 1.942926 0.569803 10.347727
H 2.657094 1.936414 13.390090
C 2.646364 1.218821 12.573061
Cl 1.156579 6.235621 9.419578

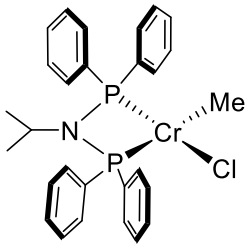
Spin state: quintet

E = -8611.17 kcal mol-1

H = -8302.17 kcal mol-1
TS = -63.48 kcal mol-1
G (298.15 K) = -8365.65 kcal mol-1

H -1.590047 7.942952 13.383682
C -1.186987 4.132213 9.926660
C -0.523700 7.784315 13.547336
C 1.624655 8.587448 14.319333
C 1.431882 6.357441 13.388119
C 0.061953 6.575918 13.171027
H -0.201942 9.737800 14.412379
H -1.724525 3.031952 14.811364
H -0.515087 4.976887 9.765201
H -1.177688 0.956274 11.182223
H -1.469169 2.163547 13.287764
C -1.228039 3.082962 13.833203
H 6.142689 3.066278 16.480258
C 0.280807 3.228974 14.044054
H 3.284854 7.227411 14.096957
H 0.437098 4.083037 14.722416
C 1.648334 1.345604 11.129046
C -0.706728 2.978284 10.565460
C -1.549631 1.864865 10.707523
C 2.937737 -1.131749 10.854730
H 3.433983 -2.096991 10.751217
C -2.862774 1.917380 10.242770
Cr 2.616571 4.678309 10.362490
H -3.513787 1.050246 10.357956
C 2.214725 7.377821 13.952839
C 0.255718 8.791265 14.123675
H -1.646895 3.927301 13.273464
C 3.287933 4.549826 15.359446
Cl 4.412321 6.059070 10.404796
P 1.009562 3.051822 11.174565
H 4.051355 -0.566060 12.620187
C 4.241255 4.066775 16.255115
H 6.521504 2.850317 14.028077
C 5.609081 3.314855 14.402392
H 2.392933 5.047702 15.734126
C 0.874481 1.977414 14.696319
H -4.370546 3.116998 9.265328
C -3.343621 3.079524 9.630333
H 1.942981 2.107387 14.905408
H 2.238206 9.375949 14.755816
H 0.361141 1.774785 15.646557
H 0.748329 1.103097 14.044943
N 1.005906 3.625570 12.800741
P 2.216792 4.849119 12.738809
C 3.482464 4.401476 13.976175
C 5.398187 3.441988 15.777538
H -0.540969 5.798747 12.700281
H 4.083678 4.179410 17.328321
H -2.868095 5.082261 8.969923
C -2.504321 4.184302 9.469649
H 1.712249 -1.393044 9.094020
C 1.968705 -0.739404 9.928076
C 4.657191 3.796317 13.502007
H 4.827818 3.725072 12.426130
C 3.281629 -0.275193 11.904643
H 0.597330 0.803776 9.311476
C 1.330706 0.494936 10.055953
H 2.944112 1.632801 12.841328
C 2.650944 0.960876 12.035443
Cl 2.185443 4.214072 8.190110

Geometry:



Spin state: singlet

E = -8958.01 kcal mol-1
H = -8628.60 kcal mol-1
TS = -62.39 kcal mol-1
G (298.15 K) = -8690.99 kcal mol-1

H -1.822466 7.608440 13.090961
C -1.256906 4.163258 10.204695
C -0.735867 7.584440 13.181126
C 1.357482 8.701373 13.653908
C 1.351296 6.355466 13.031573
C -0.046336 6.399650 12.920429
H -0.575461 9.663269 13.749716
H -1.392942 2.628654 14.906041
H -0.643216 5.058457 10.086306
H -1.011951 0.875100 11.085903
H -1.021471 1.789312 13.388622
C -0.935150 2.748069 13.914896
H 6.177720 3.734067 16.529422
C 0.529855 3.153079 14.075984
H 3.137913 7.498902 13.468259
H 0.559480 4.080964 14.671715
C 1.712244 1.313458 11.032504
C -0.663693 2.966268 10.639758
C -1.455650 1.812147 10.749325
C 2.949915 -1.192903 10.727267
H 3.424424 -2.167844 10.612524
C -2.815753 1.857520 10.441796
Cr 2.455665 4.636393 10.299699
H -3.419994 0.953777 10.530862
C 2.049773 7.519634 13.391813
C -0.036744 8.736518 13.550019
H -1.508496 3.494085 13.351681
C 3.357270 5.046022 15.134258
C 4.047844 3.485318 9.947491
P 1.111293 3.040388 11.113996
H 4.075835 -0.670122 12.497166
C 4.306373 4.728062 16.107271
H 6.509901 2.986355 14.175096
C 5.623678 3.560843 14.447083
H 2.474782 5.625038 15.407655
C 1.321429 2.075471 14.825765
H -4.466898 3.090880 9.791855

C -3.402819 3.056372 10.027889
H 2.374242 2.362181 14.938220
H 1.907716 9.599820 13.935527
H 0.897688 1.929884 15.829661
H 1.271664 1.117430 14.292040
N 1.161741 3.533915 12.781994
P 2.252519 4.849068 12.509850
C 3.534023 4.619919 13.807714
C 5.437844 3.981415 15.767393
H -0.591460 5.505753 12.616624
H 4.159576 5.061458 17.135411
H -3.067687 5.144160 9.574836
C -2.619699 4.208028 9.909676
H 1.711850 -1.408086 8.968119
C 1.987222 -0.767846 9.807003
C 4.679124 3.880756 13.471318
H 4.821972 3.558255 12.440017
C 3.311385 -0.355036 11.785746
H 0.644096 0.808366 9.215125
C 1.378638 0.479539 9.951141
H 3.011215 1.552908 12.742331
C 2.703761 0.892051 11.932936
H 3.841488 3.221351 8.889158
H 4.307517 2.560323 10.479990
H 4.907061 4.184628 9.970475
Cl 1.659458 6.216073 8.988455

Spin state: triplet

E = -8966.61 kcal mol-1
H = -8637.18 kcal mol-1
TS = -62.51 kcal mol-1
G (298.15 K) = -8699.69 kcal mol-1

H -2.049270 7.094842 13.303630
C -1.071519 4.386073 10.196891
C -0.965851 7.209565 13.256225
C 1.004827 8.612289 13.330184
C 1.232922 6.223480 12.975102
C -0.160647 6.089286 13.041660
H -1.014491 9.347211 13.562411
H -0.941458 2.020179 15.010335
H -0.339795 5.181322 10.038975
H -1.305245 1.149873 11.255328
H -0.500822 1.346313 13.429397
C -0.558727 2.275149 14.013140
H 6.227290 4.325522 16.659152
C 0.823257 2.910631 14.140719
H 2.894651 7.609390 13.051811
H 0.723967 3.833280 14.737166
C 1.517943 1.198068 10.969212
C -0.654114 3.140451 10.698469
C -1.608168 2.123705 10.872232
C 2.435843 -1.423017 10.524382
H 2.786967 -2.441223 10.354857
C -2.948549 2.351646 10.559415
Cr 2.532939 4.555770 10.319166
H -3.678456 1.553320 10.699045
C 1.811412 7.495831 13.116479
C -0.385253 8.471529 13.400367
H -1.277746 2.942779 13.524220
C 3.322281 5.268143 15.143758
C 4.128582 3.358411 10.094188
P 1.123478 2.973858 11.131629
H 3.793267 -1.052396 12.165206
C 4.282653 5.114108 16.145495
H 6.655761 3.422365 14.376227
C 5.718819 3.936143 14.594164
H 2.388923 5.788316 15.361106
C 1.791753 1.973485 14.873790
H -4.403705 3.772028 9.827660
C -3.355393 3.596797 10.071779
H 2.807444 2.385520 14.896002
H 1.460558 9.597302 13.434893
H 1.457199 1.833843 15.911574
H 1.818577 0.987848 14.392154
N 1.347500 3.370679 12.819727
P 2.287831 4.795761 12.532462
C 3.553105 4.749913 13.859433
C 5.479182 4.445222 15.874835
H -0.617006 5.109048 12.908881
H 4.094353 5.516146 17.141802
H -2.717912 5.584116 9.500463
C -2.412662 4.612800 9.890453
H 1.001920 -1.475589 8.907154
C 1.432563 -0.881784 9.714167
C 4.763933 4.091744 13.589758
H 4.949403 3.702601 12.588588
C 2.996283 -0.646078 11.541355
H 0.216931 0.839444 9.272149
C 0.982534 0.421415 9.926091
H 3.003223 1.268997 12.533998
C 2.546512 0.656612 11.758055
H 3.978593 3.007421 9.053543
H 4.315873 2.474115 10.719115
H 5.010369 4.025411 10.123080
Cl 2.102123 6.268948 8.989485

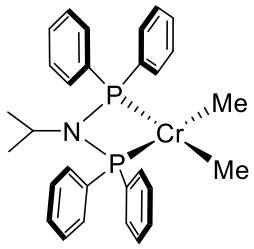
Spin state: quintet

E = -8973.11 kcal mol-1
H = -8643.40 kcal mol-1
TS = -64.37 kcal mol-1
G (298.15 K) = -8707.77 kcal mol-1

H -1.765434 7.831387 13.402626
C -1.349803 4.149034 10.165058
C -0.685194 7.733427 13.514629
C 1.453990 8.673544 14.141080
C 1.330964 6.399934 13.303074
C -0.057584 6.540455 13.154609
H -0.422474 9.734751 14.285658
H -1.590039 2.873758 14.860455
H -0.723227 5.037593 10.062330
H -1.146923 0.865285 11.074815
H -1.318967 2.028765 13.325369
C -1.131106 2.963194 13.866920
H 6.177699 3.323115 16.397009
C 0.368388 3.219422 14.027344
H 3.168057 7.390106 13.884211

H 0.486850 4.096027 14.685156
C 1.645145 1.366972 11.066965
C -0.781905 2.953933 10.637227
C -1.577132 1.800463 10.715619
C 3.010580 -1.069573 10.741505
H 3.534739 -2.017543 10.618792
C -2.921450 1.848927 10.348416
Cr 2.530405 4.855742 10.284297
H -3.532875 0.948240 10.413671
C 2.085652 7.480740 13.788563
C 0.068322 8.801231 14.009576
H -1.630747 3.773344 13.323073
C 3.317531 4.784979 15.258410
C 3.878882 6.434872 10.418937
P 0.976032 3.062071 11.122299
H 4.156153 -0.471760 12.475077
C 4.290314 4.346844 16.157080
H 6.465624 2.910770 13.957215
C 5.579246 3.428755 14.324170
H 2.441414 5.321100 15.624522
C 1.062928 2.024880 14.689855
H -4.538165 3.083151 9.618432
C -3.486426 3.048536 9.903804
H 2.129564 2.222303 14.850123
H 2.047240 9.508147 14.515773
H 0.601764 1.823999 15.666942
H 0.960737 1.124513 14.070992
N 1.026170 3.637132 12.753558
P 2.168987 4.918166 12.645779
C 3.463549 4.536639 13.884263
C 5.418555 3.663799 15.692280
H -0.642752 5.715037 12.748190
H 4.168346 4.537983 17.223774
H -3.129138 5.131873 9.449012
C -2.698531 4.198859 9.813042
H 1.740658 -1.363043 9.017740
C 2.000800 -0.704814 9.847081
C 4.608096 3.867144 13.423047
H 4.732158 3.693341 12.352114
C 3.356355 -0.204609 11.783520
H 0.564745 0.792882 9.274941
C 1.327454 0.507508 9.999218
H 2.983066 1.686350 12.739475
C 2.688624 1.009285 11.938890
H 4.297078 6.615911 9.417504
H 4.710169 6.245879 11.119242
H 3.363345 7.352239 10.752045
Cl 2.347951 4.510981 8.066358

Geometry:



Spin state: singlet

E = -9314.87 kcal mol-1
H = -8964.77 kcal mol-1
TS = -63.20 kcal mol-1
G (298.15 K) = -9027.97 kcal mol-1

H -1.971109 7.543634 13.778134
C -1.607846 4.183354 10.651414
C -0.888132 7.578481 13.650276
C 1.188286 8.813382 13.662392
C 1.197088 6.438685 13.132866
C -0.195381 6.417891 13.297751
H -0.739940 9.686765 14.108605
H -1.302581 2.441256 14.944163
H -1.121627 5.156110 10.738051
H -0.892731 0.849394 10.711013
H -0.968752 1.748122 13.343533
C -0.912606 2.666621 13.942469
H 6.209463 3.681366 16.178720
C 0.532649 3.157387 14.052324
H 2.960846 7.692621 13.163982
H 0.542373 4.058082 14.688880
C 1.706804 1.591821 10.759418
C -0.833327 3.013864 10.735480
C -1.471977 1.769083 10.629601
C 3.107863 -0.751109 10.081125
H 3.648646 -1.661234 9.819833
C -2.854240 1.697742 10.440717
Cr 2.188852 4.902669 10.242991
H -3.338156 0.723316 10.361013
C 1.879801 7.654197 13.310796
C -0.199300 8.779868 13.835994
H -1.566566 3.410288 13.470711
C 3.459643 5.255617 14.913628
C 4.098920 4.675651 10.009914
P 0.966698 3.239977 11.073120
H 4.100177 -0.511936 11.986530
C 4.448894 4.884748 15.828565
H 6.203966 2.709123 13.881521
C 5.436340 3.426892 14.174312
H 2.683180 5.957365 15.217976
C 1.418795 2.100021 14.722827
H -4.695897 2.806450 10.220881
C -3.616505 2.865347 10.364988
H 2.460436 2.437928 14.785909
H 1.732755 9.749165 13.796580
H 1.060200 1.904063 15.743574
H 1.383969 1.154227 14.165463
N 1.068326 3.624774 12.748838
P 2.078979 4.997861 12.401054
C 3.449936 4.718168 13.617469
C 5.439024 3.970555 15.462991
H -0.743071 5.490339 13.131666
H 4.440361 5.307989 16.834031
H -3.576057 5.028008 10.417062
C -2.988360 4.110894 10.474144
H 1.970417 -0.707151 8.242223
C 2.164926 -0.216678 9.196932
C 4.452194 3.800885 13.260420

H 4.437070 3.364867 12.262538
C 3.358897 -0.107295 11.296105
H 0.753621 1.369282 8.825569
C 1.475222 0.949335 9.528253
H 2.883476 1.568283 12.567678
C 2.667181 1.058081 11.631295
H 4.251497 5.459084 9.232546
H 3.838684 3.706273 9.496882
H 5.022384 4.550382 10.585447
C 1.204265 6.542183 9.932348
H 1.795470 7.166392 9.233725
H 0.534918 7.172192 10.531335
H 0.579281 5.821608 9.310744

Spin state: triplet

E = -9321.34 kcal mol-1
H = -8972.01 kcal mol-1
TS = -63.95 kcal mol-1
G (298.15 K) = -9035.96 kcal mol-1

H -1.684742 8.300472 13.559698
C -1.612064 3.812171 10.144897
C -0.635473 8.059572 13.734738
C 1.498444 8.582950 14.742707
C 1.267654 6.587932 13.374292
C -0.081295 6.920321 13.154329
H -0.281221 9.785206 14.989451
H -1.979467 3.539609 14.685797
H -1.190432 4.808948 9.998766
H -0.695689 0.695842 11.194365
H -1.834279 2.761247 13.096132
C -1.483764 3.601048 13.707192
H 6.495835 3.169975 15.306607
C 0.037431 3.562291 13.901436
H 3.108197 7.210907 14.330841
H 0.296690 4.362591 14.612864
C 1.852937 1.670894 11.109122
C -0.788121 2.784788 10.633387
C -1.323235 1.499122 10.808046
C 3.557826 -0.552931 10.916634
H 4.220045 -1.415861 10.841462
C -2.663132 1.249388 10.503669
Cr 2.073815 4.966027 10.187307
H -3.071817 0.247787 10.643391
C 2.055437 7.440944 14.164959
C 0.151812 8.893940 14.534570
H -1.798629 4.530277 13.219249
C 3.390126 4.476663 14.790810
C 3.507279 4.082318 9.031302
P 0.929698 3.249428 11.079148
H 4.390436 0.131282 12.791610
C 4.482156 3.936376 15.471758
H 6.615623 3.531405 12.842746
C 5.712555 3.798894 13.392244
H 2.489176 4.746957 15.342616
C 0.492683 2.220762 14.481221
H -4.527738 2.082663 9.798628
C -3.481034 2.279663 10.032296
H 1.560715 2.237922 14.729214
H 2.120085 9.232348 15.360486
H -0.072324 1.988557 15.394820
H 0.321033 1.411361 13.758257
N 0.792393 3.918905 12.668652
P 1.974590 5.185354 12.430587
C 3.447998 4.678209 13.401254
C 5.644301 3.594258 14.773565
H -0.690682 6.278662 12.517474
H 4.425721 3.780808 16.549876
H -3.585376 4.368252 9.480323
C -2.952018 3.562696 9.853661
H 2.546847 -0.964869 9.050242
C 2.618366 -0.300574 9.912151
C 4.620281 4.335205 12.709601
H 4.658515 4.463962 11.625787
C 3.651793 0.311974 12.009969
H 1.057761 1.007340 9.205875
C 1.774995 0.806481 10.002857
H 2.904509 2.099976 12.947446
C 2.807968 1.418889 12.104727
H 3.054692 3.951845 8.028997
H 3.880715 3.099436 9.355605
H 4.367128 4.772840 8.928601
C 0.992556 6.594161 9.695969
H 1.830155 7.279067 9.437308
H 0.315701 7.146299 10.362066
H 0.454935 6.332673 8.763476

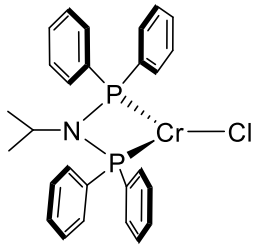
Spin state: quintet

E = -9331.09 kcal mol-1
H = -8981.02 kcal mol-1
TS = -65.97 kcal mol-1
G (298.15 K) = -9046.99 kcal mol-1

H -1.975580 7.663829 13.617715
C -1.555464 4.288922 10.375110
C -0.888237 7.630473 13.694477
C 1.207657 8.679151 14.289487
C 1.198917 6.427932 13.377634
C -0.201011 6.489156 13.279628
H -0.724298 9.620560 14.521681
H -1.390282 2.627778 14.931840
H -0.966583 5.207437 10.319993
H -1.187920 0.950893 10.979287
H -1.157402 1.903196 13.330623
C -1.004319 2.814527 13.920868
H 6.325139 3.461237 16.134576
C 0.479194 3.174040 14.007776
H 2.987621 7.515262 13.938622
H 0.575667 4.030017 14.695589
C 1.572196 1.543220 10.837897
C -0.917085 3.080486 10.701477
C -1.669749 1.896370 10.729474
C 2.987246 -0.803179 10.203394
H 3.532078 -1.715510 9.960084
C -3.036355 1.924978 10.452150
Cr 2.349246 4.979495 10.151616
H -3.612786 0.999508 10.477490
C 1.898960 7.539714 13.877898

C -0.186903 8.727764 14.201341
H -1.596633 3.615945 13.464091
C 3.377334 4.880090 15.177013
C 3.735174 6.525509 10.014483
P 0.871915 3.211672 11.067105
H 4.228653 -0.319715 11.905851
C 4.407838 4.450352 16.013641
H 6.485445 3.090403 13.675688
C 5.611030 3.585225 14.099211
H 2.509680 5.387602 15.599659
C 1.293595 2.006849 14.575764
H -4.737131 3.154264 9.936238
C -3.668324 3.135233 10.150373
H 2.354854 2.266991 14.665192
H 1.761225 9.534952 14.677126
H 0.920282 1.746227 15.576034
H 1.200032 1.121475 13.934165
N 1.030852 3.686242 12.718380
P 2.102759 5.037345 12.613132
C 3.452294 4.657451 13.792938
C 5.522113 3.796992 15.477916
H -0.750138 5.641417 12.869096
H 4.340391 4.622387 17.088439
H -3.409238 5.262641 9.862228
C -2.925047 4.318283 10.112359
H 1.614873 -0.987150 8.543474
C 1.909558 -0.396936 9.411770
C 4.584470 4.019251 13.259942
H 4.653822 3.866831 12.180551
C 3.375284 -0.021839 11.295543
H 0.393346 1.092537 9.073487
C 1.210768 0.770772 9.718628
H 3.010628 1.765935 12.439495
C 2.681659 1.147685 11.605191
H 3.996461 6.745945 8.967424
H 4.668652 6.275225 10.550143
H 3.338943 7.451340 10.469110
C 2.115429 4.366681 8.177038
H 2.776709 4.926940 7.497332
H 1.074557 4.515338 7.836955
H 2.345305 3.291687 8.066797

Geometry:



Spin state: doublet

E = -8484.96 kcal mol-1
H = -8179.01 kcal mol-1
TS = -58.41 kcal mol-1
G (298.15 K) = -8237.42 kcal mol-1

H -1.599391 7.703468 13.149250
C -0.963450 4.321317 10.031754
C -0.519610 7.617972 13.276840
C 1.610494 8.604247 13.862144
C 1.503893 6.281041 13.166060
C 0.115795 6.405318 13.003668
H -0.271347 9.665844 13.920174
H -1.579275 2.693565 14.784166
H -0.261840 5.155838 9.961389
H -1.099634 1.049020 10.988075
H -1.164792 1.869382 13.269828
C -1.051421 2.807314 13.827889
H 5.909627 3.168836 16.846822
C 0.424018 3.111213 14.088393
H 3.330150 7.311670 13.705088
H 0.477713 4.019078 14.712941
C 1.698905 1.265783 11.086060
C -0.523535 3.088438 10.541686
C -1.424539 2.013635 10.597833
C 2.763594 -1.325265 10.836360
H 3.170630 -2.332350 10.742352
C -2.740938 2.173762 10.163064
Cr 2.699191 4.538860 10.442975
H -3.432240 1.331606 10.211386
C 2.248319 7.394151 13.590099
C 0.225044 8.718513 13.708173
H -1.538224 3.602873 13.251063
C 3.316470 4.793371 15.341949
Cl 2.989856 5.733099 8.630121
P 1.203681 3.029161 11.164262
H 3.827429 -0.888869 12.667411
C 4.175274 4.359550 16.353880
H 6.296479 2.446805 14.492499
C 5.458979 3.102238 14.733546
H 2.479373 5.448058 15.585654
C 1.097010 1.963815 14.851274
H -4.203180 3.530376 9.331926
C -3.173980 3.408089 9.670978
H 2.155717 2.180349 15.039843
H 2.196621 9.462747 14.191891
H 0.600393 1.814952 15.820520
H 1.024466 1.027104 14.283365
N 1.152246 3.483923 12.845647
P 2.340639 4.734119 12.647202
C 3.521205 4.382703 14.015335
C 5.243081 3.509320 16.053955
H -0.463680 5.550569 12.653462
H 4.006146 4.681996 17.382021
H -2.608741 5.444874 9.211081
C -2.281773 4.482530 9.605805
H 1.603408 -1.450642 9.016651
C 1.882584 -0.831155 9.869728
C 4.606614 3.542023 13.721039
H 4.774390 3.227330 12.688010
C 3.129917 -0.516501 11.916088
H 0.688341 0.838364 9.216256
C 1.358762 0.456797 9.986755
H 2.910553 1.403294 12.871081
C 2.606833 0.770975 12.037551

Spin state: quartet

E = -8502.74 kcal mol-1
H = -8196.45 kcal mol-1
TS = -60.62 kcal mol-1
G (298.15 K) = -8257.07 kcal mol-1

H -0.990039 8.679012 13.173228
C -1.322885 3.788002 9.869102
C -0.054603 8.242410 13.525060
C 1.902266 8.335151 14.942144
C 1.591916 6.455263 13.436059
C 0.391606 7.036725 12.989086
H 0.352880 9.841426 14.923646
H -2.248883 4.049242 14.324298
H -0.810194 4.730896 9.664511
H -0.768488 0.740101 11.301462
H -2.033579 3.255278 12.750059
C -1.620067 4.014738 13.423803
H 6.116743 2.333943 15.805066
C -0.173818 3.691414 13.819337
H 3.293638 6.699414 14.752104
H 0.134648 4.436066 14.570867
C 1.824461 1.488492 11.330684
C -0.640371 2.766846 10.549141
C -1.289848 1.543764 10.780954
C 3.238940 -0.933070 11.435294
H 3.788642 -1.874004 11.476108
C -2.606272 1.356499 10.355337
Cr 2.495489 4.708466 10.321122
H -3.104144 0.403998 10.541150
C 2.350261 7.124501 14.409650
C 0.699583 8.895947 14.506006
H -1.682000 4.987977 12.923726
C 3.216700 3.947262 15.026850
Cl 3.533577 5.437764 8.525993
P 1.050184 3.140700 11.152501
H 3.814255 -0.321780 13.428132
C 4.162675 3.255777 15.784972
H 6.600686 2.904058 13.426180
C 5.652058 3.195704 13.877505
H 2.271395 4.243650 15.482395
C -0.056030 2.292576 14.428928
H -4.314810 2.237319 9.368810
C -3.286308 2.386005 9.699063
H 0.953565 2.110305 14.816256
H 2.498521 8.842578 15.701458
H -0.772007 2.174140 15.254041
H -0.276716 1.524627 13.674958
N 0.788353 3.888806 12.698698
P 2.177892 4.939222 12.586062
C 3.476992 4.260139 13.680390
C 5.379793 2.875712 15.211495
H -0.189183 6.537242 12.211890
H 3.949562 3.012928 16.826632
H -3.163817 4.405006 8.932955
C -2.640996 3.603477 9.455726
H 2.517320 -1.259314 9.423070
C 2.524925 -0.589133 10.283236
C 4.705653 3.881539 13.116788
H 4.912135 4.114733 12.069749
C 3.252118 -0.065161 12.529685
H 1.271423 0.882154 9.325566
C 1.823802 0.615616 10.227898
H 2.585636 1.820919 13.326478
C 2.553425 1.142372 12.476919

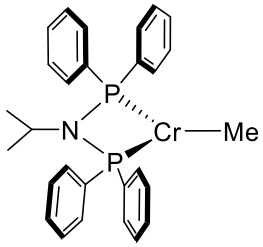
Spin state: sextet

E = -8501.70 kcal mol-1
H = -8194.45 kcal mol-1
TS = -59.76 kcal mol-1
G (298.15 K) = -8254.21 kcal mol-1

H -1.005058 8.655495 13.030797
C -1.306378 3.813433 9.852753
C -0.095783 8.219782 13.446408
C 1.750915 8.305386 15.005521
C 1.565649 6.441938 13.457495
C 0.396016 7.024354 12.929678
H 0.196606 9.803847 14.890869
H -2.122177 4.023428 14.375282
H -0.754415 4.731655 9.638627
H -0.892275 0.756256 11.317304
H -1.978093 3.289507 12.764772
C -1.525262 4.012318 13.452731
H 6.135741 2.413282 15.918814
C -0.075110 3.645133 13.790728
H 3.166238 6.684145 14.897803
H 0.267524 4.359542 14.555597
C 1.762235 1.409043 11.340163
C -0.666547 2.767004 10.539929
C -1.374190 1.577024 10.786288
C 3.164246 -1.023032 11.473375
H 3.707439 -1.967035 11.525271
C -2.697513 1.446824 10.364408
Cr 2.569937 4.718935 10.242863
H -3.238010 0.520349 10.562168
C 2.246252 7.105294 14.493094
C 0.578787 8.865319 14.489324
H -1.581299 5.007007 12.996802
C 3.211252 3.958641 15.092559
Cl 3.615388 5.523522 8.452969
P 1.037009 3.075893 11.117889
H 3.963108 -0.269918 13.336672
C 4.159679 3.286175 15.863922
H 6.651973 3.010543 13.551473
C 5.687185 3.273917 13.985509
H 2.253044 4.231009 15.535064
C 0.034953 2.228426 14.357282
H -4.367243 2.395713 9.372533
C -3.332425 2.500339 9.699474
H 1.052676 2.014478 14.704049
H 2.285954 8.806272 15.813241
H -0.654668 2.107488 15.203960
H -0.230302 1.482795 13.595917
N 0.858360 3.870638 12.644252
P 2.219665 4.956810 12.620550
C 3.487720 4.285298 13.750154
C 5.397274 2.939508 15.313332

H -0.122979 6.532278 12.105213
H 3.932431 3.032332 16.899996
H -3.119200 4.505989 8.916970
C -2.632520 3.685506 9.445117
H 2.219180 -1.486176 9.584308
C 2.328677 -0.753869 10.384862
C 4.738034 3.938357 13.210147
H 4.959185 4.179637 12.168025
C 3.305948 -0.074207 12.488868
H 0.997121 0.661125 9.453875
C 1.636838 0.455521 10.313046
H 2.746645 1.873829 13.210707
C 2.614442 1.136260 12.421836

Geometry:



Spin state: doublet

E = -8836.44 kcal mol-1
H = -8509.37 kcal mol-1
TS = -63.52 kcal mol-1
G (298.15 K) = -8572.89 kcal mol-1

H -1.057207 8.656849 13.276975
C -1.324799 3.836144 9.894362
C -0.111981 8.234864 13.621070
C 1.846035 8.349130 15.033172
C 1.566287 6.476005 13.508974
C 0.355800 7.043070 13.071555
H 0.270393 9.828233 15.034204
H -2.224618 3.998801 14.372312
H -0.819380 4.785848 9.702670
H -0.728434 0.776608 11.279574
H -2.007180 3.244228 12.778959
C -1.599911 3.993110 13.468145
H 6.057433 2.363549 15.920765
C -0.146762 3.679694 13.848911
H 3.261672 6.736515 14.829895
H 0.155309 4.414523 14.612534
C 1.853379 1.558928 11.299292
C -0.629294 2.815552 10.559991
C -1.262441 1.581378 10.773420
C 3.319929 -0.836885 11.319627
H 3.889562 -1.766816 11.327562
C -2.577191 1.382916 10.346948
Cr 2.459428 4.726134 10.311820
H -3.062967 0.421440 10.518622
C 2.312088 7.149475 14.489194
C 0.633019 8.893367 14.605953
H -1.676970 4.976515 12.990604
C 3.176855 3.994350 15.105350
C 2.800803 4.682153 8.306993
P 1.061273 3.208883 11.165435
H 3.884006 -0.282077 13.332120
C 4.109988 3.299440 15.876426
H 6.566558 2.914092 13.542850
C 5.616601 3.216821 13.984438
H 2.231137 4.302614 15.551973
C -0.011111 2.271898 14.435342
H -4.298296 2.256369 9.375514
C -3.271086 2.413335 9.706445
H 1.001670 2.096212 14.817448
H 2.435045 8.859087 15.796748
H -0.723816 2.130163 15.259806
H -0.222905 1.514150 13.668539
N 0.805396 3.907355 12.729012
P 2.178802 4.984197 12.619959
C 3.448609 4.296780 13.759793
C 5.330088 2.907235 15.316890
H -0.216618 6.541128 12.289368
H 3.885424 3.063177 16.917303
H -3.175129 4.443739 8.968024
C -2.641330 3.641614 9.479065
H 2.600524 -1.108167 9.297959
C 2.595970 -0.467846 10.180923
C 4.679072 3.903821 13.212468
H 4.890356 4.123154 12.163081
C 3.315759 -0.006293 12.443013
H 1.314786 1.012103 9.274329
C 1.870125 0.722930 10.167905
H 2.610390 1.836765 13.304904
C 2.591141 1.186904 12.432592
H 3.543983 5.513340 8.215371
H 1.945790 4.945869 7.662496
H 3.273499 3.782337 7.882121

Spin state: quartet

E = -8855.93 kcal mol-1
H = -8529.00 kcal mol-1
TS = -63.46 kcal mol-1
G (298.15 K) = -8592.45 kcal mol-1

H -1.011608 8.715222 13.333733
C -1.337475 3.802792 9.889437
C -0.077654 8.270466 13.679904
C 1.863684 8.319976 15.117840
C 1.574108 6.486354 13.546962
C 0.376482 7.083343 13.110019
H 0.311519 9.824866 15.134552
H -2.274782 4.105081 14.298533
H -0.847614 4.760976 9.701585
H -0.709718 0.752063 11.285354
H -2.047925 3.300604 12.731281
C -1.640225 4.065726 13.402176
H 6.036718 2.266147 15.843877
C -0.195280 3.749025 13.808765
H 3.259454 6.694455 14.890223
H 0.101592 4.490151 14.567878
C 1.864040 1.570019 11.327885
C -0.633339 2.793374 10.566218

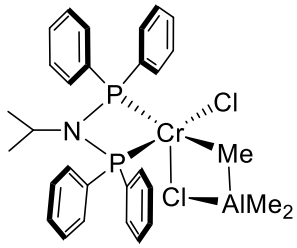
C -1.249481 1.548074 10.771894
C 3.363026 -0.801228 11.380958
H 3.947352 -1.721779 11.401112
C -2.555435 1.329648 10.328469
Cr 2.453207 4.745154 10.283964
H -3.027620 0.360543 10.494628
C 2.318813 7.128040 14.550561
C 0.664290 8.894396 14.689337
H -1.702174 5.035135 12.894646
C 3.178430 3.958569 15.074211
C 2.775704 4.601196 8.265723
P 1.045800 3.202035 11.172094
H 3.864883 -0.244650 13.409829
C 4.103990 3.232586 15.825947
H 6.546442 2.861652 13.475080
C 5.602981 3.169408 13.926748
H 2.237710 4.269455 15.529391
C -0.077979 2.346937 14.411516
H -4.278384 2.174716 9.335309
C -3.258375 2.348141 9.679255
H 0.928148 2.167137 14.808777
H 2.450926 8.801550 15.900891
H -0.801963 2.220565 15.228545
H -0.288352 1.582325 13.651014
N 0.780520 3.958435 12.701575
P 2.188412 5.016996 12.627140
C 3.452428 4.289872 13.734168
C 5.316141 2.834263 15.255025
H -0.197110 6.608663 12.312064
H 3.878200 2.976323 16.861780
H -3.184986 4.380827 8.942104
C -2.644883 3.587281 9.459565
H 2.705051 -1.076973 9.339189
C 2.666001 -0.439930 10.223493
C 4.676006 3.888791 13.174314
H 4.890090 4.128871 12.130200
C 3.315557 0.024147 12.507044
H 1.384551 1.023605 9.288118
C 1.921382 0.739328 10.194415
H 2.559949 1.854402 13.354017
C 2.572809 1.206227 12.480823
H 3.502314 5.424190 8.066948
H 1.897550 4.788800 7.626574
H 3.246842 3.668429 7.915924

Spin state: sextet

E = -8856.15 kcal mol-1
H = -8528.48 kcal mol-1
TS = -60.90 kcal mol-1
G (298.15 K) = -8589.38 kcal mol-1

H -1.036249 8.657784 13.090673
C -1.285030 3.869454 9.864392
C -0.133637 8.223141 13.522099
C 1.671237 8.296386 15.129324
C 1.542890 6.457027 13.545055
C 0.380458 7.039435 12.999425
H 0.107975 9.785669 14.999605
H -2.116420 3.994603 14.389151
H -0.738778 4.796873 9.677987
H -0.859463 0.782235 11.263734
H -1.956596 3.286423 12.768090
C -1.514397 4.002737 13.469819
H 6.101412 2.396984 15.998631
C -0.062528 3.643789 13.808749
H 3.102377 6.688723 15.030714
H 0.269662 4.347359 14.588045
C 1.794972 1.468149 11.328234
C -0.643885 2.814498 10.540237
C -1.342680 1.610044 10.744854
C 3.264916 -0.928545 11.383729
H 3.834511 -1.858110 11.405054
C -2.656431 1.475351 10.297041
Cr 2.545694 4.819502 10.244187
H -3.189485 0.538491 10.464246
C 2.188933 7.108761 14.610011
C 0.508059 8.857039 14.592448
H -1.576749 5.003714 13.028220
C 3.193960 3.974567 15.168151
C 2.732016 4.788100 8.177039
P 1.046177 3.124857 11.139339
H 4.040657 -0.214095 13.272398
C 4.133439 3.289012 15.938930
H 6.631497 3.000408 13.633901
C 5.668358 3.272530 14.066557
H 2.235764 4.250895 15.608224
C 0.058324 2.218173 14.350477
H -4.321180 2.428376 9.299029
C -3.293192 2.537000 9.645553
H 1.076492 2.008375 14.698508
H 2.181261 8.787483 15.959137
H -0.633758 2.075857 15.191923
H -0.196590 1.483866 13.574534
N 0.873132 3.899942 12.670590
P 2.233561 4.998642 12.686619
C 3.478367 4.309749 13.827814
C 5.370889 2.934077 15.393201
H -0.115520 6.555631 12.155912
H 3.898682 3.029981 16.972160
H -3.088259 4.562008 8.911420
C -2.601820 3.735474 9.430527
H 2.334422 -1.354363 9.478353
C 2.422790 -0.646237 10.303034
C 4.728467 3.949961 13.292805
H 4.951890 4.189953 12.250685
C 3.379090 -0.009593 12.430027
H 1.056046 0.762862 9.414941
C 1.698054 0.545017 10.269375
H 2.766124 1.897457 13.214433
C 2.654079 1.182638 12.401919
H 3.321791 5.647558 7.806547
H 1.753806 4.821102 7.666168
H 3.242337 3.871100 7.832261

Geometry:



Spin state: singlet

E = -10067.93 kcal mol-1
H = -9687.08 kcal mol-1
TS = -72.99 kcal mol-1
G (298.15 K) = -9760.07 kcal mol-1

H -1.227899 7.853095 12.029837
C -0.858392 3.597466 9.968718
C -0.167047 7.715595 12.242131
C 2.022340 8.643761 12.689154
C 1.722849 6.238001 12.601288
C 0.361848 6.426506 12.320586
H 0.248109 9.832863 12.358377
H -1.709187 3.107128 14.468118
H -0.288054 4.523895 9.917401
H -0.565139 0.353722 10.991216
H -1.234286 2.028305 13.141413
C -1.102433 3.035299 13.555666
H 5.424014 3.701627 17.299129
C 0.362308 3.304024 13.904573
H 3.619948 7.218955 12.963116
H 0.419123 4.295281 14.383298
C 2.033595 0.927378 11.443385
C -0.268236 2.447836 10.519955
C -1.000367 1.250814 10.552192
C 3.366039 -1.542014 11.591687
H 3.879930 -2.501663 11.651204
C -2.297319 1.205673 10.038820
Cr 3.186464 3.924001 10.396280
H -2.857081 0.270154 10.068336
C 2.554283 7.358008 12.773795
C 0.660770 8.826038 12.426660
H -1.488266 3.751830 12.821155
C 3.147637 5.110622 15.190271
Cl 5.283320 4.643844 10.749715
P 1.422511 2.634273 11.203857
H 4.058931 -0.866642 13.525082
C 3.838814 4.839149 16.372154
H 6.075791 2.556459 15.184090
C 5.247083 3.265194 15.189783
H 2.333169 5.835741 15.191546
C 0.894963 2.262495 14.894438
H -3.891374 2.315074 9.093245
C -2.878928 2.353935 9.496214
H 1.937077 2.469905 15.166297
H 2.674440 9.507569 12.821519
H 0.292320 2.279394 15.813343
H 0.832676 1.253847 14.465259
N 1.225960 3.442435 12.699739
P 2.486665 4.588107 12.475921
C 3.494741 4.449891 14.001664
C 4.884791 3.912100 16.374871
H -0.280038 5.561480 12.154262
H 3.559937 5.352377 17.293125
H -2.601381 4.447940 9.034686
C -2.156783 3.550341 9.465260
H 2.552111 -1.918076 9.624868
C 2.618309 -1.216207 10.456746
C 4.558436 3.534412 14.006772
H 4.847452 3.045651 13.075879
C 3.463959 -0.626337 12.643343
H 1.398286 0.263635 9.477173
C 1.959006 0.010657 10.377794
H 2.925493 1.328663 13.370924
C 2.812950 0.604847 12.565497
H 1.280747 2.101931 6.292573
H 0.657058 2.128766 7.954357
H 0.231223 3.421309 6.833593
Cl 1.969815 5.468626 9.118502
Al 2.659527 3.780423 7.669390
C 3.835185 4.614517 6.336887
C 3.916377 2.539842 8.837476
H 3.286094 5.291223 5.664730
H 4.327634 3.857943 5.705377
H 4.626826 5.200821 6.827195
H 4.009081 2.095801 9.859308
H 4.940040 2.753051 8.503205
H 3.522906 1.682252 8.260016
C 1.054045 2.760754 7.146696

Spin state: triplet

E = -10077.20 kcal mol-1
H = -9696.38 kcal mol-1
TS = -73.24 kcal mol-1
G (298.15 K) = -9769.61 kcal mol-1

H -1.225031 7.859865 12.007759
C -0.851547 3.590008 9.941879
C -0.171883 7.721266 12.254792
C 1.995046 8.646568 12.805262
C 1.711871 6.242860 12.642144
C 0.360637 6.433311 12.316745
H 0.227439 9.836527 12.444587
H -1.724576 3.166900 14.461899
H -0.262142 4.503468 9.867491
H -0.616897 0.367241 11.045583
H -1.279435 2.077805 13.133692
C -1.121834 3.080798 13.548011
H 5.475625 3.648430 17.270240
C 0.349335 3.314752 13.895816
H 3.589778 7.222681 13.097551
H 0.425801 4.298700 14.386445
C 2.015019 0.919961 11.452688
C -0.286275 2.444860 10.527274
C -1.036383 1.260082 10.582659
C 3.350018 -1.548001 11.596911
H 3.865202 -2.507052 11.655061
C -2.329595 1.223065 10.059668
Cr 3.210737 3.932687 10.401225

H -2.904590 0.297519 10.105981
C 2.530867 7.361335 12.874355
C 0.642937 8.830052 12.499742
H -1.491511 3.807636 12.815435
C 3.147299 5.060901 15.221685
Cl 5.267655 4.794796 10.681136
P 1.404670 2.623694 11.206840
H 4.073858 -0.858403 13.514672
C 3.855221 4.772926 16.389431
H 6.138567 2.581888 15.118348
C 5.292437 3.268921 15.150779
H 2.316751 5.766999 15.249289
C 0.864623 2.250206 14.869778
H -3.897665 2.334550 9.074040
C -2.888116 2.367454 9.484809
H 1.907972 2.440702 15.149458
H 2.637511 9.509244 12.984080
H 0.257916 2.258426 15.786067
H 0.793208 1.250055 14.422539
N 1.217201 3.451933 12.692715
P 2.480866 4.597903 12.498141
C 3.500325 4.441836 14.012400
C 4.923706 3.872095 16.356602
H -0.269877 5.570532 12.102385
H 3.572483 5.252685 17.327080
H -2.572503 4.443681 8.970247
C -2.146740 3.551095 9.429353
H 2.505038 -1.938249 9.646554
C 2.584352 -1.230562 10.472374
C 4.586832 3.554292 13.981469
H 4.879622 3.101926 13.033027
C 3.464643 -0.624365 12.641035
H 1.345313 0.240895 9.502753
C 1.922169 -0.004399 10.395191
H 2.941816 1.337409 13.361095
C 2.813890 0.606354 12.564235
H 1.312505 1.996424 6.344766
H 0.646616 2.110012 7.985715
H 0.261308 3.349447 6.791744
Cl 2.010168 5.465030 9.047390
Al 2.674452 3.727942 7.665957
C 3.873219 4.498537 6.316187
C 3.921511 2.495678 8.864105
H 3.342777 5.172091 5.626031
H 4.350180 3.715751 5.704985
H 4.675669 5.078303 6.796774
H 4.063287 2.062339 9.881227
H 4.927393 2.718944 8.485587
H 3.511120 1.632684 8.308511
C 1.069540 2.698926 7.159013

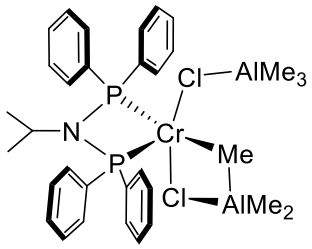
Spin state: quintet

E = -10090.02 kcal mol-1
H = -9709.81 kcal mol-1
TS = -72.46 kcal mol-1
G (298.15 K) = -9782.27 kcal mol-1

H -1.129979 7.908481 11.836845
C -0.834755 3.525752 9.853710
C -0.114539 7.756903 12.203762
C 1.957307 8.650643 13.079326
C 1.728065 6.266271 12.713073
C 0.423781 6.471352 12.237777
H 0.231099 9.853918 12.590911
H -1.779808 3.374042 14.387930
H -0.223361 4.418128 9.713804
H -0.653881 0.372535 11.158065
H -1.403816 2.261257 13.058682
C -1.170703 3.244251 13.483509
H 5.515785 3.522013 17.274923
C 0.308044 3.358483 13.860943
H 3.524933 7.218071 13.462037
H 0.440627 4.317206 14.387363
C 2.014963 0.923277 11.504748
C -0.297787 2.411764 10.518897
C -1.061121 1.241016 10.640592
C 3.363709 -1.529182 11.719735
H 3.883858 -2.483335 11.805740
C -2.349278 1.189698 10.108149
Cr 3.258929 3.951275 10.398879
H -2.937862 0.276758 10.203830
C 2.499595 7.366565 13.122042
C 0.650020 8.848078 12.625589
H -1.466093 4.005982 12.753166
C 3.111085 4.933722 15.317980
Cl 5.312088 4.889423 10.654077
P 1.378832 2.607300 11.206853
H 4.107186 -0.769757 13.602356
C 3.836059 4.611504 16.465290
H 6.235531 2.634265 15.061605
C 5.351577 3.268005 15.136108
H 2.247535 5.595870 15.387934
C 0.733606 2.227068 14.799914
H -3.890856 2.260212 9.039656
C -2.885067 2.305198 9.458202
H 1.771607 2.355534 15.130254
H 2.560976 9.501620 13.395558
H 0.089468 2.218766 15.690060
H 0.638924 1.253912 14.300696
N 1.212573 3.480530 12.677789
P 2.492921 4.624350 12.564995
C 3.496042 4.409842 14.073172
C 4.950844 3.772118 16.376316
H -0.162108 5.623284 11.884107
H 3.531683 5.016914 17.430677
H -2.532292 4.336551 8.807817
C -2.126183 3.471672 9.332527
H 2.501038 -1.990399 9.792207
C 2.585431 -1.254399 10.592158
C 4.631276 3.588763 13.984581
H 4.955046 3.225458 13.007878
C 3.486282 -0.569767 12.728653
H 1.336128 0.180431 9.581548
C 1.920102 -0.033539 10.477378
H 2.953580 1.408600 13.392855
C 2.825799 0.653734 12.618480
H 1.293868 1.901648 6.344046
H 0.690340 2.003055 8.006846
H 0.200347 3.211170 6.818326

Cl 2.001960 5.507267 8.846733
Al 2.646851 3.701757 7.576420
C 3.752120 4.412800 6.113865
C 3.949763 2.534267 8.749610
H 3.169742 5.050721 5.431225
H 4.194954 3.606134 5.507656
H 4.579474 5.021598 6.509075
H 4.186767 2.167939 9.773028
H 4.926444 2.768064 8.305234
H 3.543701 1.624584 8.273594
C 1.052594 2.603733 7.159664

Geometry:



Spin state: singlet

E = -11543.46 kcal mol-1
H = -11090.93 kcal mol-1
TS = -84.76 kcal mol-1
G (298.15 K) = -11175.69 kcal mol-1

H 1.720742 8.390496 15.045643
C -1.614439 5.056818 10.486029
C 2.428401 7.576627 14.885744
C 4.615165 6.603529 15.207182
C 2.942626 5.415056 13.902712
C 2.047333 6.474027 14.123029
H 4.014913 8.516831 16.012200
H -1.412545 4.857541 15.302805
H -0.798038 5.690497 10.146739
H -2.211208 2.041071 11.960830
H -1.929402 4.313234 13.694054
C -1.075987 4.684856 14.271565
H 5.825785 -0.132704 14.897733
C 0.085463 3.679009 14.276105
H 4.947507 4.685201 14.294434
H 0.811599 4.018325 15.031329
C 0.287544 1.503204 11.170473
C -1.336468 3.833879 11.113942
C -2.408399 3.010854 11.504926
C 0.358149 -1.243533 10.610182
H 0.388635 -2.311016 10.390400
C -3.725540 3.419870 11.304446
Cr 2.322311 4.275953 10.453840
H -4.546062 2.773029 11.616841
C 4.234375 5.493581 14.453709
C 3.713797 7.647655 15.427147
H -0.773628 5.645411 13.840584
C 3.252010 2.090290 14.683049
Cl 1.466673 6.509951 10.901575
P 0.410842 3.318608 11.363204
H 1.591863 -1.406194 12.377576
C 4.054548 1.070581 15.193524
H 6.435417 0.985913 12.755734
C 5.538925 1.288926 13.297244
H 2.381920 2.418221 15.249533
C -0.408959 2.278575 14.651473
H -5.022898 4.972357 10.542513
C -3.992306 4.652977 10.701009
H 0.415062 1.563151 14.749576
H 5.622428 6.652263 15.621600
H -0.953115 2.317948 15.605133
H -1.094828 1.892180 13.887207
N 0.858959 3.689628 12.998713
P 2.535583 4.046420 12.756469
C 3.568200 2.698882 13.457516
C 5.198078 0.664310 14.498050
H 1.055696 6.441853 13.680815
H 3.793258 0.598301 16.141121
H -3.135049 6.418790 9.797747
C -2.934939 5.465053 10.286876
H -0.853830 -0.760168 8.885688
C -0.341772 -0.375360 9.767869
C 4.728048 2.300418 12.777458
H 4.997486 2.778713 11.837618
C 1.030271 -0.737088 11.724989
H -0.914013 1.662660 9.374456
C -0.376207 0.990726 10.044165
H 1.563379 1.019913 12.847059
C 1.003757 0.630338 11.999067
Cl 3.199653 2.107924 9.904318
Al 3.593022 7.035155 10.125891
C 4.356261 8.197573 11.521072
C 3.321639 7.659373 8.276466
C 4.561825 5.242737 10.212141
H 5.258470 5.619017 9.435390
H 4.435905 4.204756 9.868302
H 5.116916 5.212084 11.159509
H 4.319988 7.713619 12.508482
H 3.814867 9.152683 11.602651
H 5.410774 8.439881 11.312248
H 4.265475 8.027393 7.841856
H 2.598522 8.487542 8.219374
H 2.956357 6.857884 7.617234
Al 2.721494 2.861279 7.759106
C 1.738679 1.385347 6.895127
C 4.418849 3.520239 6.996307
C 1.413812 4.365711 8.183205
H 1.357899 5.245942 8.847778
H 0.397962 3.952028 8.122164
H 1.627200 4.868802 7.219379
H 5.281517 2.907956 7.301484
H 4.631339 4.557656 7.295696
H 4.387900 3.502019 5.894762
H 2.403653 0.542971 6.649080
H 1.270057 1.714463 5.953470
H 0.941976 0.995084 7.544815

Spin state: triplet

E = -11544.20 kcal mol-1

H = -11091.69 kcal mol-1
TS = -86.08 kcal mol-1
G (298.15 K) = -11177.77 kcal mol-1

H -0.556573 8.213273 13.720924
C -1.362620 4.722709 10.772329
C 0.432012 7.793600 13.909011
C 2.701170 8.043601 14.710427
C 1.968702 5.918247 13.798646
C 0.702301 6.474354 13.551918
H 1.222537 9.616674 14.760024
H -1.414383 3.219026 15.596987
H -0.565029 5.437991 10.571081
H -1.843224 1.467912 11.684833
H -1.682507 3.496464 13.861552
C -0.952272 3.594788 14.673819
H 6.006233 1.557977 16.512226
C 0.321112 2.794113 14.372332
H 3.975151 6.315875 14.516158
H 1.046293 2.981715 15.179852
C 0.918394 1.252881 11.088586
C -1.043373 3.416254 11.171493
C -2.075801 2.488391 11.382849
C 1.545170 -1.369546 10.314908
H 1.788223 -2.388601 10.013700
C -3.404783 2.864077 11.192946
Cr 2.434386 4.516620 10.720366
H -4.200137 2.135339 11.350700
C 2.973513 6.718537 14.365198
C 1.431247 8.581124 14.490914
H -0.726987 4.657108 14.815400
C 3.561823 3.743789 15.582588
Cl 3.657743 6.556608 10.829939
P 0.718186 3.028683 11.465958
H 3.114200 -1.262720 11.800389
C 4.434467 3.035152 16.410759
H 6.040154 1.170258 14.050898
C 5.338523 1.883521 14.483691
H 2.879554 4.476551 16.014160
C 0.051820 1.288979 14.337630
H -4.754873 4.455714 10.637892
C -3.715242 4.167717 10.795666
H 0.977583 0.717807 14.210152
H 3.489002 8.660066 15.143857
H -0.421354 0.982414 15.279666
H -0.627252 1.021622 13.518189
N 1.011865 3.267927 13.140167
P 2.372686 4.304281 13.052397
C 3.571682 3.523479 14.195276
C 5.321032 2.104134 15.863396
H -0.066128 5.874731 13.062486
H 4.422820 3.212523 17.486524
H -2.929224 6.108628 10.260552
C -2.693281 5.096026 10.587386
H -0.065617 -1.160062 8.891219
C 0.502367 -0.684561 9.690659
C 4.470217 2.591516 13.654311
H 4.501442 2.442864 12.576423
C 2.289549 -0.738160 11.316931
H -0.594468 1.157358 9.535782
C 0.190760 0.622741 10.066664
H 2.571041 1.056364 12.473575
C 1.983965 0.566358 11.696195
Cl 1.518061 5.039365 8.674522
Al 5.327805 4.991314 10.458713
C 6.353618 4.934243 12.143756
C 6.185426 5.449812 8.752069
C 4.207468 3.274026 10.070298
H 4.229695 3.202938 8.975336
H 3.305007 2.701227 10.392933
H 5.000900 2.617818 10.472534
H 7.076211 5.765121 12.170206
H 6.931404 4.003326 12.259569
H 5.719020 5.026668 13.036972
H 6.880722 4.662334 8.419969
H 6.761663 6.385367 8.816170
H 5.433253 5.577667 7.958760
Al 0.891632 3.274910 7.120173
C 2.150381 1.799571 7.557099
C 1.273393 4.246377 5.435841
C -1.042192 3.032359 7.526992
H -1.615352 3.912914 7.195085
H -1.295387 2.881233 8.585356
H -1.442839 2.166369 6.972254
H 2.327357 4.556933 5.363372
H 0.655729 5.151689 5.326461
H 1.066049 3.609321 4.559208
H 2.262718 1.566837 8.624410
H 3.156242 2.009454 7.159937
H 1.808536 0.867751 7.074476

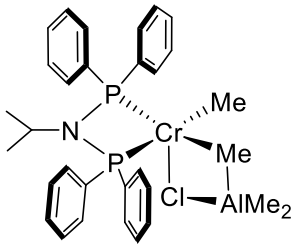
Spin state: quintet

E = -11561.54 kcal mol-1
H = -11108.99 kcal mol-1
TS = -86.76 kcal mol-1
G (298.15 K) = -11195.75 kcal mol-1

H 1.374472 8.738727 14.454408
C -1.515466 4.857780 10.652922
C 2.077774 7.918637 14.600349
C 4.081373 7.028490 15.619091
C 2.793032 5.656276 14.085748
C 1.892388 6.722619 13.912372
H 3.321787 9.016865 15.985214
H -1.525722 4.879527 15.190777
H -0.741541 5.589413 10.432807
H -1.903224 1.646280 11.744996
H -1.895792 4.240480 13.576452
C -1.111950 4.699086 14.189332
H 5.172638 -0.313189 15.403357
C 0.119291 3.792110 14.312239
H 4.621974 5.019088 15.063065
H 0.783757 4.246460 15.063187
C 0.676454 1.406492 11.393915
C -1.163333 3.590894 11.140995
C -2.167824 2.640100 11.385490
C 1.058658 -1.342737 11.000139
H 1.210880 -2.411140 10.845015
C -3.506209 2.964517 11.165930

Cr 2.579149 4.321941 10.462681
H -4.280830 2.222009 11.359321
C 3.898158 5.824002 14.938366
C 3.171833 8.075608 15.456286
H -0.850673 5.665461 13.744718
C 3.384913 2.582385 15.232585
Cl 1.570801 6.532767 10.385891
P 0.596380 3.230633 11.476445
H 1.963690 -1.330547 12.963683
C 3.973215 1.444030 15.781558
H 5.436571 0.173414 12.973131
C 4.865576 0.849029 13.609840
H 2.816353 3.259891 15.870505
C -0.263011 2.389405 14.786295
H -4.898875 4.484659 10.521138
C -3.852048 4.234737 10.696307
H 0.622736 1.788144 15.021150
H 4.942652 7.149031 16.276563
H -0.879233 2.461656 15.692902
H -0.847890 1.862615 14.021163
N 0.946948 3.791078 13.064147
P 2.624018 4.204148 13.006732
C 3.522934 2.857698 13.860721
C 4.713555 0.576125 14.970418
H 1.065054 6.618940 13.212570
H 3.856304 1.231843 16.844804
H -3.117546 6.162763 10.050898
C -2.854742 5.177737 10.436706
H 0.145451 -1.028403 9.064277
C 0.454813 -0.570189 10.003466
C 4.269785 1.983121 13.055735
H 4.351180 2.167937 11.982864
C 1.479763 -0.739164 12.185884
H -0.172780 1.394981 9.396909
C 0.268682 0.796529 10.194012
H 1.648993 1.092751 13.298054
C 1.295580 0.631191 12.380456
Cl 3.114258 2.348331 9.284823
Al 3.809195 6.978023 10.068005
C 4.440306 7.898466 11.688654
C 3.964270 7.759834 8.275788
C 4.681249 5.069501 9.950404
H 5.550680 5.724127 10.165245
H 4.810039 4.706894 8.923027
H 4.884065 4.231195 10.638224
H 3.775597 8.729684 11.967801
H 5.442925 8.327474 11.529002
H 4.504598 7.235290 12.563258
H 5.016014 7.845246 7.959976
H 3.531248 8.771315 8.239067
H 3.445893 7.152387 7.519386
Al 2.004061 2.857624 7.184405
C 1.672557 1.017178 6.522677
C 3.410366 3.958470 6.324237
C 0.376305 3.877371 7.726756
H 0.584330 4.836728 8.226538
H -0.343221 3.333045 8.357276
H -0.168322 4.135756 6.800860
H 4.379185 3.436438 6.278865
H 3.574131 4.905676 6.862759
H 3.142676 4.229930 5.289682
H 2.602773 0.436660 6.421023
H 1.189040 1.028582 5.531712
H 1.009736 0.451577 7.196497

Geometry:



Spin state: singlet

E = -10431.21 kcal mol-1
H = -10029.42 kcal mol-1
TS = -72.57 kcal mol-1
G (298.15 K) = -10101.99 kcal mol-1

H -1.200551 7.758931 11.984892
C -0.762139 3.552702 9.965203
C -0.132703 7.632194 12.167738
C 2.066957 8.578506 12.498769
C 1.771785 6.166137 12.522426
C 0.402034 6.347464 12.284607
H 0.280055 9.753511 12.180377
H -1.707948 3.104859 14.461731
H -0.175934 4.470711 9.931407
H -0.549765 0.304241 10.988477
H -1.165773 1.978092 13.200957
C -1.072856 3.007288 13.571217
H 5.368685 3.700912 17.336592
C 0.377104 3.327672 13.939150
H 3.674567 7.169235 12.773656
H 0.410274 4.352631 14.344588
C 2.029772 0.833337 11.547322
C -0.203019 2.392132 10.526074
C -0.959198 1.210031 10.542081
C 3.244574 -1.691216 11.795950
H 3.713113 -2.670765 11.893579
C -2.247363 1.190679 10.004002
Cr 3.121278 3.773085 10.369267
H -2.825630 0.266020 10.022063
C 2.601956 7.296312 12.615335
C 0.696642 8.750531 12.276542
H -1.456887 3.675595 12.791283
C 3.307719 5.215627 15.079999
C 5.036307 3.918801 10.945870
P 1.476501 2.556232 11.257666
H 3.787723 -1.051188 13.787497
C 3.968237 4.967375 16.285943
H 5.782003 2.235034 15.361632
C 5.087175 3.072385 15.286506
H 2.604952 6.045984 15.012529
C 0.889700 2.374846 15.025835
H -3.802892 2.331547 9.031281

C -2.797330 2.350252 9.452436
H 1.931328 2.595015 15.289239
H 2.722090 9.447191 12.573674
H 0.278035 2.480890 15.932999
H 0.818586 1.331095 14.691711
N 1.261202 3.382826 12.746430
P 2.539183 4.504158 12.409470
C 3.528974 4.393050 13.965324
C 4.856456 3.894929 16.393602
H -0.245069 5.477505 12.175025
H 3.781733 5.611272 17.146332
H -2.468597 4.438860 8.997752
C -2.050945 3.532305 9.436382
H 2.582165 -2.031737 9.765616
C 2.608494 -1.332907 10.602471
C 4.430594 3.321425 14.081804
H 4.600534 2.673598 13.221484
C 3.284511 -0.783750 12.857443
H 1.535566 0.199088 9.533222
C 2.010674 -0.079969 10.475070
H 2.743688 1.183145 13.553215
C 2.686429 0.471445 12.732607
H 5.425959 4.403366 11.847193
H 5.134268 4.628977 10.085909
H 5.640062 3.024129 10.720533
Cl 2.134719 5.589263 9.276358
Al 2.635423 4.076263 7.595168
C 3.934377 4.966012 6.414384
C 3.744656 2.583717 8.588996
H 3.474602 5.784492 5.840016
H 4.367499 4.261709 5.686472
H 4.767906 5.395466 6.991178
H 3.817009 2.035820 9.556835
H 4.773305 2.753456 8.234188
H 3.294999 1.805436 7.945379
C 0.944757 3.319087 6.929334
H 0.194627 4.094303 6.711469
H 0.487434 2.627108 7.651912
H 1.111560 2.760558 5.993884

Spin state: triplet

E = -10440.05 kcal mol-1
H = -10039.10 kcal mol-1
TS = -72.22 kcal mol-1
G (298.15 K) = -10111.32 kcal mol-1

H -1.469198 7.404410 11.865849
C -0.621966 3.534223 9.964225
C -0.389151 7.384926 12.015179
C 1.735398 8.531824 12.130699
C 1.640498 6.124230 12.440474
C 0.253247 6.167914 12.254479
H -0.152959 9.516877 11.761008
H -1.631168 2.905236 14.463986
H -0.009251 4.435103 9.930170
H -0.519906 0.279951 10.993267
H -1.007101 1.783124 13.238843
C -0.974988 2.823576 13.587416
H 5.369613 4.514530 17.517342
C 0.447586 3.223784 13.981214
H 3.464791 7.290093 12.464021
H 0.423492 4.254681 14.370672
C 2.087095 0.744019 11.588270
C -0.109081 2.358681 10.539066
C -0.897117 1.196642 10.540690
C 3.288723 -1.781029 11.840043
H 3.755226 -2.761428 11.937756
C -2.173739 1.213799 9.978088
Cr 3.197457 3.733823 10.431272
H -2.777339 0.305480 9.983800
C 2.378580 7.317623 12.362257
C 0.348093 8.568442 11.955848
H -1.381717 3.453198 12.787363
C 3.314613 5.648516 15.040880
C 4.915104 2.865478 11.154701
P 1.550576 2.462570 11.296949
H 3.836416 -1.142433 13.830252
C 3.999283 5.613004 16.257725
H 5.620284 2.640417 15.889437
C 4.976504 3.488585 15.654529
H 2.656060 6.487889 14.821956
C 0.975415 2.312555 15.094263
H -3.678027 2.397990 8.976593
C -2.680966 2.388891 9.417278
H 2.002416 2.574554 15.372916
H 2.319677 9.450356 12.069275
H 0.342322 2.415493 15.986779
H 0.946661 1.260356 14.781799
N 1.369574 3.299546 12.803857
P 2.555031 4.538731 12.514719
C 3.458806 4.604976 14.112344
C 4.835206 4.538104 16.567338
H -0.326295 5.246630 12.269472
H 3.871700 6.429293 16.969655
H -2.279251 4.464191 8.958277
C -1.900558 3.548654 9.412423
H 2.633521 -2.118275 9.807049
C 2.657263 -1.421021 10.644922
C 4.293354 3.518923 14.440192
H 4.396859 2.688359 13.744703
C 3.332585 -0.874043 12.901059
H 1.600835 0.119610 9.569899
C 2.066887 -0.164903 10.514115
H 2.800526 1.097919 13.592537
C 2.740123 0.383667 12.774698
H 5.583171 3.076964 10.296860
H 4.909467 1.775564 11.306361
H 5.348481 3.348530 12.039459
Cl 2.328998 5.618589 9.237257
Al 2.608227 4.144531 7.461362
C 3.800498 5.079774 6.199411
C 3.643407 2.611046 8.333096
H 3.315999 5.958267 5.745477
H 4.107831 4.419400 5.371985
H 4.720703 5.431602 6.691497
H 3.625347 2.057603 9.294672
H 4.698958 2.693878 8.035944
H 3.171120 1.861622 7.671037
C 0.809927 3.577021 6.872754

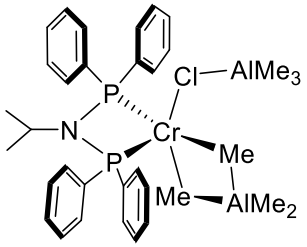
H 0.089959 4.409541 6.851563
H 0.376916 2.796112 7.515045
H 0.855829 3.170012 5.848961

Spin state: quintet

E = -10453.05 kcal mol-1
H = -10052.24 kcal mol-1
TS = -73.16 kcal mol-1
G (298.15 K) = -10125.40 kcal mol-1

H -1.202025 7.934002 12.196561
C -0.885713 3.644097 9.877957
C -0.168567 7.773546 12.505358
C 1.938482 8.640757 13.318336
C 1.703229 6.269755 12.858550
C 0.375736 6.490698 12.457912
H 0.185832 9.854905 12.967363
H -1.742115 3.287526 14.513631
H -0.246954 4.518317 9.740731
H -0.791719 0.482696 11.168835
H -1.381627 2.215197 13.147195
C -1.156119 3.192289 13.589658
H 5.668930 3.350681 17.145220
C 0.330730 3.325346 13.926225
H 3.525786 7.202614 13.569328
H 0.463447 4.273895 14.471650
C 1.932074 0.971937 11.439856
C -0.381834 2.515386 10.545807
C -1.177147 1.364914 10.657144
C 3.297210 -1.482961 11.538853
H 3.824434 -2.436504 11.578309
C -2.463697 1.349723 10.119507
Cr 3.151482 4.127041 10.386339
H -3.076454 0.451860 10.207307
C 2.486197 7.358616 13.278880
C 0.610403 8.851254 12.936546
H -1.487202 3.964503 12.885737
C 3.212322 4.868381 15.334444
C 4.829533 5.343527 10.573203
P 1.311636 2.671304 11.202624
H 4.117487 -0.764995 13.406037
C 3.982636 4.501645 16.438678
H 6.248915 2.482290 14.882843
C 5.393022 3.145251 15.012358
H 2.368079 5.546743 15.461995
C 0.801247 2.179986 14.827143
H -3.973063 2.465770 9.050342
C -2.967905 2.482292 9.472733
H 1.849461 2.312548 15.122143
H 2.553034 9.480069 13.645368
H 0.190329 2.148189 15.740127
H 0.698719 1.215626 14.312713
N 1.192073 3.488902 12.716949
P 2.466201 4.637650 12.589405
C 3.521956 4.366198 14.060295
C 5.069075 3.635851 16.280273
H -0.224673 5.654815 12.098101
H 3.733849 4.891355 17.426370
H -2.557791 4.505243 8.828656
C -2.177098 3.628269 9.352676
H 2.348543 -1.901125 9.642023
C 2.466831 -1.184165 10.455100
C 4.625901 3.512911 13.906214
H 4.875380 3.139731 12.910912
C 3.459822 -0.547063 12.563807
H 1.177741 0.270654 9.529228
C 1.793970 0.036673 10.397509
H 2.945571 1.409493 13.300096
C 2.790420 0.675647 12.510908
H 5.325708 5.307673 9.589000
H 4.549909 6.390034 10.774344
H 5.551935 5.021976 11.340235
Cl 2.108669 5.263123 8.466399
Al 2.969668 3.295054 7.595467
C 4.115983 3.814727 6.078925
C 4.223468 2.511147 9.059200
H 3.533768 4.257758 5.256031
H 4.658267 2.949500 5.663435
H 4.870383 4.557049 6.383323
H 4.374752 2.503199 10.166620
H 5.225471 2.717940 8.655169
H 3.978030 1.453554 8.860967
C 1.424442 2.099747 7.270127
H 0.875044 2.406020 6.365834
H 0.693882 2.089100 8.091969
H 1.754834 1.060198 7.106172

Geometry:



Spin state: singlet

E = -11904.88 kcal mol-1
H = -11429.05 kcal mol-1
TS = -82.45 kcal mol-1
G (298.15 K) = -11511.51 kcal mol-1

H -1.249160 8.437465 13.398024
C -1.165381 3.247688 9.377570
C -0.228325 8.104604 13.588199
C 1.926353 8.429597 14.628057
C 1.535160 6.460821 13.255204
C 0.224835 6.912640 13.024622
H 0.269814 9.802415 14.830019
H -2.103929 3.910332 14.284801
H -0.609798 4.070634 8.932359
H -0.854110 0.781189 11.713196
H -1.910759 2.950828 12.804147
C -1.521545 3.811088 13.358776
H 6.283804 3.040551 15.886957
C -0.037089 3.638464 13.706535

H 3.406403 6.919575 14.244752
H 0.231702 4.455751 14.393175
C 1.838561 1.369713 11.412378
C -0.596950 2.501438 10.420503
C -1.296723 1.390949 10.925712
C 3.309314 -0.998326 11.758070
H 3.883788 -1.915874 11.888776
C -2.550442 1.055817 10.418681
Cr 2.424025 4.688158 10.082805
H -3.083606 0.193145 10.819518
C 2.380840 7.238415 14.063381
C 0.621961 8.868360 14.391835
H -1.688693 4.706845 12.750217
C 3.238977 4.198368 14.886470
C 4.268420 5.914749 9.505937
P 1.059329 2.988617 11.042144
H 4.175403 -0.013391 13.478547
C 4.227386 3.688129 15.726572
H 6.801679 3.530158 13.498304
C 5.800852 3.710421 13.891082
H 2.251599 4.417234 15.291565
C 0.217143 2.303231 14.411441
H -4.099658 1.555293 8.996386
C -3.120405 1.821187 9.395644
H 1.253866 2.219338 14.756534
H 2.599325 9.021547 15.248667
H -0.448691 2.207750 15.280147
H 0.019153 1.459805 13.737956
N 0.853502 3.849356 12.528322
P 2.171726 4.974540 12.376889
C 3.511666 4.445289 13.528355
C 5.510676 3.438324 15.229013
H -0.447175 6.325833 12.402704
H 3.998746 3.491515 16.774535
H -2.850656 3.496918 8.058576
C -2.423859 2.911946 8.873501
H 2.283320 -1.697545 9.986937
C 2.411175 -0.878649 10.695011
C 4.806030 4.206826 13.046331
H 5.042344 4.395456 12.000970
C 3.472774 0.065936 12.648617
H 0.998647 0.381007 9.678204
C 1.679702 0.296546 10.522436
H 2.902184 2.070363 13.162636
C 2.747519 1.243884 12.473785
Cl 1.883796 4.265776 7.716024
Al 3.510030 2.637678 7.795274
C 4.940787 3.211990 6.556011
C 4.187996 2.806005 9.719647
H 4.571943 3.279541 5.520434
H 5.770477 2.485105 6.553226
H 5.375434 4.191699 6.808329
H 3.802070 3.271273 10.663298
H 5.217770 3.183834 9.636056
H 4.223036 1.752301 10.041055
C 2.568492 0.951446 7.357830
H 2.639802 0.755513 6.275946
H 1.496307 0.996886 7.602236
H 2.989885 0.076100 7.876023
H 4.757107 6.910388 9.438928
H 4.502523 5.425097 8.553689
H 4.836083 5.439673 10.317077
Al 2.698603 7.296907 9.618835
C 0.830128 6.275160 9.850661
H 0.467086 6.380790 8.820174
H 0.619309 7.213269 10.400152
H 0.171059 5.557743 10.357183
C 2.492375 8.048018 7.807227
H 3.378899 8.630291 7.508787
H 1.628871 8.728340 7.735245
H 2.351500 7.254589 7.057711
C 3.090552 8.559720 11.089636
H 3.769409 8.139094 11.846298
H 2.196917 8.907005 11.630174
H 3.582100 9.455913 10.677149

Spin state: triplet

E = -11915.12 kcal mol-1
H = -11438.93 kcal mol-1
TS = -84.53 kcal mol-1
G (298.15 K) = -11523.45 kcal mol-1

H -1.203896 8.480151 13.401456
C -1.180650 3.210467 9.380101
C -0.185074 8.138304 13.586617
C 1.983682 8.453356 14.599657
C 1.555358 6.467632 13.261621
C 0.247717 6.932123 13.037632
H 0.345630 9.849779 14.796120
H -2.117021 3.970668 14.273179
H -0.624531 4.028550 8.926897
H -0.872508 0.780359 11.754671
H -1.930633 2.988336 12.806782
C -1.533808 3.852391 13.349945
H 6.311215 3.062470 15.881066
C -0.051665 3.669967 13.702686
H 3.442112 6.920095 14.225339
H 0.222364 4.488748 14.385311
C 1.828635 1.371025 11.419486
C -0.618701 2.486846 10.442847
C -1.313346 1.376550 10.955914
C 3.311988 -0.988430 11.758414
H 3.892299 -1.902732 11.886092
C -2.559285 1.024021 10.441218
Cr 2.403995 4.684370 10.074841
H -3.089190 0.162339 10.848487
C 2.418839 7.249095 14.048343
C 0.682134 8.904793 14.369364
H -1.691523 4.740886 12.728233
C 3.254684 4.191811 14.883911
C 4.226040 5.975276 9.518902
P 1.039134 2.982943 11.048624
H 4.163869 -0.008699 13.488913
C 4.248353 3.689291 15.722508
H 6.823990 3.562641 13.493329
C 5.821284 3.731921 13.886224
H 2.265124 4.400780 15.288997
C 0.190068 2.336956 14.416238
H -4.098457 1.490450 8.997010

C -3.125529 1.770232 9.402106
H 1.225143 2.246904 14.764785
H 2.669635 9.046523 15.204711
H -0.479026 2.251357 15.283405
H -0.012481 1.491071 13.747235
N 0.846878 3.864430 12.526660
P 2.181400 4.975232 12.387494
C 3.525524 4.445082 13.526097
C 5.533987 3.453835 15.224192
H -0.438350 6.344661 12.432359
H 4.022039 3.488259 16.770132
H -2.854274 3.426563 8.040896
C -2.431639 2.858107 8.869561
H 2.299497 -1.684451 9.978057
C 2.417843 -0.869064 10.691683
C 4.822301 4.220252 13.042103
H 5.056512 4.412471 11.997014
C 3.464406 0.071158 12.656412
H 1.000653 0.388232 9.676364
C 1.679514 0.302285 10.522484
H 2.878773 2.069860 13.178507
C 2.732316 1.245699 12.485221
Cl 1.917222 4.213204 7.703460
Al 3.588758 2.633014 7.832593
C 5.035018 3.243734 6.629194
C 4.207329 2.842548 9.775149
H 4.701137 3.265624 5.579836
H 5.899114 2.559713 6.675004
H 5.411806 4.250684 6.867554
H 3.786362 3.303652 10.705748
H 5.230302 3.243551 9.720600
H 4.257568 1.793149 10.108207
C 2.717170 0.910849 7.388303
H 2.831330 0.702691 6.312479
H 1.636862 0.922010 7.597262
H 3.150232 0.058113 7.933801
H 4.654290 6.968474 9.265827
H 4.484608 5.358683 8.650246
H 4.820053 5.667215 10.388750
Al 2.604582 7.302052 9.569323
C 0.770122 6.215480 9.848925
H 0.376135 6.259068 8.825614
H 0.566766 7.185316 10.345529
H 0.127075 5.534952 10.422016
C 2.337874 7.993298 7.742220
H 3.187974 8.614626 7.417738
H 1.438280 8.624614 7.666587
H 2.230092 7.175299 7.014241
C 2.965901 8.603889 11.012260
H 3.674788 8.220520 11.760860
H 2.068784 8.920277 11.565760
H 3.412283 9.514235 10.580190

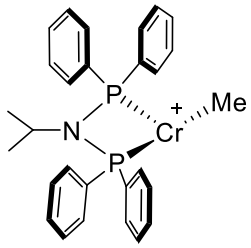
Spin state: quintet

E = -11924.95 kcal mol-1
H = -11451.42 kcal mol-1
TS = -87.41 kcal mol-1
G (298.15 K) = -11538.82 kcal mol-1

H -1.251853 8.506222 13.387290
C -1.723466 3.665073 10.204911
C -0.220984 8.185537 13.538739
C 2.020488 8.632217 14.331002
C 1.505572 6.497928 13.300052
C 0.180346 6.921497 13.110622
H 0.386284 10.035947 14.473962
H -2.033501 3.695388 14.705523
H -1.303548 4.659550 10.051722
H -0.828459 0.545711 11.271002
H -1.904293 2.788664 13.184627
C -1.526489 3.659743 13.732177
H 6.148850 2.688760 15.835361
C -0.012303 3.571665 13.956750
H 3.464192 7.059574 14.038978
H 0.273519 4.407956 14.614262
C 1.677752 1.456874 11.230309
C -0.917253 2.635427 10.714989
C -1.454642 1.350598 10.886553
C 3.326689 -0.800935 11.043859
H 3.976560 -1.672471 10.966240
C -2.790492 1.106270 10.566499
Cr 2.187959 4.753499 10.124493
H -3.205060 0.106960 10.701718
C 2.426857 7.366614 13.907941
C 0.698426 9.043422 14.148992
H -1.798643 4.558493 13.167185
C 3.319444 4.409533 15.034504
C 4.068802 5.921418 9.996727
P 0.799569 3.052196 11.164329
H 3.968652 -0.297132 13.045458
C 4.301677 3.809462 15.821089
H 6.318757 2.600584 13.345189
C 5.481146 3.107178 13.824683
H 2.485653 4.927985 15.509261
C 0.371854 2.259910 14.643260
H -4.637290 1.943454 9.822751
C -3.594514 2.138428 10.074395
H 1.431430 2.251580 14.924834
H 2.743629 9.303260 14.794464
H -0.225459 2.130181 15.555942
H 0.176330 1.404104 13.983524
N 0.757999 3.828581 12.702032
P 2.063126 4.939642 12.545031
C 3.407472 4.351240 13.632310
C 5.382094 3.156028 15.216535
H -0.533396 6.258838 12.621861
H 4.226377 3.852049 16.908070
H -3.680201 4.219347 9.493664
C -3.059077 3.416660 9.891490
H 2.541936 -1.011967 9.041189
C 2.516878 -0.435730 9.965352
C 4.496711 3.701422 13.033574
H 4.566990 3.633756 11.948016
C 3.322100 -0.031969 12.208836
H 1.103202 0.990641 9.189161
C 1.698541 0.688439 10.051123
H 2.544102 1.712013 13.195134
C 2.507692 1.096528 12.300718
Cl 2.250889 3.626572 8.054330

Al 4.405231 2.583622 7.765119
C 5.363034 4.025916 6.798440
C 5.038643 2.235423 9.630903
H 4.878568 4.273694 5.841253
H 6.405242 3.745532 6.571847
H 5.402592 4.956157 7.387067
H 4.215315 2.101032 10.348197
H 5.697674 3.033246 10.011157
H 5.623597 1.301233 9.662695
C 3.838052 0.975853 6.740924
H 3.570038 1.226367 5.702621
H 2.959505 0.488255 7.191577
H 4.638906 0.219061 6.695876
H 4.644018 6.442049 9.209691
H 4.452490 4.889599 9.898637
H 4.407130 6.317126 10.964081
Al 2.547659 7.265628 9.217125
C 0.640065 6.453626 9.418351
H 0.249257 5.655066 8.769005
H 0.268897 7.383712 8.945224
H 0.129670 6.429562 10.393743
C 2.931396 7.463460 7.290378
H 3.891703 7.970189 7.103957
H 2.156178 8.048171 6.769768
H 2.984848 6.478906 6.800197
C 2.664149 8.816793 10.444316
H 3.704732 9.131899 10.621276
H 2.216907 8.605307 11.427204
H 2.134524 9.690016 10.030480

Geometry:



Spin state: triplet

E = -8737.67 kcal mol-1
H = -8409.98 kcal mol-1
TS = -60.10 kcal mol-1
G (298.15 K) = -8470.08 kcal mol-1

H -0.914996 8.666187 13.131704
C -1.314024 3.768612 9.834794
C 0.051211 8.257556 13.427596
C 2.139066 8.471192 14.635431
C 1.680339 6.462070 13.360394
C 0.440899 6.999518 12.972806
H 0.594844 9.979670 14.613157
H -2.245563 3.999119 14.261465
H -0.824241 4.730019 9.673317
H -0.712562 0.684260 11.187687
H -1.998207 3.138079 12.731236
C -1.611572 3.942211 13.367202
H 6.040455 2.436749 16.101588
C -0.164481 3.680259 13.795181
H 3.502334 6.807685 14.485143
H 0.114554 4.459218 14.521851
C 1.886667 1.500289 11.283471
C -0.626875 2.737282 10.494718
C -1.244969 1.490751 10.683424
C 3.389251 -0.862915 11.318433
H 3.969801 -1.785334 11.334232
C -2.549927 1.290267 10.232048
Cr 2.541881 4.594773 10.399828
H -3.031539 0.324090 10.382386
C 2.534226 7.210140 14.187302
C 0.899906 8.995010 14.259256
H -1.705046 4.887678 12.821192
C 3.184998 4.035124 15.152518
C 1.701570 6.165598 9.597672
P 1.026691 3.102338 11.148404
H 3.876455 -0.335123 13.356723
C 4.108765 3.394483 15.978060
H 6.561710 2.770815 13.689723
C 5.613778 3.119549 14.098720
H 2.249451 4.405912 15.571611
C -0.004107 2.305138 14.443760
H -4.257216 2.163510 9.240966
C -3.237939 2.324886 9.591815
H 1.005135 2.166684 14.849492
H 2.801807 9.044922 15.283102
H -0.723417 2.190088 15.265050
H -0.196823 1.508216 13.712311
N 0.813117 3.871532 12.674451
P 2.216215 4.880797 12.644245
C 3.466736 4.210243 13.786636
C 5.320025 2.933538 15.451739
H -0.216745 6.426311 12.319460
H 3.886934 3.259875 17.036696
H -3.152342 4.364090 8.879561
C -2.618904 3.562713 9.390473
H 2.734940 -1.128151 9.274160
C 2.696812 -0.494408 10.160063
C 4.687884 3.752697 13.269282
H 4.919504 3.889046 12.209863
C 3.337274 -0.050338 12.453352
H 1.402965 0.961670 9.235619
C 1.950932 0.682918 10.137251
H 2.565605 1.762084 13.322857
C 2.594644 1.131022 12.437693
H 2.558022 6.873013 9.596071
H 0.831092 6.667429 10.035705
H 1.473942 5.838159 8.562882

Spin state: quintet

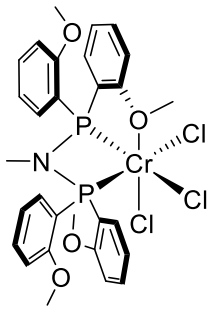
E = -8755.36 kcal mol-1
H = -8427.27 kcal mol-1
TS = -60.98 kcal mol-1
G (298.15 K) = -8488.25 kcal mol-1

H -1.519886 8.009160 13.242564
C -1.172047 4.250767 10.082221

C -0.466660 7.842646 13.468547
C 1.633224 8.627778 14.380471
C 1.484249 6.401343 13.429900
C 0.131468 6.629755 13.127080
H -0.185647 9.791653 14.355417
H -1.743626 3.061413 14.698401
H -0.561665 5.156473 10.074670
H -0.994331 0.930036 10.879136
H -1.427839 2.222756 13.171802
C -1.210956 3.133695 13.741688
H 5.964594 2.971983 16.746361
C 0.285494 3.279100 14.018590
H 3.290420 7.254307 14.280059
H 0.420427 4.137992 14.694729
C 1.772269 1.422353 11.074082
C -0.627014 3.040384 10.542074
C -1.408217 1.873993 10.525193
C 3.138989 -0.995025 10.716060
H 3.663691 -1.940615 10.580633
C -2.723133 1.926378 10.064801
Cr 2.616286 4.666370 10.342614
H -3.327298 1.019345 10.052315
C 2.236509 7.414008 14.049748
C 0.282277 8.842485 14.094938
H -1.613443 3.988650 13.186152
C 3.263742 4.618697 15.480863
C 2.488698 4.199619 8.369089
P 1.066006 3.091124 11.189388
H 4.080485 -0.562089 12.612415
C 4.156460 4.107229 16.421929
H 6.372254 2.583994 14.321206
C 5.497557 3.147203 14.646085
H 2.400747 5.198066 15.809619
C 0.856637 2.030297 14.691217
H -4.293175 3.170999 9.260022
C -3.265388 3.135800 9.621145
H 1.918895 2.154520 14.933017
H 2.220768 9.407291 14.865362
H 0.315588 1.839137 15.627400
H 0.738880 1.149983 14.046373
N 1.066684 3.674171 12.795011
P 2.297315 4.889548 12.823112
C 3.482579 4.392683 14.111253
C 5.269490 3.369129 16.006649
H -0.453764 5.854136 12.632483
H 3.984253 4.284640 17.483465
H -2.908564 5.240276 9.275953
C -2.489508 4.298698 9.630086
H 2.066056 -1.143785 8.845392
C 2.240031 -0.549926 9.742548
C 4.608725 3.659614 13.700936
H 4.787102 3.485925 12.637415
C 3.371863 -0.222784 11.856870
H 0.875757 1.003557 9.139861
C 1.561264 0.656095 9.912840
H 2.901909 1.592904 12.915732
C 2.701655 0.987522 12.033314
H 3.278327 4.819268 7.894349
H 1.528600 4.460672 7.898485
H 2.709772 3.145202 8.143816

6.3 Activation of complex 2

Geometry:



Spin state: doublet

E = -10017.52 kcal mol-1
H = -9657.19 kcal mol-1
TS = -72.65 kcal mol-1
G (298.15 K) = -9729.84 kcal mol-1

Cr -0.418731 -3.029969 -2.226180
P -2.933994 -2.880125 -2.428064
N -2.946877 -1.208125 -2.118417
P -1.330232 -0.898002 -1.680644
C -4.106174 -0.312578 -2.095421
H -4.464067 -0.130130 -3.119051
H -3.815175 0.644678 -1.645556
H -4.915257 -0.744759 -1.497515
C -4.111449 -3.108645 -3.808646
C -5.186586 -4.007613 -3.755818
C -5.980625 -4.252996 -4.876178
C -5.700541 -3.596957 -6.075238
C -4.652807 -2.677675 -6.152512
C -3.867198 -2.416540 -5.022517
H -5.399139 -4.531156 -2.825207
H -6.807192 -4.959877 -4.811699
H -6.304275 -3.793439 -6.961760
H -4.451166 -2.162260 -7.089353
C -3.685870 -3.844727 -1.050662
C -4.183657 -3.326979 0.167641
C -4.564406 -4.198427 1.198439
C -4.461765 -5.580412 1.025833
C -3.966128 -6.106782 -0.165526
C -3.573244 -5.237782 -1.183685
H -3.911184 -1.740196 2.336344
H -4.947907 -3.802162 2.136049
H -4.764956 -6.242610 1.837355
H -3.866345 -7.182845 -0.301259
H -3.137126 -5.645365 -2.095523
C -0.860910 0.660873 -2.468496
C 0.396944 1.214959 -2.135171
C 0.903298 2.297247 -2.864567
C 0.161503 2.820610 -3.926276
C -1.072851 2.269656 -4.275664
C -1.573245 1.185371 -3.553379
H 2.957146 0.592286 -1.911514
H 1.873117 2.722480 -2.613460
H 0.562740 3.662225 -4.491711

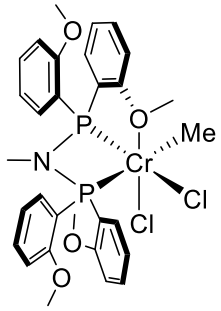
H -1.637934 2.670281 -5.116760
H -2.503914 0.712729 -3.857961
C -1.328666 -0.643240 0.119241
C -1.176512 -1.802485 0.910124
C -1.133729 -1.696974 2.304262
C -1.266028 -0.439691 2.903474
C -1.440463 0.709372 2.131919
C -1.462287 0.599690 0.739528
H -1.727615 -4.354699 1.696568
H -0.993422 -2.578646 2.924646
H -1.227321 -0.366214 3.990725
H -1.538735 1.684673 2.607626
H -1.558798 1.491339 0.118368
O -4.253476 -1.968114 0.282588
C -4.596227 -1.395383 1.548088
H -4.469761 -0.316083 1.418845
H -5.637995 -1.620418 1.824231
O -2.870587 -1.490440 -4.990885
C -2.310988 -1.033356 -6.230599
O 1.032237 0.615027 -1.094985
C 2.449672 0.789877 -0.956739
H 2.691059 1.801427 -0.595463
H 2.759030 0.041690 -0.222020
O -1.101390 -2.997020 0.234594
C -0.891102 -4.205783 1.000112
H -0.869313 -5.010205 0.261143
H 0.070604 -4.153011 1.526961
Cl 1.594173 -2.641661 -1.299916
Cl -0.406203 -5.286937 -2.278843
Cl 0.036199 -2.492727 -4.322296
H -1.422529 -0.461563 -5.948391
H -2.011018 -1.884470 -6.857613
H -3.020235 -0.388929 -6.773271

Spin state: quartet

E = -10035.44 kcal mol-1
H = -9675.11 kcal mol-1
TS = -72.66 kcal mol-1
G (298.15 K) = -9747.77 kcal mol-1

Cr -0.445936 -2.798987 -2.276999
P -2.973871 -2.765094 -2.303330
N -3.055529 -1.151567 -1.729742
P -1.411704 -0.736607 -1.521715
C -4.192436 -0.426605 -1.151246
H -4.435816 0.469867 -1.739113
H -3.961086 -0.123614 -0.120992
H -5.067904 -1.086069 -1.122100
C -3.836962 -2.733419 -3.913850
C -4.676109 -1.683168 -4.300739
C -5.144999 -1.590541 -5.612056
C -4.752637 -2.545852 -6.552292
C -3.916209 -3.601774 -6.190183
C -3.473194 -3.707521 -4.865672
H -4.952251 -0.913603 -3.582617
H -5.798424 -0.767874 -5.900795
H -5.098534 -2.469778 -7.583650
H -3.608711 -4.336750 -6.931351
C -4.032092 -3.813848 -1.231661
C -4.190240 -3.626516 0.165038
C -4.942372 -4.538575 0.918035
C -5.519370 -5.651239 0.305108
C -5.362827 -5.857861 -1.064226
C -4.629038 -4.942467 -1.816923
H -3.512082 -2.938332 2.778330
H -5.075668 -4.386147 1.986898
H -6.094953 -6.354314 0.907766
H -5.810552 -6.724083 -1.550012
H -4.506504 -5.113628 -2.884179
C -1.186639 0.886322 -2.273751
C 0.040466 1.556146 -2.067317
C 0.348203 2.698557 -2.814715
C -0.562225 3.163800 -3.766539
C -1.767585 2.495912 -3.994020
C -2.068790 1.350011 -3.257583
H 2.638111 1.110328 -2.201572
H 1.295505 3.213034 -2.665015
H -0.314097 4.052006 -4.348344
H -2.457444 2.848808 -4.759567
H -2.970568 0.778865 -3.476960
C -1.147837 -0.615442 0.271208
C -0.804650 -1.820497 0.918050
C -0.532714 -1.824992 2.288664
C -0.630610 -0.633511 3.013722
C -0.999740 0.558878 2.390125
C -1.246568 0.561640 1.015187
H -1.536297 -4.285004 1.564286
H -0.243883 -2.742144 2.795677
H -0.412838 -0.646266 4.081976
H -1.076519 1.481996 2.963746
H -1.500126 1.489959 0.501887
O -3.590611 -2.528654 0.717900
C -3.895100 -2.184720 2.072936
H -3.378372 -1.236981 2.254067
H -4.979537 -2.058956 2.216688
O -2.703274 -4.720778 -4.386925
C -1.878954 -5.446801 -5.318196
O 0.849298 1.001499 -1.125524
C 2.258482 1.268580 -1.182424
H 2.483424 2.290780 -0.841204
H 2.715708 0.536708 -0.510930
O -0.787614 -2.956940 0.139629
C -0.728691 -4.232363 0.821275
H -0.867125 -4.982260 0.038765
H 0.254812 -4.367879 1.289376
Cl 1.662685 -2.183586 -1.721571
Cl -0.166151 -5.056304 -2.361433
Cl -0.477316 -2.156248 -4.422074
H -1.198563 -6.032934 -4.695907
H -2.489530 -6.107805 -5.952115
H -1.299495 -4.741588 -5.930037

Geometry:



Spin state: doublet

E = -10389.42 kcal mol-1
H = -10008.05 kcal mol-1
TS = -73.22 kcal mol-1
G (298.15 K) = -10081.27 kcal mol-1

Cr -0.437690 -3.061074 -2.233855
P -2.918501 -2.896483 -2.422180
N -2.945464 -1.222740 -2.126850
P -1.324594 -0.922245 -1.679845
C -4.104080 -0.327696 -2.107833
H -3.814026 0.629407 -1.656740
H -4.917444 -0.757958 -1.514153
H -4.458626 -0.143925 -3.132943
C -4.073266 -3.137011 -3.821792
C -5.158904 -4.022283 -3.772730
C -5.951025 -4.262886 -4.895994
C -5.659348 -3.612457 -6.094434
C -4.597408 -2.708489 -6.170337
C -3.810485 -2.458236 -5.039173
H -5.381779 -4.537855 -2.839862
H -6.785805 -4.960215 -4.833168
H -6.262139 -3.802008 -6.983095
H -4.387075 -2.201457 -7.109642
C -3.684057 -3.860132 -1.052113
C -4.195966 -3.341490 0.159697
C -4.571693 -4.211004 1.193827
C -4.448014 -5.592609 1.031428
C -3.936134 -6.119771 -0.152866
C -3.548055 -5.252346 -1.174098
H -3.946518 -1.742767 2.318407
H -4.966222 -3.813664 2.126449
H -4.746928 -6.253652 1.845535
H -3.817212 -7.195074 -0.279406
H -3.091660 -5.659021 -2.076822
C -0.842051 0.629632 -2.483363
C 0.423260 1.171071 -2.155008
C 0.954628 2.225763 -2.907192
C 0.227619 2.740558 -3.983765
C -1.016959 2.207434 -4.324296
C -1.540878 1.148526 -3.579605
H 2.967832 0.495786 -1.900805
H 1.930928 2.638415 -2.659815
H 0.647602 3.561389 -4.565907
H -1.573140 2.603202 -5.173781
H -2.482470 0.690832 -3.874327
C -1.353587 -0.620459 0.117109
C -1.208436 -1.759209 0.941918
C -1.182913 -1.618272 2.333715
C -1.326342 -0.347072 2.899739
C -1.492522 0.781481 2.096161
C -1.495866 0.636451 0.706270
H -1.717399 -4.342177 1.752267
H -1.049206 -2.485979 2.975688
H -1.303377 -0.245460 3.985254
H -1.598819 1.768534 2.545395
H -1.584734 1.513281 0.062854
O -4.282380 -1.982487 0.264997
C -4.630914 -1.405046 1.526550
H -4.508061 -0.325778 1.392688
H -5.672526 -1.633091 1.801267
O -2.784291 -1.558538 -5.013142
C -2.301677 -1.031725 -6.255430
O 1.039618 0.584910 -1.096391
C 2.459931 0.729332 -0.954322
H 2.723343 1.743608 -0.616530
H 2.747831 -0.008993 -0.201286
O -1.120772 -2.963062 0.296340
C -0.878287 -4.158691 1.066199
H -0.814674 -4.961675 0.326293
H 0.072839 -4.073351 1.608589
Cl 1.615950 -2.658854 -1.372557
Cl -0.370785 -5.318882 -2.343494
C -0.006900 -2.593311 -4.156925
H -1.424544 -0.433032 -5.993947
H -2.003618 -1.842107 -6.936578
H -3.056631 -0.391797 -6.738646
H -0.723013 -3.100245 -4.817207
H 1.001581 -3.000100 -4.314795
H -0.005865 -1.512668 -4.356931

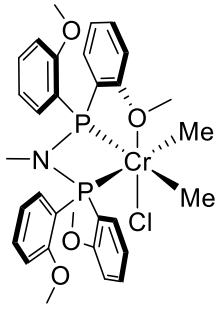
Spin state: quartet

E = -10408.48 kcal mol-1
H = -10026.47 kcal mol-1
TS = -75.22 kcal mol-1
G (298.15 K) = -10101.69 kcal mol-1

Cr -0.471674 -2.814197 -2.287892
P -2.981210 -2.815197 -2.336985
N -3.098409 -1.196907 -1.766359
P -1.460943 -0.777140 -1.496413
C -4.265485 -0.532750 -1.176699
H -4.112937 -0.373848 -0.099725
H -5.147747 -1.171267 -1.306541
H -4.455891 0.438384 -1.655275
C -3.761680 -2.768347 -3.993366
C -4.460919 -1.657584 -4.472079
C -4.870885 -1.591427 -5.805798
C -4.564568 -2.641500 -6.673048
C -3.865049 -3.762265 -6.219718
C -3.473769 -3.829161 -4.876946
H -4.669174 -0.823497 -3.804201
H -5.415334 -0.719339 -6.166853
H -4.869275 -2.591208 -7.718860
H -3.626335 -4.573025 -6.905234
C -4.159820 -3.810715 -1.342670
C -4.237144 -3.697610 0.068063

C -5.102876 -4.525718 0.795574
C -5.883213 -5.477493 0.138189
C -5.822580 -5.599483 -1.248554
C -4.969586 -4.768064 -1.973188
H -3.375980 -3.228295 2.693667
H -5.163979 -4.438429 1.878025
H -6.544289 -6.120080 0.720501
H -6.436183 -6.334321 -1.768690
H -4.933925 -4.865478 -3.055328
C -1.243567 0.874030 -2.207265
C -0.010480 1.528375 -1.979279
C 0.293938 2.710965 -2.663284
C -0.626032 3.236340 -3.574521
C -1.837942 2.588904 -3.822246
C -2.135420 1.403641 -3.146598
H 2.596517 1.119423 -2.137100
H 1.243592 3.214530 -2.492342
H -0.382498 4.158227 -4.103569
H -2.540706 2.993552 -4.549764
H -3.052416 0.861532 -3.374232
C -1.227120 -0.606676 0.301152
C -0.662146 -1.708366 0.982050
C -0.324771 -1.587678 2.336415
C -0.602683 -0.398875 3.016360
C -1.207401 0.677542 2.364712
C -1.500656 0.569599 1.003599
H -0.250943 -4.314610 1.753934
H 0.144230 -2.413644 2.865402
H -0.340207 -0.320073 4.071854
H -1.423022 1.600532 2.902005
H -1.915664 1.421489 0.462602
O -3.457894 -2.739210 0.651964
C -3.700518 -2.415544 2.026142
H -3.103584 -1.522130 2.229623
H -4.766192 -2.197979 2.197499
O -2.817700 -4.874217 -4.303588
C -2.169921 -5.837267 -5.148609
O 0.805044 0.920725 -1.077228
C 2.210430 1.207625 -1.111834
H 2.420988 2.208737 -0.704663
H 2.674655 0.438948 -0.488120
O -0.500399 -2.861777 0.264103
C 0.264177 -3.935274 0.859975
H 0.312985 -4.710562 0.090294
H 1.275895 -3.583917 1.101553
Cl 1.691920 -2.186418 -1.903675
Cl -0.178099 -5.071203 -2.418094
C -0.583729 -2.192246 -4.247011
H -1.549327 -6.432975 -4.474364
H -2.909551 -6.471832 -5.660952
H -1.526728 -5.333768 -5.885530
H -0.800275 -3.090717 -4.841544
H 0.423919 -1.823509 -4.477331
H -1.321906 -1.413350 -4.486224

Geometry:



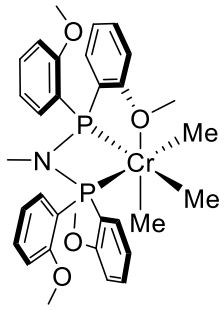
Spin state: quartet

E = -10770.73 kcal mol-1
H = -10368.68 kcal mol-1
TS = -74.32 kcal mol-1
G (298.15 K) = -10442.99 kcal mol-1

Cr -0.442797 -3.153238 -2.225638
P -2.917551 -2.917560 -2.410937
N -2.971571 -1.252009 -2.082295
P -1.356177 -0.891897 -1.646433
C -4.157061 -0.392904 -2.058081
H -3.910489 0.549825 -1.553640
H -4.972772 -0.873359 -1.507065
H -4.493343 -0.173616 -3.082526
C -4.050742 -3.140743 -3.831520
C -5.137141 -4.025173 -3.829031
C -5.890032 -4.252566 -4.982448
C -5.556029 -3.588552 -6.162416
C -4.494101 -2.681500 -6.191058
C -3.748975 -2.442506 -5.029238
H -5.392428 -4.550911 -2.909884
H -6.726931 -4.949830 -4.957496
H -6.126679 -3.768875 -7.073985
H -4.252042 -2.162928 -7.116340
C -3.696969 -3.905608 -1.060704
C -4.184499 -3.410329 0.171730
C -4.549052 -4.300796 1.192827
C -4.441998 -5.678994 0.998808
C -3.962354 -6.184793 -0.208539
C -3.587121 -5.296382 -1.216391
H -3.912867 -1.870180 2.369304
H -4.922476 -3.920832 2.141348
H -4.730875 -6.355164 1.803973
H -3.864857 -7.258489 -0.364341
H -3.171999 -5.689786 -2.144461
C -0.916446 0.665434 -2.463672
C 0.398198 1.123919 -2.208342
C 0.945229 2.170000 -2.957893
C 0.179903 2.762205 -3.967785
C -1.113072 2.311157 -4.240345
C -1.652975 1.259436 -3.494445
H 2.901611 0.292167 -2.156857
H 1.959222 2.514996 -2.763368
H 0.607145 3.578669 -4.550677
H -1.697708 2.766947 -5.039257
H -2.637264 0.869269 -3.743016
C -1.398754 -0.539387 0.143827
C -1.239702 -1.653310 1.000038

C -1.173362 -1.472207 2.385617
C -1.299289 -0.185129 2.919221
C -1.482261 0.919504 2.087190
C -1.519243 0.734179 0.702148
H -1.669032 -4.205338 1.934668
H -1.023028 -2.320510 3.049740
H -1.246696 -0.052571 4.000406
H -1.573835 1.919789 2.509819
H -1.617807 1.593059 0.036237
O -4.258531 -2.055042 0.310654
C -4.593276 -1.503107 1.587199
H -4.451589 -0.423161 1.479182
H -5.637664 -1.721222 1.859437
O -2.730679 -1.538869 -4.949866
C -2.217539 -0.970031 -6.160204
O 1.039994 0.451269 -1.214855
C 2.474331 0.488780 -1.163146
H 2.829138 1.457351 -0.778408
H 2.756417 -0.321973 -0.486107
O -1.184302 -2.878405 0.388976
C -0.881323 -4.037131 1.185735
H -0.863007 -4.872976 0.482355
H 0.104679 -3.929738 1.657282
Cl 1.620454 -2.976416 -1.289235
C -0.455781 -5.209070 -2.442168
C 0.010437 -2.774539 -4.180292
H -1.367437 -0.355173 -5.851480
H -1.873964 -1.756038 -6.848375
H -2.970768 -0.336333 -6.654295
H -0.719859 -3.236105 -4.858773
H 1.003268 -3.217137 -4.342445
H 0.059670 -1.690566 -4.364685
H 0.580895 -5.515825 -2.642311
H -1.092904 -5.551224 -3.273015
H -0.789928 -5.710621 -1.517243

Geometry:



Spin state: doublet

E = -11114.99 kcal mol-1
H = -10692.61 kcal mol-1
TS = -75.04 kcal mol-1
G (298.15 K) = -10767.65 kcal mol-1

Cr -0.370810 -3.130719 -2.186810
P -2.927568 -2.956720 -2.439199
N -2.932691 -1.274891 -2.132776
P -1.312220 -0.986333 -1.677902
C -4.082486 -0.369553 -2.108434
H -3.749911 0.624104 -1.782851
H -4.849514 -0.728749 -1.412313
H -4.520297 -0.280406 -3.113981
C -4.145643 -3.105818 -3.802349
C -5.329965 -3.854598 -3.738208
C -6.142357 -4.026947 -4.860827
C -5.778750 -3.440976 -6.073298
C -4.614461 -2.670620 -6.165508
C -3.804138 -2.497929 -5.038663
H -5.617262 -4.314227 -2.793185
H -7.055673 -4.617023 -4.784733
H -6.402259 -3.574071 -6.957763
H -4.345979 -2.209998 -7.114179
C -3.733003 -3.898835 -1.069222
C -4.165713 -3.386974 0.175620
C -4.570291 -4.260385 1.197293
C -4.557727 -5.641131 0.990298
C -4.139390 -6.165013 -0.232220
C -3.726293 -5.292081 -1.239487
H -3.843260 -1.852491 2.386403
H -4.903445 -3.865882 2.154954
H -4.875489 -6.304621 1.795206
H -4.123085 -7.241187 -0.400869
H -3.373315 -5.699027 -2.188678
C -0.846946 0.568093 -2.491414
C 0.390765 1.172288 -2.154715
C 0.898528 2.225766 -2.921218
C 0.191535 2.672727 -4.043714
C -1.011546 2.067189 -4.407826
C -1.519773 1.019421 -3.637723
H 3.008035 0.819255 -1.699370
H 1.844938 2.693603 -2.656913
H 0.596628 3.492226 -4.637778
H -1.553048 2.403397 -5.292081
H -2.434042 0.515483 -3.943803
C -1.308111 -0.670260 0.115880
C -1.126775 -1.792417 0.955151
C -1.085916 -1.635833 2.344399
C -1.239393 -0.360397 2.900902
C -1.436963 0.753799 2.084867
C -1.466546 0.590352 0.697913
H -1.787365 -4.277247 1.797298
H -0.932158 -2.491577 2.997633
H -1.201029 -0.246811 3.984677
H -1.555166 1.744675 2.523155
H -1.595202 1.455724 0.046181
O -4.157243 -2.029403 0.322062
C -4.497340 -1.466069 1.590940
H -4.320421 -0.391357 1.484803
H -5.552804 -1.652156 1.844669
O -2.665231 -1.741361 -5.023025
C -2.144544 -1.255110 -6.263672
O 1.020033 0.637159 -1.067508
C 2.379436 0.999846 -0.813878
H 2.463872 2.053676 -0.504709
H 2.706446 0.348990 0.002192
O -1.008918 -3.011217 0.324185
C -0.906459 -4.188877 1.145591
H -0.882353 -5.028357 0.448922

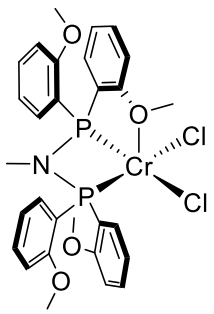
H 0.019045 -4.168220 1.738820
C 1.493542 -2.578452 -1.524279
C -0.368065 -5.189381 -2.088176
C 0.129117 -2.903578 -4.138508
H -1.204673 -0.757852 -6.007773
H -1.946286 -2.082712 -6.961220
H -2.831465 -0.530230 -6.728802
H 1.102982 -3.396556 -4.286825
H 0.235538 -1.834696 -4.383790
H -0.619550 -3.359136 -4.801352
H -0.456701 -5.602815 -3.104824
H -1.160890 -5.635948 -1.469188
H 0.610455 -5.488153 -1.674295
H 1.894122 -1.732558 -2.101797
H 2.157348 -3.447257 -1.672056
H 1.490137 -2.303365 -0.457010

Spin state: quartet

E = -11131.29 kcal mol-1
H = -10708.23 kcal mol-1
TS = -77.72 kcal mol-1
G (298.15 K) = -10785.95 kcal mol-1

Cr -0.294794 -3.184349 -2.280348
P -2.896476 -2.953479 -2.453579
N -2.860132 -1.275529 -2.131004
P -1.235602 -0.981114 -1.678879
C -3.990378 -0.355061 -1.981823
H -3.953383 0.143253 -1.003216
H -4.927900 -0.916706 -2.046303
H -3.980048 0.408923 -2.771086
C -4.184480 -3.090927 -3.746241
C -5.371644 -3.820640 -3.603435
C -6.260700 -3.971797 -4.670191
C -5.963617 -3.387620 -5.901346
C -4.790187 -2.645992 -6.072769
C -3.903781 -2.492939 -5.001087
H -5.595733 -4.284123 -2.642723
H -7.177941 -4.545238 -4.537668
H -6.647140 -3.504438 -6.742889
H -4.572415 -2.194332 -7.038580
C -3.634898 -3.913093 -1.058807
C -4.204412 -3.408483 0.131258
C -4.581124 -4.285722 1.160177
C -4.405294 -5.663516 1.009154
C -3.841341 -6.178236 -0.157638
C -3.451255 -5.299450 -1.169100
H -4.069685 -1.788959 2.275097
H -5.018655 -3.899772 2.078505
H -4.705709 -6.330925 1.817518
H -3.688119 -7.250335 -0.276444
H -2.967577 -5.692185 -2.065093
C -0.763455 0.569204 -2.494193
C 0.444734 1.200838 -2.115270
C 0.956812 2.261075 -2.870594
C 0.285046 2.676273 -4.025526
C -0.882613 2.032937 -4.436731
C -1.394530 0.979884 -3.675926
H 3.057124 0.961936 -1.507493
H 1.880639 2.754871 -2.575588
H 0.693523 3.499707 -4.611870
H -1.389937 2.341220 -5.350763
H -2.273540 0.434893 -4.016073
C -1.345545 -0.642287 0.112987
C -1.234583 -1.764614 0.965494
C -1.306266 -1.605984 2.354064
C -1.505403 -0.329913 2.892814
C -1.634347 0.783545 2.062874
C -1.548850 0.618522 0.677207
H -1.844943 -4.312980 1.757542
H -1.206081 -2.462424 3.017158
H -1.557507 -0.214329 3.975981
H -1.787934 1.774795 2.489141
H -1.619869 1.483465 0.016002
O -4.348082 -2.052973 0.216415
C -4.748466 -1.483073 1.465113
H -4.667831 -0.399759 1.330444
H -5.786404 -1.750670 1.717821
O -2.743019 -1.775866 -5.059617
C -2.277874 -1.317323 -6.333637
O 1.043482 0.679956 -1.002877
C 2.363744 1.116912 -0.666666
H 2.371093 2.176726 -0.366975
H 2.670319 0.493462 0.178215
O -1.067539 -2.976895 0.345828
C -0.936951 -4.155409 1.157997
H -0.820142 -4.979636 0.450390
H -0.048503 -4.087663 1.802234
C 1.571052 -2.805269 -1.491309
C -0.173014 -5.246502 -2.405007
C 0.189163 -2.769831 -4.221328
H -1.298861 -0.870314 -6.138133
H -2.164976 -2.154854 -7.038061
H -2.957139 -0.560836 -6.757744
H 1.199163 -3.161615 -4.412316
H 0.185063 -1.683298 -4.408094
H -0.527139 -3.259190 -4.897567
H 0.870523 -5.554503 -2.574828
H -0.782881 -5.636824 -3.237084
H -0.522190 -5.737451 -1.477374
H 2.305601 -3.511977 -1.906158
H 1.531352 -2.937321 -0.395603
H 1.906330 -1.778126 -1.702595

Geometry:



Spin state: singlet

E = -9916.01 kcal mol-1
H = -9557.60 kcal mol-1
TS = -73.63 kcal mol-1
G (298.15 K) = -9631.23 kcal mol-1

Cr -0.341701 -2.989180 -2.339740
P -2.719887 -2.803921 -2.289435
N -2.642054 -1.095201 -2.131084
P -1.140821 -1.006713 -1.313005
C -3.608864 -0.052765 -2.445870
H -4.180616 0.274112 -1.565723
H -4.315491 -0.439780 -3.189590
H -3.079125 0.806491 -2.879790
C -3.895543 -3.152723 -3.623889
C -4.959731 -4.049462 -3.467473
C -5.699520 -4.479190 -4.569574
C -5.363469 -4.019304 -5.844662
C -4.310443 -3.119854 -6.026990
C -3.584015 -2.671938 -4.917399
H -5.193252 -4.427667 -2.471909
H -6.522721 -5.180261 -4.435054
H -5.923989 -4.364015 -6.714307
H -4.058785 -2.774298 -7.027594
C -3.474726 -3.509685 -0.772294
C -4.558085 -2.917572 -0.088834
C -4.947389 -3.400036 1.167490
C -4.280968 -4.492807 1.726434
C -3.227350 -5.108524 1.050476
C -2.824516 -4.602726 -0.186190
H -5.763371 -0.721979 0.909072
H -5.761823 -2.931530 1.715494
H -4.593353 -4.860386 2.704400
H -2.716082 -5.966762 1.485521
H -1.974488 -5.046886 -0.709525
C -0.350822 0.568349 -1.761079
C 0.359200 0.578819 -2.987231
C 1.145435 1.682722 -3.335788
C 1.210559 2.784589 -2.480893
C 0.515581 2.789701 -1.270113
C -0.249918 1.679514 -0.912255
H 1.320543 -0.141463 -5.532583
H 1.707620 1.683763 -4.267382
H 1.822117 3.641984 -2.763960
H 0.583046 3.644908 -0.598323
H -0.751539 1.661397 0.054300
C -1.632738 -0.870799 0.450721
C -1.194491 -1.880698 1.340519
C -1.738272 -1.972093 2.629563
C -2.708742 -1.056824 3.037491
C -3.150072 -0.051150 2.174975
C -2.614638 0.029252 0.888034
H -0.552412 -4.479452 1.945882
H -1.415124 -2.759279 3.307171
H -3.124538 -1.135344 4.042484
H -3.902847 0.666356 2.501513
H -2.972223 0.802429 0.208623
O -5.167598 -1.876402 -0.731480
C -6.172148 -1.144904 -0.022071
H -6.476135 -0.335196 -0.692978
H -7.046003 -1.775448 0.204004
O -2.576279 -1.756642 -4.970667
C -1.931734 -1.528997 -6.228399
O 0.227075 -0.532603 -3.774430
C 1.305012 -0.843987 -4.685944
H 2.264377 -0.830154 -4.151778
H 1.095157 -1.859098 -5.037519
O -0.258440 -2.726078 0.841089
C 0.251992 -3.786330 1.655144
H 0.982969 -4.294739 1.018769
H 0.751288 -3.389883 2.552486
Cl 1.793582 -2.961577 -1.635962
Cl -0.279848 -4.127143 -4.287423
H -1.115498 -0.836861 -6.007355
H -1.523860 -2.471032 -6.622823
H -2.616167 -1.067404 -6.957231

Spin state: triplet

E = -9924.99 kcal mol-1
H = -9567.25 kcal mol-1
TS = -71.42 kcal mol-1
G (298.15 K) = -9638.67 kcal mol-1

Cr -0.309148 -3.017143 -2.295353
P -2.677411 -2.829741 -2.268018
N -2.578520 -1.115926 -2.175046
P -1.091487 -0.999004 -1.329524
C -3.533995 -0.074347 -2.531819
H -4.049618 0.337306 -1.652418
H -4.288902 -0.502023 -3.201296
H -3.008699 0.731535 -3.061952
C -3.855300 -3.194725 -3.599274
C -4.897199 -4.116004 -3.426055
C -5.643305 -4.569170 -4.514040
C -5.337617 -4.109301 -5.796516
C -4.309768 -3.184495 -5.996758
C -3.576832 -2.712730 -4.901390
H -5.109046 -4.494873 -2.425891
H -6.448624 -5.287372 -4.362273
H -5.902093 -4.471502 -6.656353
H -4.083625 -2.836316 -7.002497
C -3.455927 -3.495565 -0.747093
C -4.535695 -2.867365 -0.089126
C -4.974025 -3.339692 1.154635
C -4.359282 -4.454927 1.727981
C -3.308282 -5.103005 1.078354
C -2.857825 -4.610519 -0.147302
H -5.708467 -0.641238 0.881846
H -5.787420 -2.845976 1.681600
H -4.711020 -4.815609 2.695022
H -2.838186 -5.979249 1.524005
H -2.013061 -5.085667 -0.650863
C -0.359884 0.607596 -1.759531
C 0.300212 0.665806 -3.012734
C 1.053334 1.789432 -3.365942
C 1.144041 2.868015 -2.482189
C 0.507125 2.823737 -1.240670
C -0.230274 1.695015 -0.881632
H 1.143779 0.002174 -5.621731
H 1.569781 1.825053 -4.323172

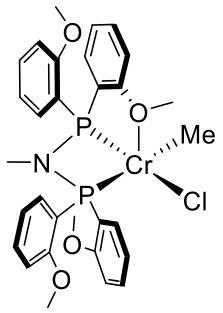
H 1.728609 3.743191 -2.767233
H 0.595275 3.658603 -0.545937
H -0.686664 1.644885 0.105576
C -1.614591 -0.890972 0.425415
C -1.226062 -1.924248 1.310231
C -1.774499 -1.997581 2.597731
C -2.709633 -1.046353 3.006615
C -3.110898 -0.023729 2.144746
C -2.566977 0.041801 0.860606
H -0.648733 -4.540940 1.950071
H -1.486600 -2.800952 3.272023
H -3.131642 -1.112429 4.009833
H -3.838891 0.719589 2.469688
H -2.891835 0.830148 0.182240
O -5.093129 -1.805646 -0.744128
C -6.098620 -1.048409 -0.064164
H -6.356107 -0.227399 -0.740723
H -6.997223 -1.654438 0.129617
O -2.597477 -1.768182 -4.978600
C -2.025951 -1.484160 -6.258213
O 0.154775 -0.433896 -3.813924
C 1.192254 -0.704630 -4.779427
H 2.179363 -0.657653 -4.299452
H 0.998100 -1.724386 -5.126274
O -0.334988 -2.815914 0.806173
C 0.164835 -3.868964 1.637076
H 0.881194 -4.402722 1.004934
H 0.679422 -3.461325 2.520325
Cl 1.793648 -3.170537 -1.538215
Cl -0.263121 -3.995258 -4.323487
H -1.230760 -0.761076 -6.060310
H -1.597726 -2.396923 -6.698280
H -2.764107 -1.037018 -6.942594

Spin state: quintet

E = -9947.59 kcal mol-1
H = -9589.67 kcal mol-1
TS = -72.25 kcal mol-1
G (298.15 K) = -9661.92 kcal mol-1

Cr -0.320314 -3.004590 -2.374172
P -2.756920 -2.758545 -2.339479
N -2.634659 -1.057660 -2.152126
P -1.157276 -0.960196 -1.286022
C -3.607170 -0.007799 -2.433840
H -3.076559 0.870756 -2.825640
H -4.189660 0.279772 -1.547813
H -4.303986 -0.368770 -3.200345
C -3.945740 -3.068216 -3.665641
C -5.132565 -3.787374 -3.481589
C -5.902029 -4.180089 -4.576943
C -5.468189 -3.869583 -5.867974
C -4.289108 -3.151053 -6.077179
C -3.534709 -2.729363 -4.975483
H -5.440488 -4.056646 -2.471487
H -6.823827 -4.740666 -4.424825
H -6.052232 -4.192126 -6.730671
H -3.963382 -2.925735 -7.090352
C -3.495302 -3.485798 -0.824601
C -4.543997 -2.897551 -0.086795
C -4.903980 -3.417015 1.163143
C -4.240375 -4.540176 1.662639
C -3.221227 -5.151556 0.932661
C -2.847680 -4.611261 -0.298571
H -5.732442 -0.738539 1.019718
H -5.690913 -2.953012 1.753402
H -4.527897 -4.934908 2.637648
H -2.712640 -6.033259 1.321291
H -2.025638 -5.054933 -0.865297
C -0.388939 0.627862 -1.705959
C 0.309830 0.668527 -2.937298
C 1.066849 1.795759 -3.276787
C 1.112447 2.887046 -2.407901
C 0.426676 2.860925 -1.191640
C -0.310343 1.729220 -0.842468
H 1.341271 -0.092570 -5.475167
H 1.618717 1.821638 -4.214457
H 1.700035 3.763203 -2.684217
H 0.479249 3.709413 -0.510104
H -0.806480 1.686118 0.126260
C -1.667863 -0.870989 0.470996
C -1.194798 -1.898026 1.325104
C -1.716813 -2.035733 2.619189
C -2.695969 -1.148640 3.066451
C -3.169259 -0.126677 2.240183
C -2.657143 -0.000113 0.947180
H -0.501788 -4.509130 1.819227
H -1.368259 -2.834552 3.270116
H -3.093821 -1.261762 4.075523
H -3.927313 0.568447 2.600899
H -3.036962 0.786206 0.295411
O -5.151972 -1.822570 -0.674036
C -6.150341 -1.123638 0.076572
H -6.464083 -0.287607 -0.556578
H -7.019278 -1.766502 0.285898
O -2.405792 -1.971689 -5.048035
C -1.692478 -1.939041 -6.291993
O 0.194385 -0.431575 -3.741073
C 1.318090 -0.752800 -4.595042
H 2.254176 -0.686937 -4.026432
H 1.163532 -1.793073 -4.900326
O -0.247406 -2.705997 0.787807
C 0.288851 -3.790280 1.554042
H 1.024157 -4.257507 0.891659
H 0.787031 -3.422327 2.463864
Cl 1.883252 -2.766858 -1.814710
Cl -0.243930 -4.570457 -4.026786
H -0.820314 -1.309753 -6.104478
H -1.369671 -2.952964 -6.568134
H -2.297866 -1.487823 -7.092883

Geometry:



Spin state: singlet

E = -10289.92 kcal mol-1
H = -9910.46 kcal mol-1
TS = -71.49 kcal mol-1
G (298.15 K) = -9981.95 kcal mol-1

Cr -0.184688 -3.041757 -1.887786
P -2.403538 -2.811507 -2.235285
N -2.405345 -1.097675 -2.308011
P -0.919124 -0.903830 -1.445091
C -3.375770 -0.112766 -2.766301
H -3.770379 0.485582 -1.931804
H -4.217140 -0.632983 -3.237256
H -2.910226 0.552711 -3.506830
C -3.478620 -3.363588 -3.619560
C -4.338852 -4.452453 -3.415913
C -5.108285 -4.984449 -4.450585
C -5.025060 -4.421433 -5.722938
C -4.180236 -3.335272 -5.959597
C -3.401217 -2.808021 -4.920383
H -4.408021 -4.887446 -2.419228
H -5.768446 -5.829987 -4.259780
H -5.618160 -4.824743 -6.544280
H -4.123548 -2.910101 -6.959419
C -3.305780 -3.423794 -0.748579
C -4.406505 -2.747442 -0.179199
C -4.934938 -3.166361 1.048868
C -4.396811 -4.282471 1.692398
C -3.333107 -4.983916 1.124807
C -2.789778 -4.545570 -0.084149
H -5.552969 -0.457933 0.655885
H -5.763138 -2.631167 1.508040
H -4.818537 -4.600013 2.646649
H -2.921759 -5.863083 1.620597
H -1.931468 -5.065141 -0.516249
C -0.397525 0.827245 -1.803922
C -0.051734 1.181199 -3.130162
C 0.478754 2.444989 -3.417690
C 0.688664 3.365146 -2.388012
C 0.384723 3.024740 -1.070742
C -0.147863 1.765073 -0.789582
H 0.094165 1.125065 -5.951556
H 0.729455 2.715488 -4.441500
H 1.099873 4.347331 -2.623203
H 0.563554 3.731799 -0.260864
H -0.357673 1.498026 0.244756
C -1.459858 -0.835419 0.310064
C -1.090605 -1.899957 1.158043
C -1.630392 -2.009807 2.443550
C -2.567477 -1.071818 2.881334
C -2.968794 -0.026360 2.048428
C -2.415885 0.082188 0.772401
H -0.534229 -4.501857 1.842758
H -1.353968 -2.835011 3.094121
H -2.992863 -1.173187 3.879891
H -3.704311 0.701628 2.391353
H -2.727903 0.895665 0.117482
O -4.902695 -1.695827 -0.900198
C -5.909370 -0.881084 -0.296586
H -6.099596 -0.072034 -1.009264
H -6.841040 -1.444588 -0.129892
O -2.554569 -1.747130 -5.084213
C -2.634843 -1.000900 -6.298194
O -0.261019 0.220819 -4.083105
C 0.485954 0.325984 -5.301409
H 1.550196 0.511659 -5.093882
H 0.377332 -0.643439 -5.796864
O -0.220879 -2.826339 0.621593
C 0.284991 -3.852469 1.503974
H 0.983245 -4.434872 0.899164
H 0.793736 -3.390342 2.361598
Cl 0.630895 -5.120494 -1.569355
C 0.389767 -2.845582 -3.803365
H -2.026344 -0.108552 -6.129708
H -2.231322 -1.567860 -7.152220
H -3.671825 -0.698499 -6.514272
H 1.379706 -2.352384 -3.748593
H -0.286297 -2.232661 -4.409403
H 0.502460 -3.843739 -4.250381

Spin state: triplet

E = -10290.71 kcal mol-1
H = -9912.11 kcal mol-1
TS = -71.95 kcal mol-1
G (298.15 K) = -9984.07 kcal mol-1

Cr -0.513326 -3.204672 -1.879710
P -2.824103 -2.909753 -1.941551
N -2.938200 -1.443746 -1.053318
P -1.252979 -1.250141 -0.787382
C -4.008151 -0.449625 -0.967658
H -4.781506 -0.762140 -0.251482
H -4.474544 -0.296003 -1.947486
H -3.580549 0.504474 -0.633184
C -3.506421 -2.755145 -3.641440
C -3.958748 -3.933359 -4.253459
C -4.322916 -3.967470 -5.600133
C -4.242448 -2.802169 -6.360615
C -3.790943 -1.613116 -5.780731
C -3.412387 -1.588517 -4.431921
H -4.020440 -4.845463 -3.658649
H -4.666812 -4.899494 -6.047966
H -4.528240 -2.808685 -7.412902
H -3.736424 -0.709637 -6.384711
C -4.044192 -4.037208 -1.158627
C -5.440208 -3.817857 -1.203669
C -6.313996 -4.722647 -0.588731

C -5.798197 -5.834337 0.086306
C -4.423667 -6.054772 0.153068
C -3.557868 -5.154205 -0.473021
H -7.761823 -2.331910 -1.082101
H -7.390809 -4.568176 -0.622520
H -6.488581 -6.530907 0.563540
H -4.026176 -6.920938 0.681005
H -2.478376 -5.312805 -0.441764
C -0.641948 0.072451 -1.903429
C -0.048341 -0.352079 -3.108069
C 0.521811 0.569903 -3.987806
C 0.482219 1.932696 -3.672595
C -0.117574 2.374948 -2.493233
C -0.671049 1.439080 -1.615521
H 0.257931 -1.792467 -5.435368
H 0.998427 0.249125 -4.910707
H 0.932722 2.647687 -4.361498
H -0.138020 3.436982 -2.249559
H -1.106964 1.764253 -0.669417
C -1.101266 -0.528820 0.876725
C 0.215871 -0.225555 1.299513
C 0.473483 0.125351 2.627926
C -0.583629 0.176797 3.542648
C -1.885756 -0.130232 3.144524
C -2.137851 -0.489179 1.817496
H 2.622243 -1.295026 1.460536
H 1.488304 0.351107 2.950838
H -0.379183 0.451903 4.577774
H -2.702714 -0.103230 3.865332
H -3.145811 -0.771461 1.517336
O -5.846573 -2.690945 -1.865501
C -7.247421 -2.474174 -2.045915
H -7.328255 -1.558757 -2.640450
H -7.713149 -3.308272 -2.593564
O -2.944972 -0.466231 -3.801587
C -2.857508 0.751015 -4.543768
O -0.067261 -1.721973 -3.368578
C 0.687389 -2.201441 -4.511181
H 1.744483 -1.927104 -4.401902
H 0.577599 -3.286718 -4.493716
O 1.162533 -0.319824 0.322463
C 2.532877 -0.502549 0.703669
H 3.045186 -0.822018 -0.208149
H 2.968757 0.436329 1.079499
Cl 1.630283 -3.464311 -1.170635
C -0.696779 -4.939554 -3.024738
H -2.449865 1.487681 -3.844946
H -2.170820 0.652241 -5.398572
H -3.848494 1.075809 -4.899274
H 0.320429 -5.271213 -3.290767
H -1.297750 -4.840155 -3.943481
H -1.153267 -5.746299 -2.424849

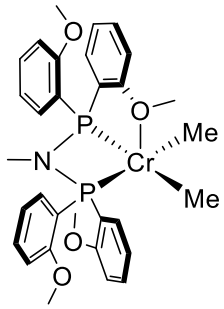
Spin state: quintet

E = -10310.37 kcal mol-1
H = -9931.80 kcal mol-1
TS = -74.70 kcal mol-1
G (298.15 K) = -10006.50 kcal mol-1

Cr -0.487012 -3.336601 -2.101454
P -2.882337 -2.929554 -2.246254
N -2.833522 -1.312970 -1.673013
P -1.231400 -1.181532 -1.068315
C -3.752329 -0.207719 -1.946587
H -4.199702 0.185949 -1.022548
H -4.558446 -0.561853 -2.597894
H -3.214247 0.602816 -2.458214
C -3.870054 -2.900865 -3.778427
C -4.957495 -3.758629 -3.981184
C -5.621751 -3.806778 -5.207808
C -5.194800 -2.986142 -6.251279
C -4.110349 -2.121681 -6.080103
C -3.442297 -2.079999 -4.849884
H -5.283139 -4.402344 -3.164198
H -6.464558 -4.483412 -5.345565
H -5.703875 -3.015121 -7.215178
H -3.787263 -1.493714 -6.907496
C -3.897742 -3.922868 -1.090814
C -5.123993 -3.485784 -0.543961
C -5.801908 -4.279360 0.389424
C -5.261937 -5.512132 0.770573
C -4.055370 -5.960537 0.235478
C -3.378379 -5.158355 -0.685432
H -6.752165 -1.630251 0.620426
H -6.745233 -3.951154 0.821318
H -5.797704 -6.122002 1.498812
H -3.636759 -6.919816 0.537434
H -2.423184 -5.484983 -1.102613
C -0.528053 0.321108 -1.837360
C 0.307163 0.155822 -2.965484
C 0.969990 1.260537 -3.517247
C 0.776378 2.529899 -2.965014
C -0.063478 2.710247 -1.865167
C -0.700143 1.601936 -1.303062
H 1.318259 -0.916698 -5.346762
H 1.636837 1.135999 -4.368116
H 1.296083 3.383308 -3.402003
H -0.207555 3.701778 -1.436536
H -1.324035 1.721070 -0.415854
C -1.416008 -0.749421 0.686324
C -0.207110 -0.597382 1.400794
C -0.215526 -0.485519 2.794179
C -1.438835 -0.521579 3.473064
C -2.640081 -0.684742 2.779254
C -2.625011 -0.809235 1.386591
H 2.051179 -1.875501 1.806132
H 0.716987 -0.378130 3.345930
H -1.445935 -0.432269 4.559833
H -3.584083 -0.732016 3.321933
H -3.549444 -0.994685 0.837818
O -5.574028 -2.273535 -0.992597
C -6.806573 -1.771275 -0.470600
H -6.957825 -0.801948 -0.955973
H -7.648075 -2.438202 -0.714690
O -2.372704 -1.274040 -4.584122
C -1.890386 -0.421603 -5.626326
O 0.398866 -1.110477 -3.469370
C 1.465001 -1.423983 -4.380484
H 2.436601 -1.152596 -3.945408

H 1.417769 -2.508416 -4.514219
O 0.907455 -0.590578 0.614171
C 2.164797 -0.967283 1.197338
H 2.820757 -1.186938 0.350393
H 2.578429 -0.147976 1.805527
Cl 1.689313 -3.479201 -1.411359
C -0.517660 -4.782769 -3.600757
H -1.078288 0.157825 -5.179566
H -1.507692 -1.008718 -6.475463
H -2.677248 0.265309 -5.975028
H 0.517449 -5.075367 -3.836358
H -0.994422 -4.378732 -4.511394
H -1.069770 -5.696205 -3.321959

Geometry:



Spin state: singlet

E = -10644.82 kcal mol-1
H = -10245.07 kcal mol-1
TS = -71.99 kcal mol-1
G (298.15 K) = -10317.07 kcal mol-1

Cr -0.293947 -3.233529 -1.884362
P -2.495863 -2.858065 -2.221685
N -2.402154 -1.148344 -2.306126
P -0.902711 -1.016361 -1.443865
C -3.305791 -0.118191 -2.799556
H -3.655029 0.534715 -1.985650
H -4.182478 -0.597191 -3.250101
H -2.802078 0.490378 -3.564006
C -3.603263 -3.347409 -3.606593
C -4.553757 -4.358041 -3.403631
C -5.335010 -4.852826 -4.448639
C -5.170835 -4.332013 -5.731142
C -4.237031 -3.320424 -5.967114
C -3.450104 -2.829477 -4.916284
H -4.683923 -4.761956 -2.399739
H -6.066342 -5.638106 -4.258464
H -5.770041 -4.709057 -6.560593
H -4.119404 -2.925783 -6.974288
C -3.450936 -3.404071 -0.738622
C -4.498876 -2.651683 -0.164842
C -5.061941 -3.041206 1.058019
C -4.612212 -4.199360 1.695154
C -3.601909 -4.973850 1.124649
C -3.026406 -4.566251 -0.079898
H -5.490323 -0.296863 0.689198
H -5.850503 -2.449925 1.518340
H -5.062065 -4.492703 2.644291
H -3.260902 -5.886715 1.613222
H -2.216889 -5.145358 -0.525021
C -0.353110 0.711781 -1.785707
C 0.058304 1.027914 -3.103235
C 0.637975 2.267438 -3.397285
C 0.834052 3.204783 -2.379334
C 0.467939 2.901356 -1.068797
C -0.114351 1.664467 -0.782406
H 0.346309 0.883999 -5.912718
H 0.940536 2.505797 -4.415260
H 1.285001 4.168576 -2.617766
H 0.637242 3.620209 -0.267028
H -0.368053 1.426839 0.249223
C -1.439434 -0.964770 0.314447
C -1.107985 -2.070402 1.123908
C -1.636587 -2.207318 2.409506
C -2.530645 -1.247672 2.891939
C -2.901637 -0.162747 2.097079
C -2.358785 -0.031420 0.818456
H -0.585165 -4.744918 1.700697
H -1.394098 -3.068970 3.025842
H -2.952326 -1.369151 3.889712
H -3.609701 0.577253 2.470964
H -2.657164 0.807488 0.189787
O -4.913713 -1.559333 -0.875863
C -5.867030 -0.685296 -0.270271
H -5.997113 0.142121 -0.975314
H -6.835745 -1.186304 -0.115277
O -2.520511 -1.840253 -5.073859
C -2.480709 -1.142970 -6.317368
O -0.132781 0.045973 -4.041221
C 0.681382 0.095772 -5.218866
H 1.737281 0.263326 -4.958861
H 0.575616 -0.885566 -5.691601
O -0.285064 -3.024160 0.541344
C 0.224389 -4.064932 1.399244
H 0.958655 -4.610762 0.803800
H 0.705000 -3.623909 2.283558
C 0.209458 -5.221598 -1.658763
C 0.330190 -3.161273 -3.796664
H -1.797335 -0.305186 -6.156610
H -2.098424 -1.781153 -7.129981
H -3.474628 -0.754052 -6.590927
H 1.381714 -2.815390 -3.714896
H -0.230978 -2.436274 -4.399064
H 0.311438 -4.143470 -4.292140
H 1.317831 -5.214002 -1.560699
H -0.025736 -5.814788 -2.554845
H -0.186336 -5.766467 -0.784341

Spin state: triplet

E = -10654.97 kcal mol-1
H = -10255.31 kcal mol-1
TS = -71.97 kcal mol-1
G (298.15 K) = -10327.29 kcal mol-1

Cr -0.148152 -3.116503 -1.832054
P -2.552629 -2.928886 -2.260782

N -2.444244 -1.203410 -2.325196
P -0.993928 -1.059080 -1.424092
C -3.338641 -0.164740 -2.823685
H -2.834259 0.425805 -3.601717
H -3.666731 0.502351 -2.012773
H -4.228300 -0.636518 -3.255234
C -3.730961 -3.335262 -3.620919
C -4.748087 -4.277694 -3.404080
C -5.581872 -4.713577 -4.434693
C -5.410315 -4.200571 -5.719469
C -4.412458 -3.255161 -5.969680
C -3.572286 -2.826070 -4.933797
H -4.891343 -4.673827 -2.398814
H -6.363694 -5.444935 -4.229845
H -6.051419 -4.531049 -6.537267
H -4.288623 -2.862367 -6.976982
C -3.513227 -3.446524 -0.775067
C -4.534871 -2.677627 -0.173707
C -5.098938 -3.078405 1.044857
C -4.679994 -4.263962 1.652157
C -3.696419 -5.054503 1.056666
C -3.119415 -4.633048 -0.142512
H -5.434104 -0.313250 0.745217
H -5.865772 -2.474950 1.525636
H -5.132441 -4.566920 2.596906
H -3.380382 -5.988640 1.521538
H -2.330724 -5.228645 -0.608168
C -0.353850 0.611143 -1.805229
C 0.088019 0.854949 -3.129703
C 0.762663 2.037250 -3.451539
C 1.007687 2.991284 -2.459610
C 0.598925 2.760194 -1.145419
C -0.066040 1.575694 -0.825944
H 0.387909 0.617830 -5.916199
H 1.099385 2.218267 -4.470728
H 1.530566 3.912051 -2.719832
H 0.806086 3.493381 -0.365989
H -0.342554 1.383745 0.209482
C -1.504425 -1.022160 0.329807
C -1.231720 -2.166193 1.111454
C -1.731213 -2.293929 2.406822
C -2.550012 -1.287263 2.930816
C -2.879159 -0.172037 2.159121
C -2.362449 -0.047752 0.868560
H -0.878401 -4.860174 1.640873
H -1.522064 -3.179828 3.000971
H -2.945792 -1.395279 3.940504
H -3.531396 0.602784 2.562882
H -2.628818 0.817457 0.261238
O -4.923733 -1.558517 -0.855484
C -5.838154 -0.666395 -0.216820
H -5.949132 0.180743 -0.901383
H -6.821600 -1.137116 -0.059431
O -2.580801 -1.898017 -5.109346
C -2.567290 -1.155586 -6.327610
O -0.175531 -0.138572 -4.033675
C 0.636794 -0.193004 -5.211767
H 1.704609 -0.137876 -4.953028
H 0.422861 -1.162564 -5.670201
O -0.492927 -3.156442 0.486462
C -0.028125 -4.260728 1.286815
H 0.607352 -4.855743 0.625712
H 0.566513 -3.894682 2.135128
C 1.840897 -3.332124 -1.303542
C 0.300035 -3.326576 -3.800486
H -1.847466 -0.348441 -6.168995
H -2.245403 -1.775171 -7.180086
H -3.557206 -0.721898 -6.541883
H 1.257225 -2.849008 -4.055202
H -0.480490 -3.012148 -4.504977
H 0.427243 -4.425595 -3.886108
H 2.513909 -2.790915 -1.984539
H 2.070011 -4.413801 -1.418147
H 2.091068 -3.040454 -0.271004

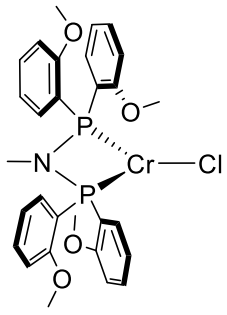
Spin state: quintet

E = -10665.25 kcal mol-1
H = -10265.71 kcal mol-1
TS = -76.14 kcal mol-1
G (298.15 K) = -10341.85 kcal mol-1

Cr -0.138266 -3.112396 -2.280366
P -2.639434 -2.870892 -2.375280
N -2.548393 -1.159964 -2.212878
P -1.079692 -0.995545 -1.339119
C -3.529737 -0.128466 -2.527425
H -3.022775 0.707428 -3.030001
H -4.051332 0.244606 -1.634786
H -4.282551 -0.545414 -3.207078
C -3.877092 -3.141567 -3.687051
C -5.027546 -3.915564 -3.495104
C -5.898263 -4.190316 -4.551467
C -5.620512 -3.682020 -5.820464
C -4.477820 -2.907575 -6.043446
C -3.602256 -2.642592 -4.983682
H -5.241142 -4.306159 -2.500081
H -6.788863 -4.794716 -4.381101
H -6.293593 -3.888012 -6.653253
H -4.272501 -2.525255 -7.041265
C -3.436520 -3.558447 -0.862848
C -4.499796 -2.946947 -0.163991
C -4.907511 -3.445926 1.080113
C -4.281099 -4.575008 1.613004
C -3.249499 -5.210145 0.921928
C -2.825557 -4.687031 -0.301377
H -5.683917 -0.757593 0.883367
H -5.705053 -2.962196 1.639713
H -4.607740 -4.955051 2.581644
H -2.769426 -6.097030 1.335166
H -1.988206 -5.142880 -0.834156
C -0.407609 0.645192 -1.750337
C 0.198847 0.748945 -3.025784
C 0.940936 1.882039 -3.372432
C 1.071599 2.928979 -2.456314
C 0.481885 2.843307 -1.193824
C -0.244308 1.703372 -0.844208
H 1.066252 0.065860 -5.646184
H 1.415855 1.948899 -4.349785
H 1.647588 3.812527 -2.733236

H 0.598867 3.654876 -0.475853
H -0.665120 1.619647 0.157024
C -1.630306 -0.884900 0.412651
C -1.205182 -1.913600 1.289685
C -1.773286 -2.035896 2.565398
C -2.749216 -1.128796 2.979057
C -3.169814 -0.098781 2.135756
C -2.611938 0.010120 0.860253
H -0.686285 -4.521066 1.828263
H -1.463834 -2.837212 3.232561
H -3.182107 -1.231658 3.974661
H -3.923103 0.615317 2.468955
H -2.948129 0.805352 0.195312
O -5.076797 -1.871843 -0.780472
C -6.082101 -1.147816 -0.066375
H -6.363110 -0.313963 -0.717684
H -6.968212 -1.772480 0.126853
O -2.459544 -1.902350 -5.093055
C -2.167017 -1.285323 -6.347519
O 0.008571 -0.318087 -3.863819
C 1.064559 -0.628477 -4.791301
H 2.038999 -0.610922 -4.284708
H 0.857398 -1.646484 -5.137095
O -0.245512 -2.749816 0.801725
C 0.169214 -3.871423 1.589591
H 0.880993 -4.412691 0.958856
H 0.666031 -3.543937 2.515946
C 1.888558 -2.650506 -2.057985
C 0.059536 -5.022123 -3.105463
H -1.278572 -0.674653 -6.168244
H -1.955389 -2.035810 -7.125532
H -2.994717 -0.636820 -6.675851
H 1.115314 -5.264642 -3.308856
H -0.501523 -5.116147 -4.052202
H -0.330381 -5.803537 -2.426165
H 2.085139 -1.574998 -1.902874
H 2.463599 -2.984670 -2.938466
H 2.296147 -3.188142 -1.183244

Geometry:



Spin state: doublet

E = -9830.80 kcal mol-1
H = -9475.55 kcal mol-1
TS = -68.15 kcal mol-1
G (298.15 K) = -9543.70 kcal mol-1

Cr -0.867168 -3.011896 -1.877217
P -3.030767 -2.764547 -1.802655
N -3.185357 -1.106564 -1.305161
P -1.459616 -0.960766 -1.420579
C -4.300700 -0.167995 -1.245720
H -3.906374 0.850687 -1.134726
H -4.950111 -0.396286 -0.390254
H -4.899500 -0.196562 -2.172528
C -3.550289 -2.693292 -3.572436
C -4.854124 -2.461027 -4.029605
C -5.105394 -2.178702 -5.374415
C -4.040818 -2.123681 -6.275007
C -2.728361 -2.351704 -5.846135
C -2.493945 -2.638101 -4.501174
H -5.677527 -2.509295 -3.315609
H -6.125068 -2.001493 -5.716668
H -4.222877 -1.902363 -7.326835
H -1.912723 -2.301752 -6.563040
C -4.423784 -3.699108 -1.029424
C -5.016556 -3.423052 0.222447
C -6.030558 -4.245976 0.725867
C -6.453556 -5.368493 0.016061
C -5.851433 -5.680060 -1.206491
C -4.851495 -4.854026 -1.713112
H -2.627509 -2.828793 0.942110
H -6.471684 -3.980574 1.686843
H -7.242488 -6.002980 0.420880
H -6.161718 -6.562354 -1.766635
H -4.390284 -5.096293 -2.672125
C -1.192701 0.483296 -2.513533
C 0.030216 1.199455 -2.524953
C 0.287365 2.144160 -3.526464
C -0.649784 2.358968 -4.542375
C -1.842654 1.636597 -4.567701
C -2.104038 0.709799 -3.557368
H 2.755624 1.380230 -2.404531
H 1.218379 2.707589 -3.529596
H -0.434739 3.094300 -5.318454
H -2.568966 1.790930 -5.365254
H -3.025520 0.129050 -3.590431
C -0.848724 -0.572225 0.243176
C -0.242058 -1.650887 0.916559
C 0.175860 -1.515849 2.242032
C -0.015338 -0.294044 2.898670
C -0.616263 0.784165 2.245665
C -1.029784 0.637393 0.921058
H -0.215766 -4.227107 1.759260
H 0.645157 -2.339062 2.774336
H 0.312118 -0.194521 3.933734
H -0.759204 1.731696 2.765210
H -1.493505 1.471437 0.391945
O -4.667601 -2.319590 0.983180
C -3.388568 -2.437695 1.633682
H -3.094751 -1.431489 1.949801
H -3.465473 -3.105171 2.507933
O -1.215623 -2.880191 -3.992455
C -0.087318 -2.513199 -4.830145
O 0.913100 0.885522 -1.529241
C 2.168392 1.567092 -1.491202
H 2.033121 2.652302 -1.356883
H 2.698261 1.156563 -0.626320

O -0.105731 -2.839372 0.193758
C 0.434844 -3.983335 0.908301
H 0.456540 -4.796274 0.179408
H 1.456656 -3.766673 1.246217
Cl 0.692681 -4.643062 -2.319444
H -0.155974 -1.446435 -5.084812
H 0.799329 -2.719753 -4.226462
H -0.065892 -3.138866 -5.731501

Spin state: quartet

E = -9836.13 kcal mol-1
H = -9481.56 kcal mol-1
TS = -68.71 kcal mol-1
G (298.15 K) = -9550.27 kcal mol-1

Cr -0.672169 -3.192466 -1.990645
P -2.918588 -2.690122 -2.087929
N -2.743937 -0.992760 -1.716344
P -1.123716 -1.119514 -1.144473
C -3.535937 0.193877 -2.046589
H -4.064816 0.595557 -1.169783
H -4.277524 -0.077706 -2.807813
H -2.884817 0.978433 -2.456415
C -3.664385 -2.720431 -3.752405
C -5.038888 -2.606546 -4.017373
C -5.538142 -2.708002 -5.317385
C -4.660864 -2.929400 -6.378988
C -3.285904 -3.060524 -6.146522
C -2.788184 -2.957014 -4.845030
H -5.721446 -2.435884 -3.186817
H -6.609183 -2.614735 -5.498040
H -5.038441 -3.008131 -7.398742
H -2.614257 -3.246358 -6.982107
C -4.108550 -3.413457 -0.904773
C -5.278137 -2.772451 -0.438014
C -6.057267 -3.355922 0.567691
C -5.677818 -4.583822 1.117746
C -4.525525 -5.231938 0.671993
C -3.754203 -4.643196 -0.329817
H -6.587393 -0.596813 0.534747
H -6.958768 -2.863927 0.927524
H -6.292882 -5.029610 1.899987
H -4.224704 -6.186095 1.103438
H -2.843383 -5.134286 -0.679592
C -0.379795 0.478296 -1.621227
C -0.255331 0.758410 -3.003506
C 0.356343 1.938515 -3.437488
C 0.854005 2.845153 -2.494426
C 0.736094 2.584871 -1.128659
C 0.119221 1.407545 -0.700800
H -1.381478 1.049876 -5.411715
H 0.453688 2.155444 -4.499546
H 1.334151 3.761635 -2.838569
H 1.117440 3.297111 -0.397101
H 0.016699 1.204458 0.365183
C -1.175406 -1.093477 0.682456
C 0.017728 -1.335168 1.399170
C -0.015480 -1.506214 2.787832
C -1.241959 -1.437886 3.458079
C -2.428229 -1.205988 2.760383
C -2.389515 -1.040028 1.373626
H 2.252270 -2.808456 1.697217
H 0.898291 -1.697710 3.347391
H -1.263011 -1.577825 4.539407
H -3.380181 -1.170295 3.289570
H -3.310674 -0.901639 0.805858
O -5.575861 -1.567145 -1.025682
C -6.697279 -0.829437 -0.536323
H -6.709727 0.101666 -1.112028
H -7.641717 -1.372413 -0.698854
O -1.451842 -3.078307 -4.539771
C -0.548400 -3.552670 -5.553588
O -0.781752 -0.192635 -3.835951
C -0.864670 0.093996 -5.232646
H 0.133169 0.121213 -5.698101
H -1.454816 -0.720057 -5.663977
O 1.146396 -1.383821 0.630722
C 2.369425 -1.815825 1.236116
H 3.093324 -1.877054 0.418467
H 2.719794 -1.092871 1.989982
Cl 1.150262 -4.424068 -2.392359
H -0.432885 -2.809522 -6.357533
H 0.405079 -3.704303 -5.037773
H -0.899310 -4.506758 -5.972781

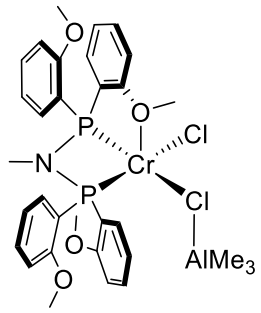
Spin state: sextet

E = -9838.51 kcal mol-1
H = -9482.11 kcal mol-1
TS = -68.84 kcal mol-1
G (298.15 K) = -9550.95 kcal mol-1

Cr -0.207684 -2.957966 -2.155806
P -2.632439 -2.823037 -2.263718
N -2.558995 -1.099918 -2.183478
P -1.121511 -0.906077 -1.250587
C -3.531700 -0.087660 -2.589768
H -3.007171 0.739381 -3.087983
H -4.106961 0.305941 -1.739471
H -4.237868 -0.537092 -3.298626
C -3.788460 -3.138916 -3.629073
C -5.006732 -3.813126 -3.469518
C -5.803970 -4.128077 -4.570961
C -5.383523 -3.767920 -5.852558
C -4.171110 -3.094198 -6.042368
C -3.374502 -2.780882 -4.936545
H -5.326584 -4.095701 -2.466679
H -6.749320 -4.651095 -4.427647
H -5.998066 -4.010940 -6.719749
H -3.856920 -2.823064 -7.048242
C -3.444242 -3.487919 -0.763313
C -4.538404 -2.864939 -0.119841
C -4.980279 -3.320520 1.127727
C -4.354492 -4.414193 1.731006
C -3.286069 -5.055923 1.101047
C -2.835484 -4.582064 -0.130648
H -5.779105 -0.650982 0.799410
H -5.804351 -2.827368 1.638533
H -4.707116 -4.759061 2.703235

H -2.802884 -5.914050 1.568080
H -1.978221 -5.054645 -0.616326
C -0.511607 0.749728 -1.680757
C 0.210909 0.845733 -2.899199
C 0.848374 2.036388 -3.256544
C 0.771897 3.147149 -2.409214
C 0.076547 3.067038 -1.200407
C -0.553281 1.875421 -0.840965
H 1.254639 0.133219 -5.463474
H 1.402522 2.102966 -4.191325
H 1.266886 4.074773 -2.697581
H 0.031202 3.927926 -0.533447
H -1.062091 1.805806 0.119522
C -1.664676 -0.864546 0.487719
C -1.173244 -1.872026 1.357330
C -1.710690 -2.026934 2.638861
C -2.738588 -1.182685 3.069878
C -3.241565 -0.189839 2.227255
C -2.710347 -0.043933 0.945252
H -0.548537 -4.459107 1.868705
H -1.344095 -2.808424 3.300397
H -3.149485 -1.313149 4.071164
H -4.044178 0.465866 2.565522
H -3.122749 0.712066 0.277247
O -5.108854 -1.822349 -0.799618
C -6.142346 -1.081665 -0.147076
H -6.410611 -0.277047 -0.839188
H -7.028516 -1.707259 0.043670
O -2.176166 -2.125244 -5.002252
C -1.687981 -1.729419 -6.285547
O 0.246381 -0.292799 -3.666050
C 1.369705 -0.469429 -4.548788
H 2.308016 -0.201778 -4.042802
H 1.389214 -1.537350 -4.790630
O -0.182509 -2.667765 0.847030
C 0.281434 -3.778159 1.626147
H 1.010025 -4.290351 0.989780
H 0.772008 -3.437281 2.550754
Cl 1.746948 -3.843979 -2.835630
H -2.388612 -1.039763 -6.782517
H -0.746140 -1.211722 -6.089338
H -1.505175 -2.601685 -6.932250

Geometry:



Spin state: singlet

E = -11405.11 kcal mol-1
H = -10975.30 kcal mol-1
TS = -80.87 kcal mol-1
G (298.15 K) = -11056.17 kcal mol-1

Cr -0.503164 -2.990373 -2.167992
P -2.820622 -2.731923 -2.551768
N -2.875039 -1.061144 -2.199170
P -1.241867 -0.877695 -1.764788
C -4.020046 -0.157189 -2.130936
H -3.678678 0.833725 -1.806847
H -4.761470 -0.523959 -1.410159
H -4.493234 -0.059550 -3.119973
C -3.951358 -2.828977 -3.992331
C -5.151310 -3.549910 -4.002617
C -5.926166 -3.651231 -5.159756
C -5.503280 -3.017733 -6.326907
C -4.322183 -2.270516 -6.341629
C -3.549344 -2.171033 -5.180215
H -5.479315 -4.048915 -3.091797
H -6.851788 -4.226037 -5.146545
H -6.093660 -3.097469 -7.240146
H -4.008741 -1.779372 -7.260344
C -3.664110 -3.765235 -1.282931
C -4.068348 -3.323521 -0.002179
C -4.485600 -4.250843 0.963341
C -4.503336 -5.615500 0.665429
C -4.105822 -6.068659 -0.591820
C -3.685032 -5.143918 -1.547668
H -3.586000 -1.970479 2.281773
H -4.801744 -3.912668 1.948011
H -4.829447 -6.323368 1.428129
H -4.107799 -7.132078 -0.827268
H -3.335265 -5.499470 -2.517167
C -0.704394 0.683896 -2.529915
C 0.600825 1.150264 -2.235231
C 1.161186 2.197857 -2.976742
C 0.426523 2.782442 -4.011751
C -0.855729 2.325118 -4.321729
C -1.409946 1.275404 -3.586519
H 3.130450 0.382269 -2.083162
H 2.165709 2.551992 -2.752826
H 0.868983 3.597925 -4.584784
H -1.419489 2.774422 -5.139020
H -2.384279 0.878133 -3.862644
C -1.127536 -0.674481 0.038051
C -0.953610 -1.861098 0.777799
C -0.788083 -1.807433 2.164055
C -0.838383 -0.569311 2.813374
C -1.047899 0.609437 2.096921
C -1.180987 0.548919 0.708254
H -1.576379 -4.287381 1.639273
H -0.605847 -2.709170 2.742641
H -0.701560 -0.535222 3.894505
H -1.081244 1.569556 2.611334
H -1.299123 1.463394 0.124845
O -4.013827 -1.977602 0.230391
C -4.258254 -1.493047 1.553489
H -4.030881 -0.423220 1.515156
H -5.307455 -1.644484 1.851956
O -2.389046 -1.452872 -5.094145
C -1.876358 -0.839469 -6.280995

O 1.227364 0.500127 -1.221327
C 2.655119 0.588768 -1.113488
H 2.963665 1.577330 -0.739463
H 2.934991 -0.193711 -0.403243
O -0.983408 -3.048363 0.063179
C -0.855763 -4.282299 0.812185
H -1.108043 -5.079005 0.111535
H 0.177291 -4.396213 1.164450
Cl 1.664851 -2.784989 -1.423589
Cl -0.425253 -5.455387 -2.273284
H -0.943988 -0.354289 -5.977844
H -1.671935 -1.590150 -7.059994
H -2.572733 -0.080490 -6.670839
Al -0.192921 -4.857431 -4.470802
C 0.325011 -2.872149 -4.312593
C -1.896435 -5.225942 -5.408693
C 1.423386 -5.769129 -5.140946
H -2.052718 -4.535637 -6.254143
H -2.796201 -5.146137 -4.783000
H -1.881490 -6.244186 -5.829039
H 2.284792 -5.584243 -4.481412
H 1.697717 -5.417437 -6.149249
H 1.281368 -6.859227 -5.206813
H 1.416586 -2.953316 -4.400422
H 0.141043 -1.930025 -3.750427
H -0.116315 -2.621826 -5.290765

Spin state: triplet

E = -11402.08 kcal mol-1
H = -10971.20 kcal mol-1
TS = -83.14 kcal mol-1
G (298.15 K) = -11054.33 kcal mol-1

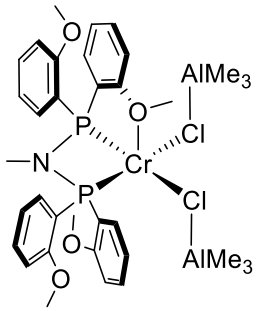
Cr -0.304693 -2.918192 -2.347602
P -2.719939 -2.744810 -2.512266
N -2.780274 -1.162211 -1.901152
P -1.144954 -0.874537 -1.496252
C -3.911087 -0.242527 -1.948827
H -4.063634 0.235640 -0.971383
H -4.818256 -0.806663 -2.189760
H -3.755810 0.527966 -2.718398
C -3.675714 -2.687840 -4.073306
C -4.792312 -3.498978 -4.317057
C -5.413791 -3.525546 -5.565800
C -4.915448 -2.730188 -6.596000
C -3.816425 -1.895205 -6.379865
C -3.200539 -1.862363 -5.123062
H -5.172745 -4.130898 -3.516180
H -6.275381 -4.171433 -5.731074
H -5.383140 -2.749295 -7.580711
H -3.448263 -1.273517 -7.192747
C -3.713012 -3.875217 -1.455260
C -4.409566 -3.514126 -0.279129
C -4.955880 -4.509380 0.544454
C -4.837978 -5.856384 0.199734
C -4.172075 -6.227727 -0.967711
C -3.610289 -5.239209 -1.774231
H -4.084587 -2.301019 2.051809
H -5.482465 -4.233193 1.455837
H -5.270037 -6.615164 0.852978
H -4.068030 -7.276508 -1.242537
H -3.055845 -5.532982 -2.663758
C -0.777402 0.774063 -2.221566
C 0.256947 0.903893 -3.177446
C 0.535010 2.153237 -3.754391
C -0.228136 3.267271 -3.403103
C -1.264989 3.154473 -2.476171
C -1.524866 1.914054 -1.890908
H 1.956109 0.098381 -5.293379
H 1.337776 2.252685 -4.482444
H -0.006681 4.231349 -3.862237
H -1.859376 4.024631 -2.199448
H -2.311577 1.836807 -1.141319
C -1.029846 -0.580507 0.310095
C -1.228118 -1.703832 1.156673
C -1.012104 -1.601205 2.535661
C -0.596248 -0.387207 3.086497
C -0.373725 0.720133 2.269544
C -0.578471 0.612160 0.892613
H -2.287358 -4.090282 2.105786
H -1.151500 -2.467479 3.178734
H -0.429771 -0.318968 4.162030
H -0.025610 1.660746 2.695265
H -0.359577 1.468007 0.257073
O -4.523162 -2.181956 0.009198
C -4.784589 -1.803926 1.362668
H -4.617600 -0.722522 1.404932
H -5.821847 -2.023721 1.660548
O -2.144538 -1.048060 -4.817207
C -1.537313 -0.309577 -5.883180
O 0.910765 -0.237770 -3.505277
C 2.137649 -0.174402 -4.241626
H 2.835383 0.540019 -3.781246
H 2.552413 -1.184263 -4.176825
O -1.624396 -2.853211 0.542342
C -1.568505 -4.089315 1.272773
H -1.849017 -4.860771 0.551252
H -0.549570 -4.272997 1.640969
Cl 1.822400 -2.583653 -1.632574
Cl -0.330918 -5.305074 -1.740564
H -0.698799 0.222125 -5.428776
H -1.166151 -0.985313 -6.668579
H -2.239983 0.419601 -6.314429
Al -0.050457 -5.324673 -4.040438
C 0.250346 -3.344841 -4.568081
C -1.735063 -5.980208 -4.853953
C 1.640191 -6.277835 -4.375882
H -1.551053 -6.225015 -5.913679
H -2.550298 -5.239842 -4.844925
H -2.112475 -6.902146 -4.384011
H 2.453630 -5.831739 -3.783395
H 1.934325 -6.224529 -5.436709
H 1.580925 -7.343921 -4.108040
H 1.331632 -3.234603 -4.728259
H -0.138304 -2.344065 -4.243895
H -0.237821 -3.435842 -5.556717

Spin state: quintet

E = -11427.08 kcal mol-1
H = -10996.61 kcal mol-1
TS = -85.66 kcal mol-1
G (298.15 K) = -11082.27 kcal mol-1

Cr -0.317493 -2.915084 -2.058867
P -2.763933 -2.723017 -2.444706
N -2.836840 -1.120108 -1.880513
P -1.222787 -0.741741 -1.471287
C -4.013155 -0.254788 -1.839129
H -4.089867 0.236803 -0.858998
H -4.913530 -0.861679 -1.981630
H -3.966934 0.504435 -2.633177
C -3.715980 -2.683847 -3.994149
C -4.946096 -3.325426 -4.174618
C -5.592647 -3.297863 -5.410722
C -5.002455 -2.620530 -6.477654
C -3.780588 -1.961406 -6.321432
C -3.135915 -1.985764 -5.079952
H -5.388114 -3.869894 -3.340710
H -6.544946 -3.810644 -5.540346
H -5.492954 -2.602602 -7.451277
H -3.336311 -1.441281 -7.167052
C -3.700475 -3.870491 -1.371266
C -4.311614 -3.552504 -0.138338
C -4.792046 -4.580902 0.685467
C -4.683685 -5.913802 0.283705
C -4.095840 -6.240039 -0.938580
C -3.600163 -5.220174 -1.749077
H -3.985175 -2.399087 2.239602
H -5.258703 -4.345222 1.639791
H -5.063198 -6.699571 0.937546
H -4.001052 -7.278532 -1.252826
H -3.098383 -5.472030 -2.684538
C -0.839075 0.842434 -2.284976
C 0.264826 0.869122 -3.172105
C 0.599224 2.056058 -3.840841
C -0.172635 3.202371 -3.646033
C -1.274721 3.186936 -2.788975
C -1.597356 2.009360 -2.112438
H 2.143718 -0.139438 -5.035537
H 1.452373 2.081627 -4.515993
H 0.093977 4.118884 -4.173519
H -1.874319 4.084528 -2.641598
H -2.445258 2.002916 -1.428315
C -1.176866 -0.424060 0.324895
C -1.241086 -1.579797 1.146044
C -1.088567 -1.475221 2.531311
C -0.886134 -0.219789 3.110199
C -0.815411 0.926346 2.318609
C -0.946987 0.815965 0.932260
H -1.966242 -4.135667 1.997916
H -1.111119 -2.365546 3.156353
H -0.767241 -0.145970 4.191619
H -0.637039 1.900358 2.773130
H -0.840601 1.704526 0.311720
O -4.401006 -2.228443 0.194296
C -4.680834 -1.889849 1.554819
H -4.521819 -0.809114 1.627764
H -5.719653 -2.128391 1.831701
O -1.945967 -1.370536 -4.816893
C -1.231110 -0.786688 -5.914936
O 0.922695 -0.305948 -3.334138
C 2.218511 -0.321689 -3.952243
H 2.879464 0.422572 -3.485420
H 2.599954 -1.329552 -3.770170
O -1.458271 -2.760047 0.494211
C -1.237080 -4.004709 1.185402
H -1.392532 -4.780697 0.429486
H -0.207315 -4.050577 1.564419
Cl 1.706410 -2.582543 -1.086374
Cl -0.218954 -5.284292 -2.249364
H -0.282036 -0.450963 -5.492766
H -1.037919 -1.534601 -6.697021
H -1.780927 0.071388 -6.329948
Al 0.007648 -5.336967 -4.634403
C 0.808049 -3.523892 -4.921500
C -1.861195 -5.597355 -5.262684
C 1.249208 -6.851216 -4.919954
H -1.881064 -5.735596 -6.357267
H -2.539143 -4.759702 -5.044624
H -2.310879 -6.506533 -4.830088
H 2.209818 -6.693493 -4.405021
H 1.475189 -6.988978 -5.990954
H 0.835953 -7.805314 -4.556258
H 1.820774 -3.481958 -4.491500
H 0.234395 -2.681005 -4.493506
H 0.902852 -3.299437 -5.998371

Geometry:



Spin state: singlet

E = -12878.20 kcal mol-1
H = -12375.87 kcal mol-1
TS = -95.68 kcal mol-1
G (298.15 K) = -12471.55 kcal mol-1

Cr -0.543194 -3.111934 -1.909656
P -2.741606 -2.702056 -2.487419
N -2.802203 -1.088745 -1.948181
P -1.182605 -0.944993 -1.424531
C -3.934917 -0.173706 -1.987981
H -4.055394 0.330996 -1.018675
H -4.847378 -0.751407 -2.176884
H -3.821451 0.571715 -2.789049
C -3.587636 -2.563366 -4.108905
C -4.742200 -3.272463 -4.461112
C -5.288363 -3.179065 -5.742601

C -4.675444 -2.363677 -6.692326
C -3.539158 -1.619530 -6.362694
C -2.999220 -1.706900 -5.075193
H -5.216603 -3.917179 -3.722538
H -6.182294 -3.747810 -5.996187
H -5.082377 -2.294271 -7.701355
H -3.080977 -0.976657 -7.111407
C -3.820795 -3.797940 -1.490356
C -4.396877 -3.452478 -0.244756
C -5.037925 -4.434745 0.524752
C -5.097000 -5.754855 0.073518
C -4.520190 -6.113354 -1.144686
C -3.883976 -5.136936 -1.909923
H -4.161715 -2.444201 2.229904
H -5.492727 -4.173572 1.478034
H -5.595178 -6.505533 0.687777
H -4.551131 -7.144546 -1.493931
H -3.398786 -5.420275 -2.844751
C -0.585566 0.679934 -2.017499
C 0.710859 0.757187 -2.586509
C 1.188267 1.976499 -3.089492
C 0.386573 3.116305 -3.025498
C -0.887707 3.060386 -2.460228
C -1.361862 1.845960 -1.960712
H 2.793161 -0.165736 -4.171970
H 2.185015 2.036127 -3.520850
H 0.769735 4.059431 -3.416123
H -1.508026 3.954103 -2.401685
H -2.351177 1.815139 -1.509412
C -1.233231 -0.842740 0.390427
C -1.235204 -2.076684 1.068885
C -1.303585 -2.118704 2.462296
C -1.386258 -0.924085 3.181166
C -1.391713 0.306745 2.525497
C -1.304631 0.340899 1.133841
H -2.286239 -4.398270 1.607970
H -1.244172 -3.061030 2.998421
H -1.417951 -0.966258 4.269813
H -1.435100 1.235381 3.093541
H -1.259335 1.298289 0.616241
O -4.276101 -2.151512 0.156556
C -4.663350 -1.803834 1.488961
H -4.320897 -0.773504 1.630224
H -5.755101 -1.859786 1.620813
O -1.914239 -0.988708 -4.653889
C -1.248559 -0.127277 -5.581815
O 1.411216 -0.399366 -2.612891
C 2.758873 -0.414882 -3.100360
H 3.390775 0.275537 -2.524454
H 3.100702 -1.440982 -2.937589
O -1.169799 -3.223416 0.285664
C -1.400367 -4.486506 0.968158
H -1.593748 -5.221507 0.187457
H -0.509418 -4.762353 1.545082
Cl 1.704637 -3.187935 -1.155463
Cl -0.559625 -5.567107 -1.973275
H -0.435430 0.335430 -5.014022
H -0.834930 -0.696000 -6.429005
H -1.925752 0.656787 -5.953410
Al -0.119199 -5.051571 -4.147878
C 0.317365 -3.033935 -4.004543
C -1.715241 -5.454116 -5.234880
C 1.582770 -5.933839 -4.597976
H -1.465659 -5.400390 -6.307363
H -2.568411 -4.781294 -5.076172
H -2.064186 -6.482766 -5.048750
H 2.349304 -5.712608 -3.839569
H 1.972885 -5.595810 -5.571829
H 1.478083 -7.028311 -4.654591
H 1.404578 -3.132782 -4.138386
H 0.202753 -2.076891 -3.452163
H -0.161737 -2.786204 -4.965942
Al 2.726143 -1.929834 0.584632
C 2.257812 0.001630 0.412064
C 4.611651 -2.316716 0.082880
C 2.036768 -2.829776 2.228516
H 2.869974 -3.169216 2.865254
H 1.443352 -3.725618 1.985488
H 1.404003 -2.169651 2.840504
H 2.442675 0.487886 1.385698
H 1.214278 0.220165 0.156098
H 2.889349 0.523091 -0.324249
H 4.860467 -1.918259 -0.914833
H 4.837445 -3.394248 0.066610
H 5.312774 -1.848666 0.794734

Spin state: triplet

E = -12888.48 kcal mol-1
H = -12386.07 kcal mol-1
TS = -95.24 kcal mol-1
G (298.15 K) = -12481.31 kcal mol-1

Cr -0.550606 -3.107336 -1.922189
P -2.768515 -2.706770 -2.489032
N -2.807743 -1.074316 -2.006188
P -1.189494 -0.907017 -1.473975
C -3.939353 -0.158313 -2.080154
H -4.074772 0.363401 -1.121845
H -4.849184 -0.738712 -2.273527
H -3.812630 0.571704 -2.893172
C -3.622347 -2.617164 -4.105906
C -4.766043 -3.353887 -4.437966
C -5.302541 -3.317151 -5.726286
C -4.693112 -2.530984 -6.702772
C -3.569276 -1.758774 -6.393985
C -3.038257 -1.790030 -5.101219
H -5.238245 -3.974761 -3.677663
H -6.187015 -3.906940 -5.964434
H -5.092975 -2.506399 -7.716662
H -3.113941 -1.138037 -7.162990
C -3.823666 -3.769906 -1.437679
C -4.376805 -3.379256 -0.194742
C -4.982172 -4.337864 0.631443
C -5.036734 -5.675725 0.234731
C -4.489622 -6.076338 -0.983849
C -3.883589 -5.124663 -1.802990
H -4.122967 -2.248950 2.225748
H -5.416678 -4.044046 1.584587
H -5.509157 -6.406582 0.891781

H -4.518923 -7.120697 -1.291678
H -3.415693 -5.440166 -2.736178
C -0.618610 0.729429 -2.063709
C 0.697188 0.830470 -2.580645
C 1.197688 2.070790 -3.002417
C 0.392146 3.207038 -2.927335
C -0.908328 3.125314 -2.428589
C -1.400432 1.892141 -1.997365
H 3.029035 0.057942 -3.906884
H 2.214318 2.148318 -3.381757
H 0.792336 4.166505 -3.256459
H -1.533635 4.015060 -2.362542
H -2.404739 1.845751 -1.582800
C -1.240298 -0.793588 0.336344
C -1.219013 -2.020153 1.029315
C -1.295270 -2.047872 2.422995
C -1.404089 -0.846992 3.129151
C -1.432134 0.375699 2.458999
C -1.339234 0.395827 1.067653
H -2.163865 -4.421118 1.582413
H -1.242792 -2.984443 2.970010
H -1.446905 -0.878337 4.217749
H -1.496098 1.309751 3.016036
H -1.309636 1.348446 0.540782
O -4.274288 -2.059451 0.143286
C -4.651212 -1.657180 1.463511
H -4.332639 -0.613441 1.550065
H -5.739415 -1.733138 1.613510
O -1.965438 -1.043080 -4.698624
C -1.292869 -0.214888 -5.651000
O 1.400797 -0.326968 -2.635826
C 2.814576 -0.289139 -2.884915
H 3.316535 0.350113 -2.144752
H 3.147755 -1.322841 -2.758478
O -1.128378 -3.174619 0.259735
C -1.251004 -4.438225 0.974196
H -1.343493 -5.207551 0.209241
H -0.352372 -4.603952 1.580346
Cl 1.710883 -3.212855 -1.204541
Cl -0.583515 -5.568441 -2.038084
H -0.485196 0.268188 -5.091827
H -0.868946 -0.812485 -6.472831
H -1.967979 0.553466 -6.057814
Al -0.088109 -5.009179 -4.187197
C 0.316318 -2.981336 -4.023710
C -1.660359 -5.408267 -5.306529
C 1.634260 -5.858897 -4.613759
H -1.458111 -5.164192 -6.362436
H -2.574859 -4.867368 -5.028657
H -1.889396 -6.485506 -5.273064
H 2.382026 -5.630918 -3.838515
H 2.039310 -5.508069 -5.576918
H 1.549594 -6.954583 -4.679789
H 1.402743 -3.087805 -4.159699
H 0.211941 -2.001727 -3.525026
H -0.172857 -2.797005 -4.994472
Al 2.726058 -2.134281 0.645996
C 2.061509 -0.256254 0.751116
C 4.614030 -2.289804 0.035669
C 2.186927 -3.318443 2.153827
H 2.883161 -3.222615 3.003902
H 2.183855 -4.381289 1.863121
H 1.186905 -3.067673 2.540583
H 1.360661 -0.105254 1.585649
H 1.552272 0.094381 -0.156942
H 2.915076 0.422449 0.918077
H 4.820553 -1.672887 -0.854433
H 4.895795 -3.324365 -0.214552
H 5.306960 -1.947642 0.823144

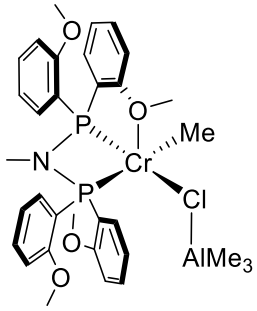
Spin state: quintet

E = -12902.18 kcal mol-1
H = -12399.67 kcal mol-1
TS = -96.89 kcal mol-1
G (298.15 K) = -12496.56 kcal mol-1

Cr -0.331965 -3.063781 -1.928831
P -2.727114 -2.684650 -2.385142
N -2.719240 -1.118858 -1.742014
P -1.119172 -0.874479 -1.180635
C -3.840000 -0.181752 -1.701630
H -3.958657 0.227341 -0.688477
H -4.762604 -0.711834 -1.961412
H -3.686403 0.637042 -2.418746
C -3.534126 -2.516387 -4.005229
C -4.770086 -3.090112 -4.326612
C -5.305448 -2.967529 -5.608511
C -4.596186 -2.264637 -6.582419
C -3.369341 -1.667904 -6.284746
C -2.835914 -1.784345 -4.995900
H -5.308234 -3.654988 -3.566782
H -6.263287 -3.428517 -5.846041
H -4.997061 -2.175156 -7.592381
H -2.834084 -1.123716 -7.059137
C -3.818746 -3.818513 -1.456536
C -4.500707 -3.523144 -0.254277
C -5.185561 -4.542390 0.424328
C -5.187312 -5.844741 -0.078900
C -4.509644 -6.150787 -1.258660
C -3.827335 -5.139907 -1.933709
H -4.522074 -2.565058 2.265817
H -5.718978 -4.324091 1.346969
H -5.722356 -6.623830 0.464643
H -4.499350 -7.167599 -1.648467
H -3.275333 -5.378309 -2.843989
C -0.596091 0.740235 -1.829229
C 0.556379 0.777326 -2.653004
C 0.996122 1.997125 -3.185421
C 0.286008 3.167848 -2.919912
C -0.864143 3.144083 -2.129477
C -1.295272 1.932334 -1.588921
H 2.376282 -0.102351 -4.577690
H 1.892089 2.033725 -3.801172
H 0.639958 4.110412 -3.338560
H -1.416344 4.060886 -1.926699
H -2.184606 1.917829 -0.960470
C -1.276318 -0.739087 0.631978
C -1.492071 -1.961118 1.318936
C -1.674573 -1.970034 2.703631

C -1.616304 -0.770753 3.415735
C -1.358450 0.434072 2.762568
C -1.183449 0.441447 1.377579
H -2.598388 -4.456557 1.696072
H -1.819287 -2.907857 3.234184
H -1.743977 -0.790118 4.498225
H -1.277142 1.362536 3.326364
H -0.943954 1.375920 0.873196
O -4.441787 -2.234285 0.196180
C -4.976940 -1.932874 1.488444
H -4.702481 -0.890871 1.680462
H -6.072378 -2.042005 1.508316
O -1.656325 -1.225578 -4.599142
C -0.860676 -0.558862 -5.590429
O 1.160179 -0.413667 -2.891927
C 2.446281 -0.439263 -3.531850
H 3.165754 0.180004 -2.978501
H 2.753191 -1.487113 -3.500046
O -1.490429 -3.093817 0.549950
C -1.626837 -4.379109 1.188302
H -1.583347 -5.107261 0.373291
H -0.800832 -4.547485 1.892596
Cl 1.905515 -3.078265 -1.274472
Cl -0.439179 -5.403659 -2.249026
H 0.048559 -0.253880 -5.070570
H -0.600456 -1.244120 -6.409273
H -1.383114 0.327417 -5.979958
Al -0.034782 -5.353125 -4.630767
C 0.849872 -3.563369 -4.784344
C -1.872047 -5.508691 -5.369636
C 1.166169 -6.903051 -4.878964
H -1.832426 -5.636236 -6.464819
H -2.516222 -4.637779 -5.181514
H -2.393085 -6.396999 -4.975926
H 2.078935 -6.811681 -4.269884
H 1.487498 -6.998953 -5.929796
H 0.683225 -7.854237 -4.605041
H 1.868864 -3.596881 -4.370195
H 0.328446 -2.716837 -4.300345
H 0.940053 -3.278121 -5.847203
Al 2.743586 -1.748573 0.545924
C 2.368971 0.163643 0.138100
C 4.653173 -2.251512 0.355552
C 1.749888 -2.503400 2.097764
H 2.440611 -2.924261 2.845769
H 1.087903 -3.323815 1.780543
H 1.125502 -1.755505 2.608796
H 2.803849 0.761901 0.958436
H 1.307923 0.442643 0.091969
H 2.842572 0.519440 -0.789410
H 5.068221 -1.951983 -0.620327
H 4.813266 -3.336160 0.457857
H 5.267489 -1.759794 1.128887

Geometry:



Spin state: singlet

E = -11759.69 kcal mol-1
H = -11309.49 kcal mol-1
TS = -80.77 kcal mol-1
G (298.15 K) = -11390.26 kcal mol-1

Cr -0.296008 -3.078175 -2.230009
P -2.528934 -2.907725 -2.103892
N -2.683682 -1.480446 -1.154302
P -0.987672 -1.256130 -0.921405
C -3.723031 -0.449095 -1.176919
H -4.256037 -0.391817 -0.217674
H -4.450429 -0.679099 -1.962837
H -3.275701 0.529501 -1.399689
C -3.494972 -2.698930 -3.652724
C -4.242136 -3.776104 -4.150188
C -4.892015 -3.708541 -5.382962
C -4.807258 -2.541045 -6.139405
C -4.064779 -1.452468 -5.675327
C -3.394993 -1.534068 -4.447752
H -4.317269 -4.684138 -3.552616
H -5.465194 -4.562283 -5.743585
H -5.316152 -2.468684 -7.101088
H -4.002104 -0.549329 -6.278901
C -3.458343 -4.255760 -1.272706
C -4.765205 -4.076604 -0.769602
C -5.410025 -5.117164 -0.092164
C -4.761230 -6.345442 0.067769
C -3.481123 -6.545091 -0.443906
C -2.838313 -5.498202 -1.106021
H -6.680060 -2.698765 0.596572
H -6.411092 -4.982797 0.312527
H -5.269049 -7.147670 0.604123
H -2.972112 -7.498721 -0.311462
H -1.824238 -5.636079 -1.476086
C -0.470772 0.200576 -1.915909
C 0.216695 -0.058155 -3.111788
C 0.681138 0.985056 -3.915730
C 0.454445 2.307651 -3.518309
C -0.226470 2.587502 -2.333344
C -0.680487 1.531671 -1.539606
H 0.680088 -1.327274 -5.510305
H 1.211733 0.795428 -4.844871
H 0.818412 3.119100 -4.148707
H -0.395373 3.618766 -2.023977
H -1.181523 1.734623 -0.592111
C -0.869770 -0.588372 0.774717
C 0.376549 -0.091801 1.220809

C 0.527817 0.365673 2.533329
C -0.554356 0.302240 3.415175
C -1.779808 -0.218026 3.000752
C -1.929822 -0.660249 1.685331
H 3.015804 -0.480141 1.546351
H 1.486087 0.744262 2.881365
H -0.424598 0.649184 4.440787
H -2.613616 -0.291394 3.698159
H -2.871422 -1.101766 1.366021
O -5.328482 -2.849921 -1.000717
C -6.643279 -2.601862 -0.499855
H -6.875841 -1.569970 -0.782289
H -7.381411 -3.280596 -0.955369
O -2.620089 -0.522869 -3.946580
C -2.715264 0.765637 -4.561965
O 0.421845 -1.406637 -3.430679
C 1.217081 -1.669908 -4.615997
H 2.190929 -1.170759 -4.529767
H 1.348133 -2.750857 -4.660139
O 1.382369 -0.112592 0.292597
C 2.710905 0.194335 0.731952
H 3.352274 0.031866 -0.139693
H 2.791953 1.244250 1.054762
Cl 0.556090 -4.629290 -0.807688
C -0.420232 -4.290895 -3.897298
H -2.158120 1.445145 -3.911655
H -2.261065 0.769566 -5.564952
H -3.764362 1.092883 -4.630292
H 0.594690 -4.673284 -4.121118
H -0.806314 -3.764030 -4.786019
H -1.062469 -5.171803 -3.737563
Al 0.175014 -4.493428 1.586865
C 0.615620 -6.371529 2.057043
C 1.541099 -3.109564 2.015512
C -1.740947 -4.000509 1.769149
H -1.904277 -3.456072 2.713668
H -2.392033 -4.888017 1.774171
H -2.102189 -3.349150 0.962370
H 2.505658 -3.562140 2.294791
H 1.229857 -2.442615 2.834443
H 1.718202 -2.479844 1.130896
H 1.640291 -6.650879 1.764472
H -0.070848 -7.085017 1.573027
H 0.535480 -6.539858 3.144563

Spin state: triplet

E = -11774.85 kcal mol-1
H = -11323.38 kcal mol-1
TS = -83.51 kcal mol-1
G (298.15 K) = -11406.89 kcal mol-1

Cr -0.563107 -3.367300 -1.405967
P -2.846607 -2.962926 -1.596022
N -2.886598 -1.523021 -0.658760
P -1.171227 -1.296055 -0.559190
C -3.967313 -0.561761 -0.415052
H -4.749981 -1.015709 0.209040
H -4.412793 -0.224748 -1.356879
H -3.554253 0.303480 0.117461
C -3.231775 -2.745700 -3.388813
C -3.321202 -3.937663 -4.118401
C -3.443189 -3.939629 -5.509479
C -3.470588 -2.724068 -6.191478
C -3.401195 -1.517830 -5.488215
C -3.298377 -1.523043 -4.089247
H -3.281647 -4.885735 -3.580288
H -3.507895 -4.883045 -6.050703
H -3.553364 -2.703469 -7.278596
H -3.439690 -0.577000 -6.033314
C -4.315571 -3.932251 -1.072663
C -5.633111 -3.545123 -1.413172
C -6.715488 -4.380902 -1.114688
C -6.490444 -5.599297 -0.466027
C -5.198469 -5.995276 -0.121528
C -4.121378 -5.163294 -0.435330
H -7.780657 -1.830458 -1.847199
H -7.731026 -4.092047 -1.379305
H -7.340136 -6.243289 -0.237000
H -5.025329 -6.950278 0.373346
H -3.105365 -5.483528 -0.204275
C -0.612038 -0.149160 -1.855641
C -0.184709 -0.729991 -3.069896
C 0.293862 0.066042 -4.111573
C 0.357220 1.454317 -3.943031
C -0.063976 2.046702 -2.751404
C -0.548369 1.242123 -1.719920
H -0.540523 -2.332553 -5.234338
H 0.628848 -0.375788 -5.046312
H 0.744504 2.068536 -4.756043
H -0.007355 3.127660 -2.623660
H -0.861846 1.688384 -0.775018
C -0.912530 -0.489870 1.050470
C 0.396846 -0.036254 1.356125
C 0.720512 0.376716 2.652354
C -0.239568 0.298503 3.665764
C -1.514599 -0.199063 3.396468
C -1.841633 -0.593374 2.097316
H 3.016699 -0.580535 1.370686
H 1.724133 0.728515 2.881710
H 0.025115 0.611275 4.676013
H -2.252343 -0.289057 4.193419
H -2.825243 -1.015417 1.898091
O -5.750376 -2.334303 -2.039382
C -7.008494 -1.982274 -2.618054
H -6.833064 -1.040404 -3.147423
H -7.345110 -2.748873 -3.333003
O -3.272630 -0.385057 -3.334432
C -3.230638 0.878283 -4.002104
O -0.273788 -2.116140 -3.174229
C 0.101459 -2.726809 -4.435325
H 1.164650 -2.545435 -4.637557
H -0.078556 -3.794015 -4.304392
O 1.278765 -0.076658 0.318152
C 2.674336 0.107224 0.584507
H 3.178342 -0.135247 -0.355406
H 2.890388 1.149204 0.868128
Cl 1.901352 -3.141885 -1.342292
C -0.522113 -5.245646 -2.349521
H -3.140479 1.623488 -3.206617

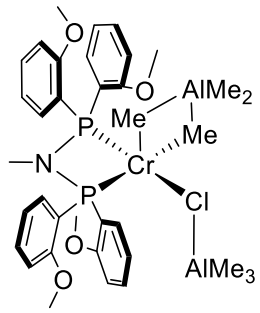
H -2.349870 0.950059 -4.657102
H -4.150119 1.058150 -4.581779
H 0.531679 -5.482952 -2.572670
H -1.096467 -5.326485 -3.287350
H -0.898024 -6.032801 -1.675716
Al 1.489431 -4.304940 0.584927
C 2.189954 -6.123301 0.274031
C 2.183678 -3.239867 2.100142
C -0.561736 -4.342873 0.735389
H -0.545067 -5.387880 1.096055
H -1.449336 -4.382043 0.062657
H -0.861748 -3.685452 1.563275
H 3.244210 -2.973051 1.966196
H 2.115026 -3.804660 3.044361
H 1.614457 -2.309022 2.243863
H 3.274805 -6.119678 0.084399
H 1.707292 -6.591456 -0.598047
H 2.017387 -6.784577 1.139273

Spin state: quintet

E = -11789.04 kcal mol-1
H = -11338.76 kcal mol-1
TS = -86.52 kcal mol-1
G (298.15 K) = -11425.28 kcal mol-1

Cr -0.427741 -3.190918 -1.986725
P -2.811556 -2.889074 -2.138529
N -2.805637 -1.243316 -1.649918
P -1.236274 -1.068061 -0.980612
C -3.733055 -0.170701 -2.010506
H -4.208877 0.270492 -1.123174
H -4.517241 -0.577584 -2.657861
H -3.194798 0.616193 -2.557892
C -3.748069 -2.965484 -3.693195
C -4.820052 -3.845211 -3.880224
C -5.428767 -3.981299 -5.128730
C -4.960271 -3.229181 -6.205963
C -3.890496 -2.343699 -6.048465
C -3.279881 -2.211963 -4.795956
H -5.173020 -4.435446 -3.034402
H -6.259951 -4.673605 -5.258272
H -5.424949 -3.330060 -7.187150
H -3.535192 -1.771376 -6.902735
C -3.786928 -3.845425 -0.930982
C -5.029041 -3.408955 -0.420559
C -5.664751 -4.132949 0.593854
C -5.064422 -5.294208 1.093118
C -3.841485 -5.740361 0.595236
C -3.206570 -5.008218 -0.408417
H -6.665262 -1.496422 0.606856
H -6.618506 -3.804094 1.001621
H -5.565147 -5.847236 1.888495
H -3.368989 -6.635964 0.995283
H -2.231531 -5.329204 -0.780212
C -0.490377 0.386453 -1.798646
C 0.397262 0.162366 -2.875336
C 1.059314 1.239381 -3.477441
C 0.821220 2.539421 -3.021356
C -0.061575 2.776693 -1.967685
C -0.702893 1.696664 -1.358033
H 1.436357 -0.993937 -5.182027
H 1.762161 1.074244 -4.291360
H 1.342398 3.371033 -3.496688
H -0.237689 3.791623 -1.612401
H -1.366183 1.861561 -0.507506
C -1.488544 -0.566032 0.740510
C -0.312481 -0.421403 1.506503
C -0.386382 -0.248002 2.890909
C -1.640596 -0.234063 3.509173
C -2.810078 -0.404936 2.765522
C -2.730519 -0.580726 1.381825
H 1.896151 -1.728933 2.111967
H 0.519475 -0.150500 3.486286
H -1.697513 -0.106753 4.590551
H -3.779122 -0.421165 3.263577
H -3.630299 -0.775871 0.797429
O -5.528595 -2.262840 -0.981062
C -6.753507 -1.735360 -0.464698
H -6.939656 -0.816537 -1.029808
H -7.589641 -2.435050 -0.618481
O -2.229387 -1.378128 -4.533475
C -1.698145 -0.596889 -5.607177
O 0.547418 -1.139199 -3.284166
C 1.608566 -1.462152 -4.201324
H 2.579877 -1.150228 -3.793137
H 1.580629 -2.550871 -4.300880
O 0.840965 -0.504526 0.781400
C 2.055102 -0.852065 1.468704
H 2.769223 -1.111281 0.682499
H 2.430280 -0.003360 2.060640
Cl 1.768949 -3.374733 -1.102152
C -0.328331 -4.584874 -3.520034
H -0.915372 0.021929 -5.159759
H -1.266785 -1.239255 -6.390389
H -2.468924 0.055993 -6.045284
H 0.699271 -4.973748 -3.601979
H -0.606138 -4.088463 -4.467668
H -1.002928 -5.446142 -3.392388
Al 1.153510 -4.830013 0.718097
C 0.645621 -6.486810 -0.258030
C 2.845040 -4.841525 1.760757
C -0.385467 -3.921774 1.610913
H -0.877880 -4.650391 2.278841
H -1.176398 -3.557716 0.935762
H -0.097848 -3.066160 2.240590
H 3.666017 -5.332210 1.214485
H 2.724278 -5.381399 2.715045
H 3.189573 -3.825250 2.012824
H 1.506605 -6.948453 -0.766724
H -0.112244 -6.304068 -1.037750
H 0.228312 -7.244569 0.426775

Geometry:



Spin state: singlet

E = -13239.07 kcal mol-1
H = -12714.79 kcal mol-1
TS = -92.11 kcal mol-1
G (298.15 K) = -12806.89 kcal mol-1

Cr -0.626485 -3.489092 -2.163520
P -2.861140 -2.939665 -2.467578
N -2.827836 -1.411217 -1.696456
P -1.159626 -1.270518 -1.317212
C -3.858199 -0.376173 -1.795706
H -4.003071 0.114750 -0.823480
H -4.803491 -0.850209 -2.077919
H -3.595069 0.374165 -2.554394
C -3.750161 -2.569080 -4.038867
C -4.873776 -3.295963 -4.457025
C -5.443435 -3.107028 -5.716884
C -4.884353 -2.174952 -6.587922
C -3.784775 -1.410049 -6.191713
C -3.227514 -1.588090 -4.919446
H -5.302846 -4.039759 -3.788021
H -6.309434 -3.696422 -6.016336
H -5.304342 -2.028723 -7.583442
H -3.370553 -0.674739 -6.877666
C -4.013078 -4.111238 -1.640957
C -4.875881 -3.831559 -0.558775
C -5.597688 -4.869242 0.049191
C -5.495815 -6.174894 -0.433465
C -4.681630 -6.461140 -1.528352
C -3.946702 -5.432387 -2.114091
H -5.479136 -2.719028 1.862319
H -6.249441 -4.665300 0.895737
H -6.064637 -6.968043 0.052343
H -4.608734 -7.474939 -1.919827
H -3.307441 -5.649297 -2.970032
C -0.614670 0.399229 -1.909008
C 0.585197 0.543200 -2.641785
C 1.018637 1.812542 -3.052410
C 0.271186 2.943692 -2.716695
C -0.889671 2.823870 -1.954010
C -1.311177 1.556118 -1.544367
H 1.939083 1.921589 -3.622369
H 0.616092 3.926144 -3.040918
H -1.456425 3.708141 -1.663791
H -2.184770 1.472324 -0.900050
C -1.132492 -0.938604 0.477038
C 0.073973 -0.504141 1.063066
C 0.123992 -0.207683 2.429797
C -1.019566 -0.389159 3.213199
C -2.206861 -0.860162 2.649520
C -2.256940 -1.135274 1.280340
H 2.805135 -0.452474 1.459547
H 1.050178 0.130916 2.889490
H -0.969968 -0.171926 4.280484
H -3.087417 -1.016583 3.272371
H -3.162668 -1.523908 0.817009
O -4.980368 -2.521369 -0.167094
C -5.821155 -2.209728 0.947763
H -5.736079 -1.126502 1.082812
H -6.871452 -2.471986 0.747788
O -2.186764 -0.835021 -4.444138
C -1.547155 0.073991 -5.345290
O 1.270296 -0.603373 -2.884082
C 2.491829 -0.558622 -3.624421
O 1.127811 -0.433828 0.205106
C 2.354993 0.147530 0.656096
H 3.015054 0.137579 -0.216473
H 2.197092 1.183983 0.992946
Cl 1.758111 -3.501973 -1.706882
C -0.672783 -5.756218 -2.334254
H -0.749695 0.547566 -4.766918
H -1.116877 -0.461482 -6.205596
H -2.246798 0.847881 -5.696518
Al 1.304440 -4.380248 0.398439
C 1.961085 -6.250553 0.359481
C 2.237385 -3.241195 1.729142
C -0.722360 -4.219529 0.426060
H -0.962009 -3.590875 1.297385
H -1.128829 -5.227990 0.601794
H -1.444778 -3.793330 -0.328276
H 2.557246 -3.845257 2.593744
H 1.612519 -2.425084 2.117865
H 3.148702 -2.796213 1.298840
H 3.033381 -6.283092 0.107783
H 1.443967 -6.915566 -0.348109
H 1.857760 -6.705548 1.359396
Al -0.412246 -5.083151 -4.301599
C -1.986099 -5.494203 -5.438018
C 1.293573 -5.937622 -4.820378
C -0.063131 -3.030792 -4.302081
H 0.964319 -3.185623 -4.670659
H -0.023283 -2.077326 -3.760751
H -0.741799 -2.849620 -5.149818
H -1.719161 -5.356999 -6.499137
H -2.871824 -4.869343 -5.257209
H -2.300425 -6.546718 -5.338232
H 2.095529 -5.656605 -4.119497
H 1.619150 -5.644726 -5.831677
H 1.224915 -7.037084 -4.815470
H 2.325074 -0.188389 -4.648183
H 2.841930 -1.594454 -3.653811
H 3.240567 0.070113 -3.118151
H -1.022001 -6.615750 -2.943469
H 0.289315 -6.062497 -1.907323
H -1.423982 -5.724262 -1.537052

Spin state: triplet

E = -13237.24 kcal mol-1
H = -12714.12 kcal mol-1
TS = -93.01 kcal mol-1
G (298.15 K) = -12807.12 kcal mol-1

Cr -0.345029 -3.040771 -2.292074
P -2.737977 -2.791620 -2.525967
N -2.849558 -1.374588 -1.571758
P -1.222532 -1.231235 -1.121476
C -3.867725 -0.327543 -1.598209
H -4.025662 0.072592 -0.587402
H -4.811402 -0.756724 -1.949457
H -3.569312 0.487763 -2.273138
C -3.716010 -2.462199 -4.036281
C -4.698389 -3.357926 -4.480703
C -5.350319 -3.173377 -5.699789
C -5.020473 -2.076377 -6.493433
C -4.057319 -1.157716 -6.070396
C -3.407380 -1.342356 -4.845142
H -4.949238 -4.219523 -3.864342
H -6.103059 -3.889325 -6.027424
H -5.511594 -1.926270 -7.455231
H -3.808490 -0.311630 -6.706174
C -3.689237 -4.129024 -1.697661
C -4.604016 -3.961227 -0.633248
C -5.128520 -5.085475 0.019921
C -4.795577 -6.370577 -0.407715
C -3.943289 -6.552177 -1.495835
C -3.394067 -5.434480 -2.118113
H -5.407627 -2.878918 1.738689
H -5.806490 -4.965783 0.861778
H -5.212520 -7.230877 0.116249
H -3.692833 -7.550971 -1.850383
H -2.722723 -5.572897 -2.962566
C -0.502660 0.218969 -1.967403
C 0.432024 -0.068677 -2.972473
C 1.118505 0.954413 -3.628509
C 0.828828 2.282534 -3.297628
C -0.124236 2.588174 -2.323922
C -0.776847 1.551808 -1.653067
H 1.858296 0.737399 -4.395027
H 1.358387 3.083154 -3.814154
H -0.340353 3.626316 -2.073516
H -1.482701 1.770998 -0.850790
C -1.244324 -0.790762 0.636845
C -0.054770 -0.355427 1.263706
C -0.026909 -0.163960 2.650474
C -1.170020 -0.425222 3.408526
C -2.342694 -0.880249 2.802482
C -2.371153 -1.068903 1.421234
H 2.524620 -0.883997 1.686103
H 0.887454 0.159229 3.143202
H -1.131551 -0.286967 4.489284
H -3.222534 -1.106603 3.403844
H -3.257120 -1.475145 0.934827
O -4.955893 -2.677992 -0.301020
C -5.840454 -2.483059 0.806584
H -5.962360 -1.398396 0.894518
H -6.822511 -2.947358 0.627475
O -2.465339 -0.484730 -4.348075
C -2.112044 0.655034 -5.140894
O 0.624272 -1.417161 -3.270686
C 1.837957 -1.774495 -3.993262
O 1.008975 -0.162491 0.435843
C 2.316313 -0.038948 1.015395
H 3.009435 -0.064189 0.169671
H 2.423417 0.915785 1.553067
Cl 1.597884 -3.130558 -0.920413
C -0.156100 -5.073540 -2.715586
H -1.410823 1.230867 -4.532495
H -1.624704 0.342172 -6.076771
H -2.995289 1.273060 -5.363445
Al 0.898871 -4.540444 0.947486
C 1.763795 -6.247855 0.432101
C 1.728917 -3.513518 2.433889
C -1.097657 -4.564525 0.968806
H -1.401416 -4.902695 1.976223
H -1.561079 -5.263265 0.255347
H -1.574070 -3.585066 0.821614
H 1.738879 -4.112798 3.360016
H 1.175417 -2.589632 2.660789
H 2.775689 -3.242848 2.221369
H 2.837461 -6.124878 0.219772
H 1.302156 -6.694323 -0.462703
H 1.678917 -6.994032 1.240203
Al -0.388063 -4.720205 -4.937002
C -1.978577 -5.836994 -5.401499
C 1.380772 -5.538802 -5.363844
C -0.620625 -2.897065 -5.767894
H 0.236290 -2.710900 -6.436495
H -0.746767 -2.010894 -5.136869
H -1.521193 -2.958971 -6.400016
H -1.930468 -6.028599 -6.487788
H -2.941810 -5.331102 -5.230433
H -2.028515 -6.826519 -4.918039
H 2.239706 -4.960923 -4.983780
H 1.509566 -5.614288 -6.456734
H 1.483139 -6.556850 -4.956416
H 1.773667 -1.408786 -5.023969
H 1.870512 -2.866474 -3.997626
H 2.708406 -1.370564 -3.462639
H -0.646781 -5.999161 -3.052697
H 0.881632 -5.330519 -2.470653
H -0.704054 -4.897472 -1.734917

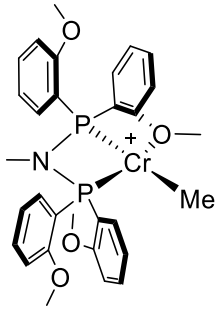
Spin state: quintet

E = -13261.44 kcal mol-1
H = -12738.20 kcal mol-1
TS = -94.11 kcal mol-1
G (298.15 K) = -12832.31 kcal mol-1

Cr -0.471305 -3.288869 -2.364864
P -2.886887 -2.844360 -2.527574
N -2.822494 -1.365806 -1.674640
P -1.156445 -1.142920 -1.336176
C -3.921097 -0.393889 -1.648636
H -3.830425 0.253121 -0.767083
H -4.871712 -0.932431 -1.575971
H -3.921764 0.223177 -2.558911

C -3.887376 -2.469571 -4.008356
C -5.078350 -3.139892 -4.312874
C -5.768208 -2.881625 -5.497681
C -5.263489 -1.939710 -6.393331
C -4.087431 -1.242418 -6.107808
C -3.399335 -1.498773 -4.916059
H -5.459829 -3.886428 -3.617588
H -6.688463 -3.420044 -5.720759
H -5.785716 -1.738167 -7.329001
H -3.711399 -0.508283 -6.816590
C -3.863214 -4.121974 -1.659408
C -4.586195 -3.991835 -0.455843
C -5.100191 -5.135061 0.171928
C -4.934300 -6.392684 -0.407628
C -4.263252 -6.530582 -1.622767
C -3.725252 -5.399187 -2.229089
H -4.792237 -3.092387 2.098483
H -5.628591 -5.052694 1.118594
H -5.334211 -7.269409 0.102006
H -4.136825 -7.509084 -2.083579
H -3.173379 -5.498877 -3.164815
C -0.577817 0.419861 -2.116576
C 0.691963 0.433582 -2.744850
C 1.139818 1.589522 -3.401409
C 0.339198 2.733275 -3.419766
C -0.896106 2.745754 -2.772536
C -1.337231 1.594191 -2.116494
H 2.109755 1.600488 -3.893870
H 0.696180 3.625097 -3.935803
H -1.508921 3.646633 -2.765681
H -2.285464 1.622334 -1.584786
C -1.104308 -0.764652 0.444189
C 0.137551 -0.422797 1.017482
C 0.241638 -0.208617 2.396183
C -0.890213 -0.349379 3.201767
C -2.119779 -0.709614 2.647696
C -2.218499 -0.923546 1.272191
H 2.629636 -1.270652 1.305110
H 1.201968 0.040751 2.842762
H -0.799474 -0.193228 4.276867
H -2.993175 -0.844455 3.285166
H -3.150110 -1.264823 0.829330
O -4.762394 -2.725164 0.036064
C -5.382073 -2.584190 1.320673
H -5.400958 -1.507894 1.520920
H -6.413302 -2.968678 1.316718
O -2.259738 -0.851299 -4.536359
C -1.682831 0.098642 -5.442417
O 1.414289 -0.709977 -2.648527
C 2.704735 -0.784952 -3.259514
O 1.168641 -0.338729 0.135759
C 2.511502 -0.409613 0.633271
H 3.137785 -0.550510 -0.252359
H 2.795373 0.522587 1.145716
Cl 1.476933 -3.492371 -1.038239
C -0.436959 -5.510617 -2.658659
H -0.781471 0.466493 -4.946372
H -1.412119 -0.381362 -6.394110
H -2.370430 0.938674 -5.621525
Al 0.664605 -4.697542 0.899611
C 1.334106 -6.525408 0.522496
C 1.589086 -3.697492 2.349182
C -1.326750 -4.492293 0.896782
H -1.676965 -4.686727 1.926598
H -1.861348 -5.205700 0.250776
H -1.688991 -3.484543 0.645995
H 1.532126 -4.257943 3.297774
H 1.137317 -2.711776 2.535911
H 2.660217 -3.547824 2.136915
H 2.395434 -6.521443 0.227783
H 0.772837 -7.021031 -0.284440
H 1.251961 -7.170013 1.414013
Al -0.223101 -4.788651 -4.663043
C -1.928916 -5.115511 -5.642286
C 1.347756 -5.829238 -5.278005
C 0.293752 -2.801947 -4.721413
H 1.389136 -2.742120 -4.784043
H -0.051890 -1.922622 -4.155796
H -0.105166 -2.622831 -5.736051
H -1.756725 -4.987026 -6.724473
H -2.762190 -4.446007 -5.382840
H -2.290570 -6.149764 -5.513629
H 2.229943 -5.629521 -4.648665
H 1.624711 -5.579685 -6.315206
H 1.169091 -6.915822 -5.248085
H 2.637003 -0.657546 -4.350478
H 3.068110 -1.790111 -3.026515
H 3.386879 -0.032248 -2.834415
H -1.008564 -6.310234 -3.161243
H 0.555213 -5.909340 -2.413995
H -0.976130 -5.397186 -1.701687

Geometry:



Spin state: singlet

E = -10071.22 kcal mol-1
H = -9693.82 kcal mol-1
TS = -69.16 kcal mol-1
G (298.15 K) = -9762.98 kcal mol-1

Cr -0.206063 -2.673945 -2.096672
P -2.546387 -2.830271 -2.025911
N -2.788123 -1.254406 -1.402919
P -1.194846 -0.808401 -0.960367
C -3.927597 -0.354429 -1.585107
H -4.152838 0.161225 -0.641442
H -4.801867 -0.938850 -1.884353
H -3.713314 0.384471 -2.371640

C -3.528792 -2.956725 -3.544782
C -4.457883 -3.987644 -3.744370
C -5.165985 -4.093202 -4.940193
C -4.945188 -3.158762 -5.951978
C -4.018315 -2.127335 -5.783687
C -3.297910 -2.029212 -4.588151
H -4.625376 -4.715418 -2.951258
H -5.884910 -4.899444 -5.079142
H -5.493848 -3.229998 -6.891160
H -3.855956 -1.417539 -6.591421
C -3.245532 -4.101090 -0.921876
C -4.519587 -3.999243 -0.318704
C -4.980321 -5.027820 0.514036
C -4.182296 -6.153225 0.736951
C -2.923460 -6.267774 0.146028
C -2.462890 -5.236455 -0.674379
H -6.476340 -2.689024 1.065971
H -5.958591 -4.964299 0.985395
H -4.556238 -6.947357 1.383275
H -2.305955 -7.147395 0.321118
H -1.479260 -5.313990 -1.142343
C -0.647904 0.543661 -2.065319
C 0.423926 0.268589 -2.939615
C 0.920144 1.249449 -3.799381
C 0.313390 2.509056 -3.824110
C -0.782506 2.788964 -3.008578
C -1.250524 1.809600 -2.132288
H 1.849448 -1.189207 -4.819937
H 1.758078 1.052419 -4.462506
H 0.702069 3.268976 -4.501366
H -1.262934 3.765710 -3.045815
H -2.089430 2.031788 -1.473454
C -1.301618 -0.085303 0.701247
C -1.745544 -0.950305 1.735929
C -1.834964 -0.482272 3.051801
C -1.448716 0.826204 3.350477
C -0.961951 1.671505 2.353742
C -0.887512 1.211911 1.038878
H -3.356759 -2.895912 2.849096
H -2.191998 -1.132183 3.847444
H -1.520017 1.178747 4.379490
H -0.640478 2.683583 2.595182
H -0.489348 1.869338 0.268461
O -5.229577 -2.874505 -0.613704
C -6.533705 -2.716218 -0.032293
H -6.905556 -1.756469 -0.402607
H -7.211569 -3.520855 -0.352853
O -2.351295 -1.069971 -4.338564
C -2.187029 -0.027197 -5.313820
O 0.944753 -1.037865 -2.926220
C 2.112011 -1.303112 -3.760978
H 2.929257 -0.628660 -3.478956
H 2.390038 -2.339896 -3.562714
O -2.046204 -2.225373 1.352258
C -2.407219 -3.175077 2.369327
H -2.527279 -4.128648 1.849320
H -1.615487 -3.261242 3.127861
C 0.357688 -4.158521 -3.377257
H -3.139455 0.491388 -5.497583
H -1.469281 0.672279 -4.879694
H -1.791937 -0.425504 -6.260023
H 1.427484 -4.409976 -3.236252
H 0.227818 -3.826585 -4.422991
H -0.204509 -5.100616 -3.274838

Spin state: triplet

E = -10080.02 kcal mol-1
H = -9702.57 kcal mol-1
TS = -68.79 kcal mol-1
G (298.15 K) = -9771.36 kcal mol-1

Cr -0.143538 -2.691340 -2.021826
P -2.461108 -2.818872 -1.972651
N -2.729587 -1.256894 -1.337613
P -1.139517 -0.810795 -0.902803
C -3.895840 -0.381773 -1.445031
H -4.324192 -0.177551 -0.454114
H -4.653258 -0.872680 -2.063629
H -3.614094 0.562249 -1.932066
C -3.368171 -2.975316 -3.540260
C -4.087882 -4.143806 -3.832077
C -4.717558 -4.315344 -5.063063
C -4.635101 -3.304693 -6.020908
C -3.917647 -2.135015 -5.762378
C -3.267335 -1.971377 -4.533085
H -4.156129 -4.928509 -3.079403
H -5.271256 -5.230178 -5.269618
H -5.127761 -3.423558 -6.985885
H -3.857712 -1.364144 -6.527343
C -3.225130 -4.081147 -0.895790
C -4.582664 -4.025053 -0.504133
C -5.114654 -5.027832 0.317185
C -4.301029 -6.082264 0.742345
C -2.958949 -6.147960 0.366900
C -2.431745 -5.143418 -0.446920
H -6.848530 -2.785998 0.420875
H -6.157503 -4.998664 0.625620
H -4.728626 -6.857453 1.378421
H -2.329253 -6.971017 0.701331
H -1.383722 -5.184167 -0.747694
C -0.652800 0.560981 -2.016291
C 0.248563 0.253066 -3.053116
C 0.670333 1.230822 -3.954196
C 0.161707 2.528718 -3.843730
C -0.768179 2.848243 -2.855437
C -1.165838 1.865373 -1.948180
H 0.995027 -1.211043 -5.221861
H 1.381901 1.008504 -4.744495
H 0.496158 3.288636 -4.549477
H -1.175028 3.856073 -2.784978
H -1.874329 2.114349 -1.158455
C -1.167933 -0.097171 0.766282
C -1.724157 -0.884469 1.808813
C -1.705906 -0.413684 3.127532
C -1.102384 0.809838 3.423029
C -0.503262 1.569045 2.418120
C -0.535957 1.111610 1.101643
H -3.624316 -2.502928 2.957336
H -2.147443 -1.000874 3.929339

H -1.092330 1.161942 4.454609
H -0.012590 2.512092 2.654571
H -0.050743 1.700333 0.325447
O -5.293059 -2.964342 -0.980397
C -6.691574 -2.877605 -0.664230
H -7.049071 -1.971895 -1.162669
H -7.239480 -3.749683 -1.050199
O -2.513129 -0.873395 -4.212661
C -2.594524 0.269286 -5.079557
O 0.691069 -1.083873 -3.146573
C 1.534940 -1.420365 -4.290334
H 2.474055 -0.856568 -4.238943
H 1.731110 -2.491177 -4.210011
O -2.238096 -2.091588 1.435075
C -2.754377 -2.956948 2.460190
H -3.060418 -3.870176 1.944498
H -1.979941 -3.193494 3.204615
C 0.196370 -4.343541 -3.179801
H -3.641281 0.567569 -5.238736
H -2.060598 1.069816 -4.561991
H -2.113839 0.072509 -6.049427
H 1.291322 -4.522964 -3.184579
H -0.130614 -4.206887 -4.223782
H -0.272228 -5.273983 -2.820592

Spin state: quintet

E = -10105.78 kcal mol-1
H = -9727.67 kcal mol-1
TS = -71.80 kcal mol-1
G (298.15 K) = -9799.47 kcal mol-1

Cr -0.222879 -2.603466 -2.306262
P -2.595353 -2.884526 -2.033112
N -2.776043 -1.289293 -1.418276
P -1.198588 -0.817169 -0.950418
C -3.916047 -0.387732 -1.608589
H -4.037012 0.242599 -0.716717
H -4.825403 -0.977935 -1.747555
H -3.765051 0.246893 -2.494523
C -3.632915 -2.963186 -3.513763
C -4.675595 -3.885506 -3.669608
C -5.402948 -3.945899 -4.857510
C -5.082759 -3.079797 -5.903440
C -4.040561 -2.157420 -5.778168
C -3.310728 -2.098806 -4.586880
H -4.913044 -4.565948 -2.852642
H -6.211533 -4.667383 -4.966253
H -5.644780 -3.119965 -6.836552
H -3.803822 -1.499002 -6.610658
C -3.271918 -4.129530 -0.894975
C -4.518348 -4.016804 -0.238576
C -4.954124 -5.045179 0.607490
C -4.158728 -6.179621 0.790819
C -2.926309 -6.303577 0.148500
C -2.489139 -5.272493 -0.684549
H -6.414699 -2.702874 1.229573
H -5.910631 -4.974353 1.120620
H -4.513556 -6.973219 1.448533
H -2.311325 -7.190276 0.294078
H -1.525669 -5.351850 -1.192277
C -0.620367 0.527025 -2.057787
C 0.548673 0.290557 -2.817280
C 1.052118 1.261424 -3.683479
C 0.367861 2.472032 -3.829857
C -0.809304 2.714571 -3.123360
C -1.288645 1.748140 -2.238696
H 2.361313 -1.147481 -4.403665
H 1.957688 1.088548 -4.259426
H 0.763085 3.223330 -4.512993
H -1.344357 3.654846 -3.249730
H -2.191785 1.947164 -1.662732
C -1.350726 -0.079233 0.695944
C -1.758603 -0.956491 1.734964
C -1.878585 -0.480664 3.045386
C -1.565923 0.850706 3.330072
C -1.126589 1.713475 2.325782
C -1.017530 1.244684 1.016395
H -3.280552 -2.966470 2.853708
H -2.202618 -1.140587 3.846981
H -1.659530 1.209461 4.355158
H -0.867884 2.745418 2.558105
H -0.657443 1.914225 0.237191
O -5.227478 -2.881310 -0.494238
C -6.510042 -2.720441 0.133853
H -6.888956 -1.755382 -0.214940
H -7.203255 -3.518612 -0.169631
O -2.269899 -1.236454 -4.358823
C -1.890080 -0.342124 -5.417048
O 1.161421 -0.967245 -2.682227
C 2.459209 -1.167733 -3.310905
H 3.161877 -0.402105 -2.960681
H 2.790807 -2.158714 -2.990950
O -1.998142 -2.245014 1.356428
C -2.320524 -3.207611 2.374299
H -2.402875 -4.165383 1.854179
H -1.525507 -3.261180 3.132301
C 0.222167 -3.880674 -3.857250
H -2.724867 0.318896 -5.692297
H -1.070695 0.257918 -5.012974
H -1.545597 -0.899866 -6.299974
H 1.090341 -3.529626 -4.442319
H -0.628407 -3.976335 -4.550753
H 0.458097 -4.892784 -3.485027

6.4 Monocationc Cr^{II}/Cr^{IV} mechanism for complex 1

Structure: C_2H_4

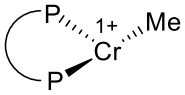
Spin state: singlet

E = -727.28 kcal mol-1
H = -693.80 kcal mol-1
-TS = -15.63 kcal mol-1
G (298.15 K) = -709.43 kcal mol-1

C 0.0 0.666922 0.0
C 0.0 -0.666922 0.0

H -0.930015 1.239355 0.0
H 0.930015 1.239355 0.0
H -0.930015 -1.239355 0.0
H 0.930015 -1.239355 0.0

Structure:



Spin state: singlet

E = -8685.41 kcal mol-1
H = -8358.34 kcal mol-1
TS = -60.42 kcal mol-1
G (298.15 K) = -8418.75 kcal mol-1

H -1.210960 8.309286 13.115307
C -1.308164 3.972784 10.017548
C -0.176517 8.037912 13.329610
C 1.997782 8.602861 14.237869
C 1.625728 6.415263 13.259738
C 0.299085 6.775968 12.971014
H 0.298758 9.938143 14.242691
H -2.049260 3.504713 14.474112
H -0.788743 4.931715 9.970531
H -0.772751 0.708013 10.897716
H -1.770714 2.637425 12.952342
C -1.465125 3.507885 13.544537
H 5.878424 2.762098 16.591575
C 0.023779 3.460432 13.894629
H 3.512551 7.071912 14.108411
H 0.233715 4.301988 14.574155
C 1.867235 1.434104 11.137106
C -0.632357 2.833858 10.487607
C -1.291151 1.594383 10.530944
C 3.338452 -0.947760 11.009355
H 3.904284 -1.878738 10.962567
C -2.623371 1.503880 10.122364
Cr 2.631855 4.543950 10.412920
H -3.137114 0.542626 10.160486
C 2.478411 7.339894 13.886767
C 0.671538 8.951990 13.963646
H -1.723555 4.411022 12.979198
C 3.193048 4.423606 15.307449
C 1.812104 6.185859 9.705645
P 1.055618 3.070701 11.127003
H 3.997443 -0.463180 13.011351
C 4.058871 3.878726 16.256445
H 6.385099 2.509937 14.166344
C 5.487140 3.039646 14.485507
H 2.311225 4.977202 15.631806
C 0.403453 2.152925 14.591919
H -4.341932 2.567891 9.361874
C -3.299848 2.642911 9.674661
H 1.448614 2.170627 14.925935
H 2.660177 9.315153 14.730786
H -0.235102 1.998049 15.472350
H 0.263206 1.298551 13.915365
N 0.911304 3.730939 12.716292
P 2.267509 4.812507 12.665477
C 3.463696 4.266116 13.936224
C 5.202666 3.184270 15.846884
H -0.358614 6.064519 12.470643
H 3.843135 3.999803 17.318594
H -3.166932 4.761550 9.259149
C -2.641210 3.876571 9.619062
H 2.521051 -1.164326 9.017663
C 2.560777 -0.547465 9.915887
C 4.619583 3.578066 13.533341
H 4.841644 3.452438 12.470688
C 3.391322 -0.154402 12.158992
H 1.226237 0.947926 9.117808
C 1.832656 0.640928 9.971838
H 2.711776 1.651729 13.119575
C 2.664542 1.036211 12.223398
H 2.690299 6.866034 9.686035
H 0.983221 6.690793 10.217251
H 1.523240 5.908729 8.671175

Spin state: triplet

E = -8686.89 kcal mol-1
H = -8360.16 kcal mol-1
TS = -59.14 kcal mol-1
G (298.15 K) = -8419.30 kcal mol-1

H -1.578903 7.943367 13.253878
C -1.147178 4.293103 10.103181
C -0.522056 7.799336 13.481540
C 1.552321 8.614924 14.430242
C 1.467852 6.410409 13.419263
C 0.110492 6.610605 13.113384
H -0.299106 9.729422 14.428391
H -1.705734 3.032267 14.679979
H -0.531072 5.195351 10.087778
H -0.971149 0.959032 10.850007
H -1.382142 2.191139 13.155141
C -1.175104 3.107000 13.721722
H 5.895855 2.952999 16.791386
C 0.320107 3.270183 13.997539
H 3.247514 7.288500 14.303047
H 0.443145 4.130906 14.673879
C 1.792626 1.425350 11.046725
C -0.596495 3.071113 10.526087
C -1.388624 1.911522 10.522306
C 3.091958 -1.035153 10.725165
H 3.589270 -1.998202 10.604573
C -2.721608 1.982045 10.114586
Cr 2.653687 4.660963 10.303891
H -3.335031 1.080544 10.114784
C 2.190873 7.426737 14.068921
C 0.196724 8.801639 14.141211
H -1.587352 3.955356 13.162729
C 3.252358 4.655677 15.473748
C 2.449464 4.019273 8.379321
P 1.111290 3.110328 11.159436
H 4.059513 -0.591985 12.608236
C 4.116620 4.125568 16.432687

H 6.345202 2.561086 14.373185
C 5.474999 3.141537 14.681066
H 2.391983 5.247805 15.787167
C 0.906144 2.028796 14.672399
H -4.313242 3.254688 9.396598
C -3.270342 3.203805 9.711501
H 1.966141 2.168763 14.917355
H 2.115603 9.395662 14.942556
H 0.364350 1.829321 15.607327
H 0.802989 1.146836 14.026494
N 1.098206 3.676847 12.775843
P 2.316093 4.914136 12.797178
C 3.492969 4.424507 14.107967
C 5.223388 3.365527 16.038330
H -0.452172 5.831441 12.597326
H 3.925564 4.304364 17.491444
H -2.905884 5.309593 9.376228
C -2.482042 4.359566 9.703007
H 2.001812 -1.190720 8.863619
C 2.197964 -0.583891 9.748309
C 4.614396 3.672221 13.718129
H 4.809115 3.493929 12.657637
C 3.355096 -0.247113 11.850332
H 0.870564 0.995932 9.125215
C 1.553139 0.644375 9.899746
H 2.938770 1.601115 12.878651
C 2.718115 0.984203 12.008266
H 3.153230 4.662823 7.809916
H 1.440117 4.168686 7.964624
H 2.742193 2.969613 8.221598

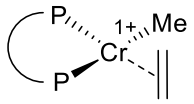
Spin state: quintet

E = -8714.07 kcal mol-1
H = -8386.71 kcal mol-1
TS = -61.43 kcal mol-1
G (298.15 K) = -8448.14 kcal mol-1

H -1.462560 8.085667 13.217089
C -1.197646 4.199793 10.062676
C -0.420806 7.894583 13.477625
C 1.646059 8.600987 14.524139
C 1.515988 6.430914 13.445911
C 0.179707 6.693769 13.097000
H -0.160044 9.786721 14.489462
H -1.781068 3.244272 14.644404
H -0.604445 5.116247 10.021120
H -0.930251 0.893293 10.904902
H -1.519736 2.397145 13.110880
C -1.246553 3.289069 13.686378
H 5.875349 2.816283 16.745823
C 0.256440 3.345016 13.965298
H 3.293180 7.213580 14.419986
H 0.433615 4.182949 14.657497
C 1.810233 1.434170 11.086542
C -0.616089 3.005668 10.521453
C -1.373906 1.823359 10.548197
C 3.177084 -0.996120 10.823037
H 3.701333 -1.947418 10.724968
C -2.706496 1.844773 10.134391

Cr 2.619940 4.707527 10.258532
H -3.294984 0.927175 10.158744
C 2.251893 7.398979 14.152235
C 0.310585 8.849043 14.192149
H -1.596326 4.170996 13.137364
C 3.228457 4.547744 15.474114
C 2.372605 4.222372 8.276487
P 1.085757 3.103482 11.154686
H 4.090438 -0.507014 12.721687
C 4.086430 3.983702 16.418715
H 6.359390 2.542256 14.318397
C 5.478466 3.097706 14.641402
H 2.359710 5.118743 15.803419
C 0.759230 2.056268 14.615648
H -4.330223 3.051880 9.377196
C -3.287393 3.039439 9.696428
H 1.819328 2.132692 14.886874
H 2.219094 9.344401 15.079381
H 0.186070 1.859841 15.532305
H 0.625397 1.199055 13.942371
N 1.065159 3.724430 12.752142
P 2.323899 4.923789 12.801230
C 3.486278 4.379789 14.101687
C 5.207205 3.255250 16.003936
H -0.391391 5.952440 12.536491
H 3.880664 4.112132 17.481987
H -2.981477 5.144571 9.302433
C -2.532304 4.216579 9.657607
H 2.131430 -1.201062 8.940869
C 2.293175 -0.579135 9.821990
C 4.621892 3.659644 13.692596
H 4.830553 3.529909 12.627998
C 3.395168 -0.189204 11.943798
H 0.939333 0.958609 9.151708
C 1.615347 0.634445 9.944033
H 2.909256 1.657609 12.941428
C 2.724026 1.027278 12.072925
H 3.053322 4.900567 7.722460
H 1.350179 4.382584 7.901816
H 2.669401 3.184816 8.055949

Geometry:



Spin state: singlet

E = -9450.86 kcal mol-1
H = -9088.97 kcal mol-1
TS = -63.97 kcal mol-1
G (298.15 K) = -9152.94 kcal mol-1

H -1.937726 7.341656 13.420923
C -1.080128 4.496309 10.195085
C -0.849902 7.360005 13.497053
C 1.199179 8.530749 14.043026
C 1.287849 6.233127 13.262746
C -0.112796 6.224925 13.152751

H -0.773421 9.397756 14.212259
H -1.313774 2.212267 14.806316
H -0.348887 5.309819 10.193272
H -1.381677 1.167300 10.909963
H -0.837222 1.532618 13.241402
C -0.855333 2.454296 13.838699
H 6.361169 3.715086 16.493234
C 0.559685 2.975048 14.071807
H 3.028607 7.417149 13.796087
H 0.494556 3.891223 14.681358
C 1.461886 1.236173 10.934141
C -0.700165 3.203148 10.598573
C -1.657797 2.174698 10.598351
C 2.413691 -1.359040 10.460739
H 2.775600 -2.371917 10.281856
C -2.970630 2.440922 10.209209
Cr 2.624642 4.680641 10.386549
H -3.708741 1.637952 10.213586
C 1.941637 7.399054 13.703504
C -0.196357 8.512942 13.941503
H -1.490863 3.187254 13.327830
C 3.427400 4.926219 15.249014
C 3.998999 3.300166 9.980058
P 1.038866 2.995514 11.133820
H 3.624853 -1.067457 12.228232
C 4.424357 4.617898 16.175954
H 6.656205 3.077014 14.104000
C 5.749426 3.590735 14.424758
H 2.524629 5.443405 15.574874
C 1.414637 1.951129 14.825529
H -4.369523 3.934920 9.514507
C -3.341782 3.732324 9.818282
H 2.455681 2.283558 14.918027
H 1.711308 9.428177 14.391366
H 1.010201 1.815954 15.838071
H 1.392424 0.976446 14.322041
N 1.208058 3.433418 12.795564
P 2.256427 4.798253 12.676916
C 3.589907 4.563700 13.900372
C 5.583392 3.950828 15.765975
H -0.628373 5.330578 12.802711
H 4.294938 4.898063 17.221951
H -2.680142 5.767993 9.502331
C -2.395644 4.761536 9.811347
H 1.125413 -1.344409 8.724547
C 1.484761 -0.783739 9.588006
C 4.756191 3.895117 13.492564
H 4.883455 3.612696 12.447530
C 2.887355 -0.628727 11.555220
H 0.300276 0.952834 9.118561
C 1.013384 0.510793 9.815066
H 2.819348 1.246841 12.619621
C 2.425247 0.668020 11.785023
H 3.737653 3.129835 8.913475
H 4.024587 2.332552 10.495759
H 4.977486 3.806530 10.033994
C 3.169184 6.382092 9.284150
C 3.559488 6.634824 10.612931
H 2.277063 6.869876 8.874849
H 3.896897 6.042983 8.539765
H 2.993445 7.337033 11.227250
H 4.592889 6.473819 10.931632

Spin state: triplet

E = -9461.06 kcal mol-1
H = -9099.04 kcal mol-1
TS = -63.83 kcal mol-1
G (298.15 K) = -9162.87 kcal mol-1

H -1.910121 7.420858 13.411726
C -1.188111 4.438512 10.240780
C -0.822210 7.420059 13.488507
C 1.246858 8.554825 14.037816
C 1.295772 6.257719 13.254788
C -0.104691 6.273065 13.142529
H -0.710864 9.455057 14.206178
H -1.378274 2.319015 14.809790
H -0.488321 5.278707 10.234560
H -1.341044 1.086298 10.889977
H -0.940913 1.608333 13.247301
C -0.920675 2.535200 13.835560
H 6.326242 3.644654 16.483708
C 0.513086 3.009315 14.053944
H 3.056976 7.409241 13.792678
H 0.482424 3.922286 14.670942
C 1.479942 1.259925 10.922073
C -0.748676 3.153863 10.608778
C -1.663993 2.088010 10.605894
C 2.505633 -1.307840 10.453643
H 2.896815 -2.310080 10.276428
C -2.995141 2.309915 10.252338
Cr 2.611516 4.723107 10.366362
H -3.700395 1.478010 10.254795
C 1.970128 7.411091 13.698051
C -0.148858 8.560799 13.934883
H -1.535289 3.284301 13.322429
C 3.407461 4.896822 15.245640
C 4.023693 3.351288 9.960310
P 1.005336 3.007312 11.113433
H 3.686242 -0.989974 12.236946
C 4.399165 4.569584 16.171544
H 6.620564 3.027694 14.088883
C 5.717987 3.546757 14.412769
H 2.509910 5.421557 15.573954
C 1.342894 1.953835 14.791281
H -4.469305 3.762116 9.628534
C -3.427067 3.593903 9.902306
H 2.391369 2.260407 14.889755
H 1.773838 9.442697 14.388399
H 0.934883 1.812094 15.801545
H 1.298581 0.988225 14.271955
N 1.165651 3.460826 12.775536
P 2.239546 4.805475 12.675527
C 3.569015 4.544111 13.894104
C 5.552252 3.894905 15.757221
H -0.634795 5.386957 12.792978
H 4.271269 4.842450 17.219641
H -2.853529 5.660239 9.615289
C -2.522361 4.659770 9.895670

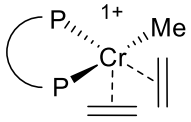
H 1.239141 -1.321979 8.701281
C 1.573056 -0.754613 9.570557
C 4.729919 3.869235 13.481193
H 4.858043 3.598390 12.433339
C 2.946037 -0.568611 11.555813
H 0.348629 0.951472 9.091424
C 1.065158 0.526355 9.795210
H 2.814956 1.300260 12.625281
C 2.446673 0.714691 11.783637
H 5.020824 3.813987 10.000185
H 3.751485 3.158381 8.901542
H 4.001474 2.400194 10.506088
C 3.409611 6.366689 9.317170
C 3.729725 6.570914 10.674337
H 2.595289 6.940582 8.859122
H 4.156394 5.979414 8.618240
H 3.182385 7.315337 11.256643
H 4.723513 6.328542 11.058540

Spin state: quintet

E = -9463.58 kcal mol-1
H = -9102.03 kcal mol-1
TS = -65.55 kcal mol-1
G (298.15 K) = -9167.58 kcal mol-1

H -1.448164 8.051459 13.071860
C -1.303533 4.113109 10.152437
C -0.398398 7.869059 13.305082
C 1.722108 8.640205 14.185522
C 1.513693 6.372685 13.342661
C 0.167365 6.623470 13.026084
H -0.065873 9.851252 14.100595
H -1.749899 3.130423 14.733577
H -0.712953 5.030264 10.091183
H -0.997558 0.807141 10.975420
H -1.502864 2.257077 13.212153
C -1.237275 3.166497 13.763215
H 5.875193 2.904587 16.788616
C 0.270154 3.259504 14.005947
H 3.341008 7.215077 14.161022
H 0.445759 4.114960 14.677886
C 1.732644 1.350109 11.069967
C -0.701985 2.920355 10.588094
C -1.456397 1.737125 10.638190
C 3.058790 -1.101208 10.772153
H 3.565260 -2.060739 10.661755
C -2.803385 1.755804 10.273872
Cr 2.534641 4.728907 10.238984
H -3.388342 0.836566 10.317179
C 2.292993 7.394644 13.914951
C 0.377420 8.878956 13.883270
H -1.618474 4.028057 13.202447
C 3.245226 4.613542 15.452532
C 2.129849 4.186344 8.278011
P 1.027090 3.030619 11.152490
H 4.006145 -0.637324 12.660137
C 4.112835 4.098198 16.416418
H 6.286021 2.430562 14.378475
C 5.430978 3.036994 14.678865
H 2.398828 5.230106 15.757521
C 0.812923 1.995717 14.674192
H -4.457377 2.960605 9.580729
C -3.403410 2.950010 9.861072
H 1.878446 2.097570 14.914892
H 2.328326 9.424661 14.639877
H 0.268347 1.811527 15.610642
H 0.676673 1.120952 14.024540
N 1.042548 3.628639 12.769298
P 2.295238 4.822081 12.774727
C 3.463558 4.335537 14.091784
C 5.200926 3.306785 16.031536
H -0.436965 5.838915 12.568899
H 3.939150 4.312316 17.471649
H -3.117054 5.056542 9.462028
C -2.652734 4.128790 9.797777
H 1.981468 -1.278563 8.905297
C 2.167223 -0.664003 9.786927
C 4.567448 3.553029 13.710680
H 4.743166 3.339232 12.653761
C 3.305549 -0.303659 11.893587
H 0.823717 0.896066 9.148127
C 1.509535 0.559067 9.926700
H 2.860433 1.543446 12.910084
C 2.654968 0.922725 12.039082
H 2.637395 4.862340 7.569929
H 1.051683 4.191657 8.051279
H 2.504019 3.161790 8.108111
C 3.098517 7.047551 9.868358
C 4.283498 6.384273 9.872436
H 2.712042 7.527176 10.772120
H 2.549243 7.219670 8.939738
H 4.891239 6.314596 10.777660
H 4.722506 6.002569 8.947474

Geometry:



Spin state: singlet

E = -10187.48 kcal mol-1
H = -9789.74 kcal mol-1
TS = -67.40 kcal mol-1
G (298.15 K) = -9857.14 kcal mol-1

H -2.121822 6.999166 13.572283
C -1.257665 4.370143 10.344198
C -1.036794 7.096882 13.623209
C 0.932891 8.390868 14.174873
C 1.172056 6.145407 13.279133
C -0.227301 6.039773 13.206317
H -1.091152 9.106088 14.420009
H -1.187437 2.136082 14.850253
H -0.617747 5.249097 10.296231
H -1.106915 1.009955 10.947774
H -0.775092 1.466833 13.263990

C -0.758054 2.381501 13.869992
H 6.590630 5.482115 16.300211
C 0.670843 2.877817 14.071686
H 2.829782 7.421475 13.861763
H 0.623448 3.775087 14.709313
C 1.569031 1.332646 10.771295
C -0.699158 3.126308 10.682947
C -1.522689 1.986238 10.700379
C 2.499732 -1.233558 10.127698
H 2.856256 -2.234106 9.880572
C -2.881384 2.096867 10.404975
Cr 2.624732 4.649789 10.249124
H -3.511035 1.206732 10.422236
C 1.746552 7.329652 13.774425
C -0.458478 8.277272 14.100571
H -1.400905 3.127725 13.390017
C 3.484308 4.630088 15.179661
C 1.717232 4.127359 8.529495
P 1.080854 3.058392 11.122937
H 3.589263 -1.133572 11.993366
C 4.546594 4.819411 16.064547
H 6.857679 6.072560 13.893048
C 5.917480 5.654812 14.254609
H 2.529081 4.282798 15.569328
C 1.521861 1.808980 14.766055
H -4.496484 3.425561 9.858685
C -3.433776 3.342531 10.089468
H 2.581924 2.088896 14.800295
H 1.387859 9.306806 14.553471
H 1.170983 1.671530 15.798360
H 1.429702 0.843650 14.251758
N 1.315764 3.366096 12.803835
P 2.242186 4.805114 12.623012
C 3.643835 4.911594 13.811529
C 5.765443 5.328236 15.604068
H -0.687857 5.132068 12.819412
H 4.416047 4.584088 17.121403
H -3.041174 5.448862 9.794896
C -2.619062 4.477988 10.056474
H 1.321810 -1.036675 8.324327
C 1.638118 -0.561962 9.253684
C 4.863357 5.445081 13.362226
H 4.987303 5.712552 12.313290
C 2.909328 -0.617943 11.314381
H 0.496734 1.226685 8.883616
C 1.175067 0.716561 9.568469
H 2.801711 1.155453 12.537187
C 2.456070 0.663706 11.630135
H 2.345428 4.851666 7.964398
H 0.666109 4.271269 8.266766
H 2.045264 3.102085 8.282118
C 4.733695 4.283177 9.934774
C 4.338345 3.356823 10.902408
H 5.357601 5.138717 10.198910
H 4.762122 4.001692 8.877051
C 1.528820 6.493081 10.114325
C 2.897943 6.707997 10.447645
H 0.772905 6.727199 10.863294
H 1.194195 6.638392 9.085294
H 4.687072 3.414184 11.930764
H 4.008668 2.363525 10.589321
H 3.184031 7.183284 11.388290
H 3.627631 6.884805 9.646844

Spin state: triplet

E = -10202.41 kcal mol-1
H = -9804.58 kcal mol-1
TS = -69.57 kcal mol-1
G (298.15 K) = -9874.15 kcal mol-1

H -1.547628 7.999036 13.839606
C -1.726707 3.897902 10.375580
C -0.466079 7.865875 13.795757
C 1.772096 8.742514 14.092902
C 1.456350 6.455118 13.343928
C 0.066013 6.640940 13.386475
H -0.031705 9.874451 14.463356
H -1.649012 2.959470 14.911675
H -1.327568 4.910060 10.340641
H -0.773818 0.674065 11.013781
H -1.477394 2.185820 13.326275
C -1.219467 3.078251 13.908266
H 6.126256 3.354413 16.530216
C 0.295944 3.251671 14.035692
H 3.392291 7.383590 13.669752
H 0.480275 4.081373 14.736659
C 1.778523 1.619640 10.932923
C -0.888025 2.819571 10.704898
C -1.412893 1.516249 10.747572
C 3.513981 -0.522499 10.397082
H 4.184101 -1.357461 10.189592
C -2.762219 1.299821 10.466293
Cr 2.430194 4.654450 10.129249
H -3.166650 0.287692 10.504361
C 2.309027 7.517964 13.693339
C 0.384943 8.917779 14.146609
H -1.694191 3.943057 13.428371
C 3.280570 4.771095 15.297322
C 2.029610 3.858352 8.264161
P 0.842297 3.182228 11.132714
H 4.485116 0.006662 12.255920
C 4.237885 4.361016 16.225825
H 6.459041 2.864783 14.110647
C 5.563593 3.389662 14.444737
H 2.404278 5.327064 15.631989
C 0.963454 1.990527 14.586477
H -4.648552 2.203421 9.923243
C -3.594493 2.376737 10.143367
H 2.032973 2.152489 14.770147
H 2.437809 9.561503 14.367628
H 0.494569 1.709530 15.539327
H 0.845275 1.150235 13.889043
N 0.932648 3.725076 12.760566
P 2.184078 4.916657 12.680011
C 3.450454 4.479243 13.931329
C 5.377320 3.668185 15.801942
H -0.598370 5.823932 13.103528
H 4.097411 4.586852 17.283537
H -3.722568 4.514276 9.842224

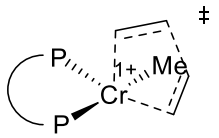
C -3.075806 3.674552 10.098612
H 2.344534 -0.811864 8.600091
C 2.479479 -0.216705 9.504003
C 4.605337 3.795909 13.513535
H 4.757663 3.575232 12.456417
C 3.684796 0.242731 11.553529
H 0.834621 1.094693 9.046664
C 1.621505 0.851268 9.761016
H 2.961895 1.894921 12.727039
C 2.824888 1.310213 11.819809
H 2.393021 4.588858 7.522076
H 0.962017 3.668685 8.077757
H 2.589290 2.919031 8.130319
C 4.684414 5.609473 10.202820
C 4.613005 4.352256 9.665654
H 4.789488 5.772481 11.276269
H 4.835411 6.481767 9.569183
C 0.916542 6.199759 9.947255
C 2.172215 6.806778 9.808924
H 0.332298 6.379636 10.849948
H 0.351360 5.911256 9.059864
H 4.673296 3.453311 10.293821
H 4.722401 4.188007 8.593882
H 2.572395 7.422956 10.615674
H 2.582706 6.999127 8.816234

Spin state: quintet

E = -10209.58 kcal mol-1
H = -9812.45 kcal mol-1
TS = -69.99 kcal mol-1
G (298.15 K) = -9882.44 kcal mol-1

H -1.948950 7.502608 13.573257
C -1.436957 4.077482 10.398141
C -0.859119 7.513636 13.616799
C 1.213484 8.685106 14.060262
C 1.262024 6.361935 13.354414
C -0.140952 6.362260 13.285616
H -0.746632 9.573593 14.261424
H -1.323076 2.494461 14.954319
H -0.895125 5.024811 10.366603
H -0.922331 0.752060 11.006309
H -1.001711 1.736890 13.385749
C -0.904237 2.669587 13.954693
H 6.204156 3.635259 16.610092
C 0.560233 3.081253 14.097814
H 3.026959 7.548713 13.792375
H 0.601262 3.963616 14.756854
C 1.796548 1.445053 10.939539
C -0.752636 2.896508 10.731518
C -1.443489 1.674421 10.747717
C 3.316958 -0.835595 10.337641
H 3.903222 -1.725699 10.106676
C -2.805400 1.640687 10.445203
Cr 2.366406 4.839101 10.169438
H -3.339772 0.690159 10.459800
C 1.936579 7.535842 13.735538
C -0.184436 8.675664 14.003246
H -1.507238 3.437188 13.454860
C 3.341343 4.985577 15.341705
C 1.689917 4.247092 8.279524
P 1.010537 3.075477 11.165362
H 4.417293 -0.384381 12.143522
C 4.311467 4.623756 16.277935
H 6.513225 3.029931 14.213848
C 5.621923 3.572577 14.530289
H 2.456494 5.536682 15.661817
C 1.391642 1.962848 14.731695
H -4.549731 2.789861 9.893650
C -3.485200 2.821515 10.129067
H 2.441480 2.258321 14.849374
H 1.742579 9.589307 14.362986
H 0.991571 1.730415 15.728185
H 1.342421 1.048703 14.125939
N 1.152527 3.576847 12.807259
P 2.217120 4.935073 12.724048
C 3.504404 4.637187 13.989881
C 5.448272 3.914865 15.875257
H -0.669102 5.462658 12.968225
H 4.178686 4.893557 17.326318
H -3.327657 4.960504 9.847922
C -2.800864 4.041278 10.106129
H 2.053545 -1.022942 8.592323
C 2.278385 -0.441977 9.487618
C 4.655451 3.936158 13.591066
H 4.792509 3.668162 12.542478
C 3.604969 -0.083057 11.480872
H 0.725992 1.002685 9.101594
C 1.523663 0.695810 9.779130
H 3.099341 1.651153 12.658371
C 2.855683 1.056913 11.777912
H 2.254014 4.844434 7.542315
H 0.615295 4.441682 8.143690
H 1.871857 3.181229 8.073510
C 4.813160 4.816164 9.774652
C 4.430570 3.516361 9.705960
H 5.167294 5.261240 10.707768
H 4.908692 5.422658 8.872132
C 1.163970 6.973318 9.879193
C 2.489867 7.256324 9.778129
H 0.633821 7.101465 10.825322
H 0.567251 6.749536 8.993782
H 4.449230 2.855322 10.574628
H 4.187142 3.044432 8.753983
H 3.057051 7.615697 10.639676
H 2.991940 7.278189 8.808853

Geometry:



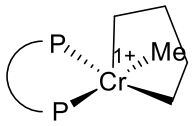
Spin state: triplet

E = -10197.04 kcal mol-1
H = -9799.11 kcal mol-1
TS = -67.01 kcal mol-1

G (298.15 K) = -9866.11 kcal mol-1

H -1.608744 7.905300 13.666367
C -1.558700 3.965683 10.415335
C -0.525064 7.786163 13.696161
C 1.675297 8.687945 14.157556
C 1.443609 6.406326 13.362639
C 0.050155 6.574041 13.309147
H -0.165212 9.790312 14.420451
H -1.617196 2.898828 14.882103
H -1.093341 4.950444 10.426743
H -0.812856 0.666420 10.927879
H -1.371239 2.081981 13.328171
C -1.161687 3.001233 13.888343
H 6.118229 3.111079 16.479628
C 0.342131 3.226722 14.055584
H 3.340351 7.358462 13.823525
H 0.481394 4.093596 14.721491
C 1.796405 1.472635 11.006978
C -0.789089 2.824429 10.698072
C -1.395022 1.557170 10.691245
C 3.346261 -0.830462 10.592928
H 3.941420 -1.730859 10.435981
C -2.755624 1.438678 10.402977
Cr 2.424436 4.767363 10.155762
H -3.223937 0.453737 10.402356
C 2.256062 7.476272 13.779872
C 0.285387 8.843914 14.119847
H -1.649879 3.833392 13.366815
C 3.378898 4.756353 15.290037
C 2.050457 3.817495 8.361500
P 0.953647 3.087686 11.160769
H 4.286254 -0.342023 12.478587
C 4.318528 4.275502 16.203144
H 6.355865 2.571581 14.059969
C 5.518415 3.178739 14.405257
H 2.549075 5.371908 15.638879
C 1.022988 2.013046 14.692006
H -4.580740 2.479165 9.899209
C -3.518056 2.577341 10.123894
H 2.088602 2.200167 14.873860
H 2.309020 9.511632 14.488244
H 0.548431 1.792111 15.657948
H 0.919178 1.126236 14.052762
N 1.009131 3.660046 12.779611
P 2.217294 4.892074 12.700060
C 3.499847 4.442868 13.924436
C 5.385420 3.484658 15.763173
H -0.581210 5.753258 12.967301
H 4.217080 4.516942 17.261826
H -3.511340 4.729760 9.911458
C -2.918755 3.841114 10.131741
H 2.239477 -1.050532 8.747480
C 2.389300 -0.449849 9.645393
C 4.581401 3.658108 13.487910
H 4.683695 3.412121 12.430187
C 3.539638 -0.053029 11.737838
H 0.887160 0.989209 9.091287
C 1.621105 0.697847 9.843031
H 2.939169 1.699710 12.832422
C 2.775387 1.097459 11.941350
H 2.298932 4.520600 7.551774
H 1.039021 3.424913 8.190878
H 2.762895 2.972660 8.356481
C 4.129142 6.185654 9.312432
C 4.460299 5.135188 10.252131
H 4.508993 7.179106 9.544854
H 4.209803 5.941437 8.251331
C 1.057638 6.276909 9.783330
C 2.235283 7.005931 9.351324
H 0.576995 6.632954 10.699860
H 0.364443 5.935428 9.010679
H 4.917386 5.429241 11.199314
H 4.835558 4.179762 9.858325
H 2.539195 7.820742 10.008781
H 2.306152 7.253151 8.290822

Geometry:



Spin state: singlet

E = -10198.56 kcal mol-1
H = -9801.17 kcal mol-1
TS = -66.51 kcal mol-1
G (298.15 K) = -9867.67 kcal mol-1

H -1.583534 7.894504 13.509421
C -1.552137 3.915641 10.320269
C -0.508473 7.727023 13.582983
C 1.706229 8.522873 14.161847
C 1.414067 6.275783 13.297587
C 0.031313 6.501598 13.190935
H -0.095767 9.696692 14.371154
H -1.745983 2.853628 14.877003
H -1.025944 4.869188 10.290832
H -1.033462 0.605244 11.011975
H -1.463797 1.983526 13.358383
C -1.268716 2.922418 13.890741
H 6.401225 3.036469 15.991227
C 0.231039 3.155244 14.078081
H 3.328258 7.133737 13.854179
H 0.358787 4.051834 14.706733
C 1.639682 1.263491 11.120634
C -0.863059 2.743508 10.676035
C -1.550117 1.518087 10.716149
C 3.109563 -1.111939 10.838215
H 3.674055 -2.039073 10.732689
C -2.909204 1.472019 10.402671
Cr 2.385586 4.594360 10.262436
H -3.439619 0.519833 10.438668
C 2.252579 7.296921 13.777681
C 0.327599 8.738713 14.067455
H -1.744251 3.735738 13.328934
C 3.476619 4.543494 15.096014
C 2.619908 3.324054 8.702348

P 0.881014 2.923874 11.183339
H 4.115511 -0.516321 12.658182
C 4.513364 4.085055 15.910666
H 6.480345 2.618922 13.536996
C 5.636404 3.153355 13.974344
H 2.641186 5.089817 15.535548
C 0.905125 1.970385 14.773341
H -4.653387 2.600223 9.808658
C -3.591101 2.641730 10.052426
H 1.971203 2.162170 14.947943
H 2.358877 9.311489 14.537914
H 0.427349 1.795773 15.747097
H 0.802103 1.055902 14.174656
N 0.908780 3.531040 12.794477
P 2.115263 4.740694 12.620321
C 3.513457 4.304146 13.711382
C 5.590902 3.389230 15.352111
H -0.617750 5.715248 12.802916
H 4.481361 4.272892 16.984512
H -3.441434 4.776435 9.737237
C -2.912267 3.863907 10.013576
H 1.950817 -1.427155 9.039738
C 2.140627 -0.770023 9.889127
C 4.601977 3.610067 13.156453
H 4.641331 3.420219 12.081398
C 3.356624 -0.259556 11.918123
H 0.672020 0.673748 9.264617
C 1.413147 0.413899 10.020850
H 2.843875 1.587996 12.893106
C 2.633176 0.926030 12.055274
H 3.034513 4.027044 7.954549
H 1.752088 2.809790 8.270191
H 3.384994 2.579357 8.978773
C 3.243895 7.402689 10.290472
C 3.793402 6.029695 10.659035
C 1.193891 6.137089 9.705316
C 2.164139 7.214194 9.214230
H 0.578261 6.496995 10.544395
H 0.546548 5.721938 8.913968
H 4.497670 6.019286 11.500970
H 4.306548 5.550725 9.781251
H 4.046441 8.082565 9.957183
H 2.794664 7.861792 11.186158
H 1.641174 8.159646 8.991166
H 2.638682 6.899389 8.268583

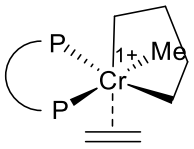
Spin state: triplet

E = -10209.03 kcal mol-1
H = -9811.74 kcal mol-1
TS = -67.02 kcal mol-1
G (298.15 K) = -9878.75 kcal mol-1

H -1.358854 8.173238 13.490392
C -1.595781 3.772011 10.228779
C -0.307891 7.909419 13.612856
C 1.928645 8.479247 14.353201
C 1.500016 6.313297 13.350199
C 0.149247 6.663247 13.183688
H 0.223113 9.794610 14.526587
H -1.945349 3.259434 14.748409
H -1.116740 4.748207 10.159337
H -0.916588 0.524286 11.067274
H -1.764466 2.410781 13.201445
C -1.441776 3.288513 13.773131
H 6.344873 2.808926 15.926964
C 0.072412 3.292573 13.996266
H 3.443865 6.972484 14.055429
H 0.308570 4.133720 14.667823
C 1.694382 1.305836 11.176458
C -0.854115 2.652381 10.642373
C -1.478203 1.396245 10.732592
C 3.227205 -1.037917 11.003890
H 3.816679 -1.953056 10.940342
C -2.831544 1.269292 10.416047
Cr 2.393610 4.609395 10.225987
H -3.314839 0.294611 10.492336
C 2.391786 7.231388 13.931858
C 0.581210 8.819112 14.195428
H -1.776967 4.184754 13.237871
C 3.387559 4.290092 15.101167
C 2.540048 3.400779 8.589659
P 0.868596 2.935049 11.164432
H 4.104400 -0.410089 12.878507
C 4.410559 3.772762 15.896479
H 6.543285 2.722743 13.445611
C 5.656346 3.155753 13.909384
H 2.514430 4.747256 15.568979
C 0.555334 1.994388 14.642551
H -4.625799 2.283280 9.768070
C -3.568090 2.387777 10.012465
H 1.622677 2.044263 14.891148
H 2.622344 9.187862 14.806651
H -0.003439 1.813328 15.570986
H 0.389631 1.139550 13.973167
N 0.831345 3.624822 12.744028
P 2.115317 4.765455 12.622566
C 3.489329 4.232656 13.699763
C 5.544114 3.206056 15.301976
H -0.540966 5.955837 12.723001
H 4.327210 3.817344 16.982940
H -3.521563 4.510313 9.599313
C -2.949384 3.638736 9.918603
H 2.188558 -1.390446 9.139531
C 2.311695 -0.723544 9.993485
C 4.631243 3.665129 13.110304
H 4.720399 3.615357 12.023136
C 3.387918 -0.174722 12.090777
H 0.851899 0.684220 9.271019
C 1.552792 0.444495 10.071174
H 2.775363 1.666188 13.019009
C 2.632341 0.996122 12.174364
H 2.955069 4.123433 7.861202
H 1.629358 2.957591 8.167218
H 3.279991 2.608352 8.788670
C 3.104192 7.463564 10.290432
C 3.745696 6.117179 10.592689
C 1.104345 6.105534 9.692616
C 2.008586 7.250344 9.234659
H 0.496801 6.398210 10.563338

H 0.459214 5.700991 8.897451
H 4.473406 6.120184 11.414775
H 4.256487 5.700047 9.683101
H 3.849581 8.205767 9.957164
H 2.655082 7.863704 11.214336
H 1.428012 8.172899 9.061257
H 2.475732 7.000954 8.266244

Geometry:



Spin state: singlet

E = -10923.10 kcal mol-1
H = -10489.77 kcal mol-1
TS = -68.14 kcal mol-1
G (298.15 K) = -10557.90 kcal mol-1

H -0.643392 8.319800 13.580627
C -1.362576 3.692506 9.923207
C 0.349973 7.889034 13.709987
C 2.601343 8.023745 14.585186
C 1.908079 6.062242 13.328412
C 0.635953 6.637215 13.166045
H 1.113334 9.571530 14.832024
H -2.026292 3.841308 14.227674
H -0.872519 4.655332 9.816428
H -0.794277 0.485719 10.953141
H -1.940862 2.969857 12.684534
C -1.441773 3.722005 13.305537
H 6.444432 2.579789 16.038948
C -0.015612 3.292727 13.678850
H 3.879497 6.338018 14.199554
H 0.345115 3.977359 14.462257
C 1.666697 1.049054 11.122893
C -0.645253 2.583853 10.403832
C -1.318725 1.357427 10.566031
C 2.894945 -1.473280 11.120236
H 3.371670 -2.453998 11.120388
C -2.674869 1.249807 10.253868
Cr 2.807783 4.272775 10.123727
H -3.183482 0.294919 10.391761
C 2.889211 6.767111 14.051032
C 1.334621 8.589248 14.413329
H -1.460053 4.672791 12.763156
C 3.324424 3.256582 14.838536
C 2.022343 3.687407 8.328892
P 1.088101 2.783091 10.993873
H 3.555831 -0.973869 13.117048
C 4.319565 2.790931 15.699751
H 7.069277 3.701473 13.902208
C 6.019476 3.569711 14.166135
H 2.281282 3.154218 15.130957
C -0.021139 1.858324 14.212377
H -4.437927 2.271870 9.534122
C -3.377874 2.358682 9.775499
H 0.954799 1.548404 14.602210
H 3.369746 8.560925 15.142166
H -0.757839 1.773241 15.022439
H -0.309488 1.154551 13.420058
N 0.971910 3.485631 12.559568
P 2.352379 4.496136 12.492190
C 3.667698 3.862270 13.618283
C 5.668513 2.943322 15.364416
H -0.135483 6.104905 12.614544
H 4.039404 2.316915 16.641162
H -3.259555 4.450125 9.240593
C -2.717200 3.579114 9.609835
H 2.108768 -1.680083 9.115654
C 2.186736 -1.039231 9.994632
C 5.024820 4.024382 13.297345
H 5.315371 4.506770 12.365235
C 2.997254 -0.643386 12.240695
H 1.029024 0.546909 9.107174
C 1.576457 0.216297 9.991499
H 2.518016 1.272922 13.098896
C 2.395075 0.615461 12.239801
H 2.524211 2.710474 8.198561
H 2.463405 4.438383 7.653667
H 0.953969 3.581249 8.124566
C 3.059316 7.372209 10.439589
C 3.784679 6.050610 10.436063
C 1.244756 5.817927 9.852880
C 1.873471 7.163322 9.504793
H 0.658962 5.908711 10.776140
H 0.562714 5.504785 9.057614
H 4.680484 6.003327 11.072714
H 4.077607 5.781699 9.384249
H 3.723600 8.191961 10.115487
H 2.726161 7.626945 11.456627
H 1.139242 7.983199 9.578700
H 2.231364 7.154906 8.461247
C 4.891522 3.436242 9.696724
C 4.303934 2.475390 10.488993
H 5.637430 4.121110 10.102304
H 4.884455 3.351276 8.607416
H 4.555090 2.354277 11.540001
H 3.796129 1.627675 10.032023

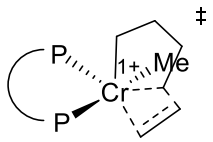
Spin state: triplet

E = -10945.28 kcal mol-1
H = -10511.85 kcal mol-1
TS = -72.98 kcal mol-1
G (298.15 K) = -10584.83 kcal mol-1

H -0.736431 8.325813 13.579733
C -1.435703 3.681198 9.975828
C 0.263428 7.912012 13.714133
C 2.522484 8.110195 14.565981
C 1.845803 6.101975 13.383987
C 0.563705 6.647776 13.206948
H 1.010754 9.639194 14.776918
H -2.046862 3.620637 14.382633
H -0.941677 4.646010 9.878584
H -0.836810 0.464892 10.977212

H -1.920667 2.795662 12.817356
C -1.476878 3.576466 13.445174
H 6.305221 2.272042 15.988696
C -0.009000 3.278188 13.772324
H 3.824182 6.427554 14.215268
H 0.316882 4.015792 14.522480
C 1.718718 1.149861 11.119849
C -0.724299 2.571577 10.461277
C -1.373882 1.331434 10.592822
C 3.100814 -1.288574 11.050916
H 3.636230 -2.238172 11.025470
C -2.720713 1.210870 10.247265
Cr 2.609083 4.400117 10.120610
H -3.221487 0.248133 10.355688
C 2.826011 6.841381 14.069680
C 1.244128 8.647703 14.387513
H -1.592305 4.535617 12.927685
C 3.287416 3.537910 15.031738
C 2.195095 3.505375 8.304355
P 0.987929 2.824879 11.038955
H 3.815943 -0.755116 13.019990
C 4.261463 2.962030 15.847569
H 6.864557 2.899007 13.642436
C 5.859042 3.066199 14.029893
H 2.301175 3.750834 15.443421
C 0.156408 1.869104 14.342099
H -4.479231 2.222002 9.504376
C -3.426346 2.320285 9.771283
H 1.178710 1.687279 14.693393
H 3.286615 8.679932 15.095787
H -0.528414 1.729752 15.189430
H -0.087822 1.113362 13.582986
N 0.903493 3.535117 12.606197
P 2.306215 4.538026 12.571347
C 3.585332 3.854754 13.693616
C 5.546040 2.719544 15.346284
H -0.199934 6.079297 12.677411
H 4.022417 2.712053 16.882003
H -3.329973 4.419220 9.259736
C -2.782262 3.554032 9.634469
H 2.236709 -1.543061 9.083574
C 2.314187 -0.899274 9.960374
C 4.881143 3.631201 13.207167
H 5.124930 3.909360 12.183740
C 3.200922 -0.457635 12.169999
H 1.024191 0.615828 9.131979
C 1.627495 0.314855 9.989538
H 2.631918 1.415815 13.065780
C 2.521687 0.761631 12.202583
H 2.647882 2.516310 8.157030
H 2.720721 4.242484 7.665857
H 1.139321 3.483121 8.005652
C 3.252446 7.308285 10.372473
C 3.947494 5.959841 10.437319
C 1.255207 5.942582 9.776633
C 2.078857 7.173335 9.395785
H 0.669745 6.132461 10.688350
H 0.577801 5.625995 8.971367
H 4.775429 5.894184 11.156066
H 4.341895 5.680246 9.428179
H 3.946997 8.108787 10.063016
H 2.882458 7.588511 11.371444
H 1.453307 8.082229 9.385393
H 2.471708 7.059780 8.370944
C 5.292995 3.152292 9.509243
C 4.714841 2.111585 10.121673
H 5.975460 3.824303 10.032550
H 5.151536 3.337871 8.442855
H 4.890713 1.890463 11.173674
H 4.074693 1.411565 9.586269

Geometry:



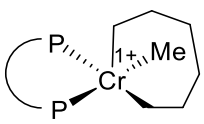
Spin state: triplet

E = -10922.77 kcal mol-1
H = -10489.63 kcal mol-1
TS = -69.02 kcal mol-1
G (298.15 K) = -10558.65 kcal mol-1

H -0.550897 8.409213 13.788427
C -1.399722 3.381157 9.684821
C 0.449046 7.979865 13.862562
C 2.755368 8.138643 14.573392
C 1.968436 6.126631 13.453512
C 0.691226 6.702093 13.353587
H 1.290284 9.702358 14.861693
H -2.008985 3.871175 14.190717
H -0.959360 4.318763 9.364272
H -0.666414 0.504284 11.368879
H -1.895928 2.882417 12.722515
C -1.425276 3.702037 13.275752
H 5.896450 1.924882 16.335198
C 0.023673 3.376729 13.663609
H 3.995493 6.423055 14.175805
H 0.338117 4.129737 14.402336
C 1.763935 1.156413 11.152912
C -0.641015 2.460172 10.422801
C -1.237388 1.242300 10.807728
C 3.061189 -1.332785 11.214248
H 3.561900 -2.301257 11.239486
C -2.566618 0.973019 10.484296
Cr 2.638143 4.582317 9.980872
H -3.016160 0.029763 10.796516
C 3.000236 6.858920 14.072864
C 1.480683 8.704000 14.466681
H -1.487826 4.603728 12.654499
C 3.199194 3.680204 15.209845
C 2.194356 4.258657 7.964569
P 1.074387 2.850811 10.966698
H 3.681096 -0.776655 13.209687
C 4.039824 3.006190 16.095574
H 6.541489 2.147727 13.938975
C 5.600449 2.568927 14.294545
H 2.281714 4.138744 15.580354

C 0.137017 1.995571 14.307303
H -4.358458 1.695290 9.512613
C -3.318542 1.907066 9.764531
H 1.138128 1.822841 14.719290
H 3.561504 8.693200 15.055281
H -0.589169 1.914012 15.127812
H -0.083726 1.202140 13.581950
N 0.986028 3.591332 12.526211
P 2.414905 4.556658 12.619090
C 3.541101 3.783628 13.848671
C 5.239143 2.446353 15.638417
H -0.123446 6.146509 12.893094
H 3.765236 2.924233 17.147991
H -3.304384 3.833649 8.784988
C -2.729366 3.106698 9.359614
H 2.297273 -1.601841 9.208002
C 2.351546 -0.940791 10.073700
C 4.752917 3.233342 13.404185
H 5.035954 3.323338 12.356437
C 3.128102 -0.479149 12.318108
H 1.155136 0.592129 9.146368
C 1.709438 0.297265 10.039404
H 2.567216 1.427156 13.143605
C 2.489163 0.763006 12.285936
H 1.333947 3.579944 7.870489
H 3.051051 3.822912 7.429376
H 1.935336 5.215260 7.484983
C 3.375707 6.866762 10.167375
C 4.320204 5.868107 9.474823
C 0.926997 5.747012 10.013258
C 1.828035 6.954429 9.778498
H 0.338835 5.805134 10.932350
H 0.279620 5.566352 9.154230
H 5.327970 6.014383 9.865128
H 4.307395 5.970823 8.384154
H 3.763431 7.848681 9.848229
H 3.498338 6.837940 11.258539
H 1.463341 7.798499 10.382305
H 1.791980 7.249099 8.721373
C 4.899663 3.756166 9.587144
C 3.935790 2.779418 9.865135
H 5.641586 3.984736 10.352238
H 5.242580 3.901579 8.562980
H 3.970438 2.277373 10.830169
H 3.512820 2.190840 9.052007

Geometry:



Spin state: singlet

E = -10958.93 kcal mol-1
H = -10524.23 kcal mol-1
TS = -70.87 kcal mol-1
G (298.15 K) = -10595.11 kcal mol-1

H -1.292469 8.197652 12.282939
C -1.429531 3.932829 10.538411
C -0.682338 7.656204 13.006629
C 0.032876 7.284190 15.291630
C 0.973630 5.947635 13.497916
C 0.180017 6.648256 12.575256
H -1.430164 8.762039 14.705797
H -0.780546 4.798688 10.405202
H -1.305502 0.632819 11.413888
C -1.253154 3.438696 14.202171
H 6.523844 4.084736 16.312584
C 0.140072 2.803609 14.297558
H 1.514163 5.744808 15.588465
C 1.376259 0.924277 11.209339
C -0.882670 2.710770 10.958537
C -1.719733 1.591001 11.099535
C 2.361094 -1.645602 10.665974
H 2.739274 -2.646952 10.457617
C -3.086894 1.703730 10.841492
Cr 2.483872 4.248584 10.612776
H -3.732446 0.832053 10.955235
C 0.897927 6.275882 14.862360
C -0.758064 7.972834 14.366758
C 3.726234 3.148401 14.604733
C 1.560641 3.784712 8.798940
P 0.881970 2.666724 11.439257
H 3.326925 -1.510256 12.595592
C 4.867492 3.037770 15.401075
H 5.821196 6.312266 15.447569
C 5.236937 5.423400 15.206995
H 3.132407 2.264830 14.373201
C 0.060721 1.300908 14.559818
H -4.695772 3.014566 10.239096
C -3.627150 2.929408 10.439508
H 1.045315 0.869403 14.775666
H -0.022862 7.533696 16.351843
H -0.591466 1.114054 15.422971
H -0.365786 0.772035 13.696748
N 0.998007 3.104448 13.104939
P 1.958445 4.520527 12.911601
C 3.331765 4.398370 14.105541
C 5.629063 4.172445 15.695484
H 0.234177 6.403467 11.513776
H 5.163353 2.063817 15.792483
H -3.213835 4.995624 9.954854
C -2.795892 4.043237 10.282545
H 1.285443 -1.490044 8.795894
C 1.545834 -0.996706 9.732911
C 4.092828 5.539994 14.416766
H 3.782851 6.522327 14.057054
C 2.691150 -1.008295 11.865559
H 0.414138 0.774444 9.266497
C 1.056050 0.282892 9.998087
H 2.476487 0.770647 13.061704
C 2.209541 0.274102 12.131218
H 2.317615 3.484136 8.057910
H 1.191211 4.793790 8.530098
H 0.716744 3.089121 8.734195
C 5.483599 5.716435 9.689835
C 5.990588 4.297134 9.981953

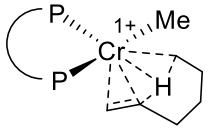
C 3.234905 6.124783 10.910680
C 3.949253 5.846757 9.615040
H 3.894354 6.316252 11.762583
H 2.437017 6.876215 10.856592
H 5.912718 6.052416 8.734782
H 5.853274 6.410887 10.459867
H 3.624156 6.551125 8.833582
H 3.579983 4.866186 9.146985
C 5.417599 3.623903 11.239820
C 4.022480 3.010473 11.100756
H 3.809344 2.376560 11.971843
H 3.952725 2.363248 10.201158
H -1.194161 4.501484 13.941972
H -1.757012 3.351307 15.174382
H -1.871314 2.931220 13.452562
H 0.682459 3.274107 15.134409
H 6.100017 2.801067 11.519724
H 5.440535 4.319497 12.095887
H 7.086256 4.341936 10.068413
H 5.782326 3.652216 9.110423

Spin state: triplet

E = -10967.93 kcal mol-1
H = -10533.95 kcal mol-1
TS = -69.59 kcal mol-1
G (298.15 K) = -10603.53 kcal mol-1

H -1.352629 8.148305 12.329231
C -1.365743 3.928450 10.409285
C -0.726794 7.621305 13.050058
C 0.016455 7.276079 15.330814
C 0.958583 5.940994 13.537200
C 0.146138 6.623305 12.616860
H -1.474142 8.727734 14.748891
H -0.674004 4.747071 10.205046
H -1.416072 0.713753 11.566349
C -1.203662 3.380427 14.261009
H 6.548857 4.113683 16.308539
C 0.200108 2.764248 14.315899
H 1.521418 5.758644 15.623561
C 1.337504 0.887829 11.234160
C -0.886945 2.724699 10.948777
C -1.778928 1.660142 11.164250
C 2.285485 -1.697935 10.703816
H 2.649050 -2.705833 10.501224
C -3.132913 1.811794 10.863552
Cr 2.471029 4.267519 10.575090
H -3.821423 0.983773 11.035557
C 0.891291 6.277057 14.900223
C -0.793527 7.946305 14.408774
C 3.740013 3.161099 14.628286
C 1.720495 3.641470 8.710697
P 0.868922 2.636271 11.445344
H 3.404414 -1.493167 12.542810
C 4.890272 3.057064 15.412649
H 5.826075 6.337038 15.449650
C 5.243518 5.445220 15.215952
H 3.150000 2.273267 14.401925
C 0.149163 1.258286 14.564834
H -4.664386 3.136050 10.107350
C -3.605700 3.021164 10.342676
H 1.145883 0.835805 14.738119
H -0.033587 7.531539 16.389885
H -0.466996 1.055932 15.450709
H -0.303056 0.730233 13.714554
N 1.019370 3.098676 13.103116
P 1.963739 4.535525 12.941212
C 3.332801 4.409290 14.135137
C 5.647381 4.196363 15.700626
H 0.191667 6.371641 11.556535
H 5.196380 2.084694 15.800109
H -3.084119 5.014097 9.685289
C -2.720193 4.077813 10.109593
H 1.066678 -1.607938 8.919913
C 1.397036 -1.082637 9.816471
C 4.091384 5.555527 14.436902
H 3.774683 6.534981 14.074892
C 2.708964 -1.018322 11.850079
H 0.227109 0.671730 9.378664
C 0.923952 0.204839 10.074992
H 2.587618 0.802074 12.994748
C 2.246642 0.272165 12.107626
H 1.406775 4.599588 8.253693
H 0.853339 2.969631 8.698377
H 2.504704 3.199220 8.078523
C 5.482636 5.750838 9.682633
C 6.020773 4.352240 10.016768
C 3.198741 6.175577 10.827044
C 3.946424 5.842946 9.568494
H 3.831729 6.408980 11.687796
H 2.382749 6.902454 10.724548
H 5.926091 6.079295 8.731804
H 5.814862 6.469326 10.447544
H 3.623452 6.485708 8.734944
H 3.610459 4.822096 9.146209
C 5.413444 3.691983 11.265430
C 4.048296 3.036926 11.064127
H 3.773283 2.463911 11.960751
H 4.050126 2.336664 10.209830
H -1.164894 4.449837 14.025487
H -1.689157 3.261834 15.239175
H -1.827093 2.882078 13.509825
H 0.755706 3.233366 15.144737
H 6.105238 2.895429 11.595345
H 5.378584 4.408290 12.103400
H 7.110615 4.431674 10.142857
H 5.862686 3.684643 9.152197
Geometry:

‡



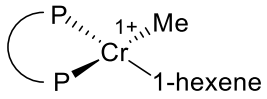
Spin state: triplet

E = -10952.37 kcal mol-1
H = -10517.34 kcal mol-1

TS = -72.21 kcal mol-1
G (298.15 K) = -10589.55 kcal mol-1

H -1.175286 8.316482 12.337949
C -1.498326 3.889751 10.526385
C -0.586680 7.749519 13.059970
C 0.109292 7.342199 15.347194
C 1.015578 5.991135 13.549161
C 0.251646 6.722693 12.624774
H -1.311511 8.862050 14.763990
H -0.837469 4.744465 10.368439
H -1.437994 0.623707 11.532430
C -1.208040 3.463685 14.255461
H 6.558309 3.985132 16.267370
C 0.184449 2.820121 14.280775
H 1.548421 5.759631 15.638219
C 1.330982 0.902589 11.260208
C -0.973357 2.672070 10.989137
C -1.832801 1.576568 11.179069
C 2.424737 -1.635771 10.777759
H 2.842819 -2.626109 10.594908
C -3.197486 1.706114 10.918337
Cr 2.395874 4.280623 10.396755
H -3.860348 0.853244 11.068867
C 0.947345 6.312972 14.915436
C -0.660117 8.056665 14.422440
C 3.672591 3.131887 14.663404
C 1.765891 3.562154 8.562786
P 0.799700 2.637809 11.421492
H 3.663454 -1.257474 12.508837
C 4.824157 2.994317 15.442063
H 5.964513 6.206143 15.307044
C 5.323482 5.342777 15.125107
H 3.027878 2.271463 14.487938
C 0.108330 1.311478 14.508425
H -4.781904 3.023384 10.266340
C -3.714760 2.925787 10.468906
H 1.100433 0.858930 14.623338
H 0.055228 7.587869 16.408437
H -0.469983 1.109795 15.419640
H -0.399488 0.810196 13.673487
N 0.987907 3.156021 13.056560
P 1.974178 4.568514 12.918061
C 3.337182 4.378223 14.114756
C 5.655423 4.095337 15.665858
H 0.322406 6.491673 11.559727
H 5.072931 2.024558 15.874501
H -3.264669 4.965800 9.911416
C -2.863807 4.017520 10.270869
H 1.085332 -1.715500 9.082248
C 1.436831 -1.125706 9.929458
C 4.169287 5.487490 14.355570
H 3.909354 6.466224 13.947591
C 2.882519 -0.869641 11.853864
H 0.128635 0.529464 9.489595
C 0.894103 0.139444 10.161256
H 2.724533 1.004028 12.910014
C 2.348282 0.398419 12.086914
H 0.744415 3.948893 8.400308
H 1.747835 2.466837 8.472115
H 2.443485 3.973711 7.797999
C 5.279557 5.835336 10.689432
C 6.195036 4.598324 10.683576
C 2.815841 6.337850 10.140733
C 4.065281 5.713349 9.767245
H 2.791392 6.955237 11.042796
H 2.142773 6.683590 9.346895
H 5.849090 6.730094 10.391629
H 4.928697 6.013427 11.718828
H 4.305439 5.702375 8.694934
H 4.023112 4.263337 9.854799
C 5.484352 3.333620 11.201157
C 4.303272 2.894971 10.333304
H 3.733670 2.066684 10.769878
H 4.606319 2.597819 9.318016
H -1.150418 4.535216 14.033373
H -1.680585 3.341567 15.239605
H -1.852264 2.986910 13.507625
H 0.760189 3.267888 15.107300
H 6.208035 2.501987 11.252713
H 5.145045 3.508597 12.234654
H 7.076406 4.801967 11.307981
H 6.570456 4.420084 9.661650

Geometry:



Spin state: singlet

E = -10956.50 kcal mol-1
H = -10522.68 kcal mol-1
TS = -69.35 kcal mol-1
G (298.15 K) = -10592.03 kcal mol-1

H -1.626465 7.900503 13.563757
C -1.753552 3.952846 10.591557
C -0.547535 7.754753 13.628329
C 1.655457 8.593603 14.180086
C 1.397769 6.328085 13.342675
C 0.010987 6.533357 13.246777
H -0.164330 9.742020 14.387489
H -1.657697 2.862651 14.940951
H -1.294600 4.938001 10.652959
H -0.988249 0.629189 10.844417
H -1.502825 2.101040 13.347530
C -1.243637 2.991633 13.932266
H 6.319209 3.198085 16.213811
C 0.270810 3.174081 14.042458
H 3.296680 7.227495 13.891059
H 0.456226 4.029206 14.712801
C 1.622677 1.406534 10.966398
C -0.967121 2.798119 10.751142
C -1.577001 1.533512 10.692298
C 3.261853 -0.811629 10.437835
H 3.895281 -1.675313 10.232804
C -2.951239 1.431388 10.467895
Cr 2.437470 4.462671 10.186524

H -3.418945 0.447034 10.426157
C 2.218528 7.371980 13.808029
C 0.272752 8.787599 14.092492
H -1.730447 3.856992 13.466991
C 3.393796 4.632455 15.207795
C 3.006683 3.399424 8.558660
P 0.802507 3.032942 11.129142
H 4.286001 -0.290845 12.269937
C 4.415291 4.209942 16.059355
H 6.474358 2.733680 13.771726
C 5.608518 3.259858 14.174903
H 2.539280 5.176374 15.612003
C 0.944919 1.935038 14.634421
H -4.800969 2.497987 10.137256
C -3.727586 2.583167 10.310146
H 2.018990 2.099039 14.787163
H 2.297691 9.395805 14.545434
H 0.495565 1.701127 15.609239
H 0.807182 1.064878 13.978834
N 0.908397 3.605215 12.750364
P 2.140614 4.808410 12.654303
C 3.470526 4.366062 13.829267
C 5.521069 3.523153 15.545307
H -0.629277 5.730014 12.881356
H 4.350234 4.418025 17.128008
H -3.730067 4.745550 10.258087
C -3.127004 3.844622 10.376552
H 2.061613 -1.072708 8.657503
C 2.230338 -0.474354 9.553577
C 4.588265 3.681936 13.321140
H 4.660389 3.471970 12.251250
C 3.481879 -0.035579 11.578643
H 0.644562 0.903969 9.090191
C 1.420668 0.632125 9.806536
H 2.859439 1.675882 12.725837
C 2.672059 1.071483 11.840141
H 3.739995 3.948613 7.946541
H 2.189941 3.042239 7.914203
H 3.502753 2.516344 9.011418
C 3.168689 7.098043 9.999968
C 4.496419 6.314688 10.141324
C 0.905695 5.915333 9.699299
C 2.168613 6.287177 9.210491
H 0.498467 6.394665 10.593952
H 0.171314 5.501748 9.006195
C 5.419733 6.853649 11.234774
H 5.011249 6.272112 9.169295
H 3.379568 8.063345 9.508967
H 2.765431 7.339492 10.995827
H 2.395110 6.135585 8.150873
H 4.331887 5.226455 10.400238
C 6.744385 6.096883 11.338466
H 4.885704 6.811015 12.198209
H 5.602764 7.921308 11.030363
H 7.303389 6.140680 10.393129
H 6.575101 5.037214 11.581405
H 7.382270 6.518176 12.126421

Spin state: triplet

E = -10967.46 kcal mol-1
H = -10533.62 kcal mol-1
TS = -69.56 kcal mol-1
G (298.15 K) = -10603.17 kcal mol-1

H -1.585813 7.953412 13.550095
C -1.751048 3.928564 10.568655
C -0.511390 7.786593 13.635060
C 1.693746 8.574325 14.250294
C 1.414153 6.331387 13.361793
C 0.033737 6.563346 13.240339
H -0.109848 9.749992 14.444744
H -1.693849 2.929412 14.915649
H -1.299785 4.917473 10.626067
H -0.959987 0.612881 10.845978
H -1.559354 2.172354 13.318215
C -1.274173 3.051128 13.908296
H 6.308389 3.168188 16.229855
C 0.245040 3.187986 14.023467
H 3.316959 7.185157 13.966835
H 0.451398 4.029897 14.704092
C 1.640837 1.409545 10.979585
C -0.955873 2.781262 10.737530
C -1.555454 1.511429 10.686384
C 3.280234 -0.819953 10.500929
H 3.912985 -1.688687 10.315967
C -2.928453 1.396873 10.460158
Cr 2.439437 4.489892 10.176150
H -3.388304 0.408591 10.424301
C 2.243511 7.350773 13.864362
C 0.316837 8.794458 14.138268
H -1.732972 3.933977 13.447779
C 3.365635 4.572741 15.232386
C 2.866103 3.427703 8.490320
P 0.810237 3.033590 11.120638
H 4.294166 -0.267002 12.329414
C 4.385177 4.144317 16.083183
H 6.501974 2.783096 13.776564
C 5.620118 3.277528 14.185327
H 2.497571 5.090405 15.642284
C 0.881577 1.924033 14.603303
H -4.786082 2.446513 10.119840
C -3.713624 2.541368 10.293419
H 1.956962 2.059973 14.773034
H 2.341810 9.356899 14.646557
H 0.413426 1.684184 15.567786
H 0.733417 1.068320 13.931172
N 0.900665 3.617411 12.739190
P 2.144679 4.809639 12.665877
C 3.462748 4.348846 13.847429
C 5.511145 3.496539 15.561872
H -0.612104 5.778864 12.844966
H 4.304004 4.318841 17.156713
H -3.733406 4.703256 10.227655
C -3.123189 3.807967 10.352260
H 2.091256 -1.110326 8.717680
C 2.255352 -0.496445 9.604027
C 4.600366 3.703647 13.332820
H 4.689164 3.528933 12.257935
C 3.494813 -0.023427 11.628480

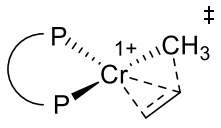
H 0.675248 0.876045 9.105553
C 1.445998 0.615987 9.831767
H 2.866588 1.707394 12.742103
C 2.684831 1.089086 11.864912
H 3.576161 3.971960 7.847497
H 2.005942 3.108055 7.884569
H 3.363472 2.520928 8.889462
C 3.160615 7.102418 9.969269
C 4.498199 6.328116 10.084968
C 0.893829 5.934015 9.709366
C 2.147783 6.302109 9.184717
H 0.504431 6.428290 10.603742
H 0.145719 5.518015 9.033025
C 5.418295 6.852610 11.188376
H 5.008119 6.316144 9.109612
H 3.361273 8.075544 9.490009
H 2.771791 7.330958 10.974318
H 2.346784 6.167812 8.118199
H 4.353122 5.231182 10.312188
C 6.744755 6.098199 11.284264
H 4.881895 6.794523 12.149838
H 5.599999 7.923422 11.001245
H 7.307476 6.159205 10.342215
H 6.578684 5.033977 11.508844
H 7.378250 6.508084 12.081698

Spin state: quintet

E = -10980.57 kcal mol-1
H = -10546.89 kcal mol-1
TS = -69.81 kcal mol-1
G (298.15 K) = -10616.70 kcal mol-1

H -1.999877 7.586625 13.370278
C -1.728156 3.693106 10.467279
C -0.912671 7.551739 13.450530
C 1.190395 8.636891 13.965839
C 1.166779 6.312708 13.259791
C -0.232528 6.371797 13.142342
H -0.736776 9.606003 14.100194
H -1.404456 2.626438 15.108098
H -1.257266 4.670490 10.336032
H -0.960100 0.462612 11.284456
H -1.207081 1.771052 13.569711
C -1.032918 2.725946 14.079638
H 6.324453 3.515498 16.167406
C 0.454682 3.074528 14.123517
H 2.963236 7.427605 13.756155
H 0.570690 3.973629 14.750403
C 1.681850 1.301856 10.995843
C -0.950972 2.586828 10.850094
C -1.555606 1.327242 10.989488
C 3.245229 -0.961706 10.452400
H 3.848011 -1.846801 10.245580
C -2.924317 1.182906 10.759297
Cr 1.929790 4.753445 10.062258
H -3.390798 0.203233 10.868918
C 1.875978 7.458205 13.665159
C -0.203724 8.685244 13.860985
H -1.623914 3.496481 13.569934
C 3.395118 4.918617 15.129021
C 1.398432 4.059540 8.180473
P 0.814594 2.894830 11.187697
H 4.382163 -0.401161 12.204011
C 4.432872 4.544334 15.984368
H 6.417909 2.883231 13.759855
C 5.567641 3.446552 14.145134
H 2.550732 5.489704 15.516648
C 1.278547 1.941889 14.739898
H -4.765109 2.171958 10.209594
C -3.696170 2.289980 10.390943
H 2.338576 2.213756 14.818322
H 1.745926 9.518197 14.288059
H 0.906831 1.726948 15.751103
H 1.188686 1.024647 14.143109
N 0.989781 3.510920 12.787611
P 2.061032 4.858064 12.610012
C 3.438378 4.555463 13.771993
C 5.516066 3.806025 15.495391
H -0.786198 5.492066 12.811614
H 4.393754 4.824416 17.037717
H -3.696535 4.406312 9.944503
C -3.097854 3.545799 10.244724
H 1.943752 -1.257514 8.750270
C 2.175131 -0.632774 9.613746
C 4.534215 3.821866 13.286221
H 4.575091 3.540288 12.232167
C 3.544946 -0.150832 11.551248
H 0.573739 0.751813 9.208700
C 1.398237 0.496681 9.875762
H 3.020413 1.614364 12.670716
C 2.773582 0.981647 11.819443
H 1.795134 4.731896 7.401029
H 0.306078 3.990008 8.053542
H 1.822419 3.053545 8.020545
C 4.133273 7.165112 10.382092
C 5.204177 6.061621 10.373707
C 1.698161 7.087541 9.666292
C 3.022814 6.921509 9.402523
H 1.359752 7.460077 10.638413
H 0.955852 7.013407 8.868278
C 6.261836 6.243725 11.465306
H 5.684338 6.023111 9.382247
H 4.613265 8.125815 10.122154
H 3.716419 7.294171 11.394000
H 3.324495 6.656124 8.381387
H 4.715941 5.076348 10.509531
C 7.360295 5.179995 11.407610
H 5.766792 6.215445 12.450281
H 6.708566 7.246893 11.370864
H 7.912475 5.229268 10.458284
H 6.936181 4.168265 11.491196
H 8.082907 5.306936 12.224421

Geometry:

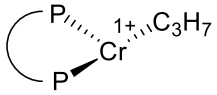


Spin state: quintet

E = -9454.32 kcal mol-1
H = -9092.24 kcal mol-1
TS = -65.05 kcal mol-1
G (298.15 K) = -9157.29 kcal mol-1

H -1.824646 7.672847 13.515052
C -1.340098 4.256526 10.279876
C -0.738426 7.613913 13.593481
C 1.385562 8.636384 14.155022
C 1.315939 6.348014 13.352752
C -0.080585 6.435389 13.234499
H -0.524050 9.632350 14.334371
H -1.529250 2.621569 14.863810
H -0.702835 5.144182 10.251676
H -1.212626 0.912055 10.979464
H -1.196708 1.836856 13.311337
C -1.070412 2.768170 13.877133
H 6.033051 3.255580 16.661119
C 0.407809 3.104623 14.064524
H 3.135431 7.401667 13.895634
H 0.472989 3.985726 14.723489
C 1.605839 1.331529 11.009073
C -0.795391 3.015672 10.655388
C -1.619318 1.878645 10.680623
C 2.911740 -1.117049 10.578843
H 3.410036 -2.073794 10.418666
C -2.969091 1.987116 10.344435
Cr 2.653334 4.736769 10.356522
H -3.604925 1.101476 10.369014
C 2.049249 7.459554 13.805339
C -0.007928 8.713662 14.053697
H -1.616472 3.562537 13.354030
C 3.285814 4.815038 15.378144
C 2.874318 4.409203 8.212605
P 0.962921 3.035635 11.149953
H 4.089942 -0.612612 12.320504
C 4.213446 4.370014 16.321886
H 6.355789 2.699025 14.255154
C 5.492592 3.286654 14.569365
H 2.428775 5.409801 15.696089
C 1.162162 1.947000 14.724686
H -4.565024 3.308364 9.729079
C -3.508535 3.227739 9.987374
H 2.221480 2.189005 14.873345
H 1.957106 9.493501 14.512567
H 0.720401 1.738076 15.708738
H 1.086356 1.035482 14.118083
N 1.063786 3.566354 12.791684
P 2.196857 4.866658 12.752793
C 3.455987 4.491234 14.021617
C 5.311760 3.602625 15.920047
H -0.650696 5.580915 12.867952
H 4.077364 4.620005 17.374672
H -3.109978 5.329786 9.669279
C -2.693245 4.363470 9.955220
H 1.603914 -1.332325 8.870425
C 1.896387 -0.702811 9.711645
C 4.569980 3.733269 13.621739
H 4.710817 3.487358 12.566311
C 3.291410 -0.298168 11.647269
H 0.470006 0.834534 9.222518
C 1.249887 0.518224 9.916205
H 2.962960 1.561656 12.684493
C 2.652262 0.924624 11.856447
H 3.052907 3.342659 8.441043
H 3.335602 4.629312 7.248888
H 1.792486 4.618844 8.124828
C 4.200581 5.872251 8.972312
C 4.196427 6.193465 10.360586
H 3.800489 6.607756 8.272854
H 5.047725 5.308694 8.578846
H 3.755214 7.143087 10.676767
H 5.018263 5.831333 10.984468

Geometry:



Spin state: singlet

E = -9444.62 kcal mol-1
H = -9081.72 kcal mol-1
TS = -62.16 kcal mol-1
G (298.15 K) = -9143.88 kcal mol-1

H -0.875556 8.531180 13.141844
C -1.476084 3.931613 10.098629
C 0.136781 8.170436 13.327168
C 2.389563 8.557399 14.131837
C 1.773667 6.381257 13.253656
C 0.475616 6.855830 13.003574
H 0.826380 10.049689 14.142295
H -2.058910 3.730619 14.561081
H -0.952558 4.882993 9.991056
H -0.926098 0.700779 11.082346
H -1.898781 2.860085 13.023315
C -1.503418 3.694007 13.614652
H 5.953617 2.487989 16.390634
C -0.013143 3.516618 13.917878
H 3.745856 6.883865 14.007234
H 0.284699 4.325288 14.604965
C 1.698355 1.382434 11.152663
C -0.787248 2.806624 10.581705
C -1.454499 1.577249 10.706333
C 3.085903 -1.051561 11.020690
H 3.619590 -2.001375 10.972168
C -2.804870 1.483167 10.363464
Cr 2.531210 4.523894 10.381350
H -3.323747 0.529153 10.464652
C 2.733715 7.242340 13.813868
C 1.092658 9.022537 13.890193
H -1.698347 4.622738 13.065083
C 3.282455 4.268718 15.243244
C 4.106369 6.245712 9.460657
P 0.937643 3.048232 11.123609

H 3.779476 -0.580520 13.013954
C 4.167681 3.680352 16.147584
H 6.335043 2.232657 13.942708
C 5.476644 2.798019 14.306771
H 2.441818 4.858381 15.611281
C 0.275298 2.170278 14.584322
H -4.549725 2.533908 9.644471
C -3.492892 2.610145 9.902870
H 1.323127 2.100950 14.902645
H 3.134760 9.219377 14.574268
H -0.361161 2.046415 15.471179
H 0.061687 1.343052 13.893450
N 0.855159 3.740233 12.716796
P 2.268505 4.734253 12.642515
C 3.483462 4.113066 13.860097
C 5.261899 2.943120 15.680862
H -0.264507 6.192235 12.555543
H 4.007239 3.801701 17.219449
H -3.363168 4.709715 9.400054
C -2.827577 3.833926 9.767869
H 2.240008 -1.247360 9.038763
C 2.310253 -0.628996 9.934274
C 4.589534 3.380513 13.399722
H 4.752356 3.252686 12.326864
C 3.176027 -0.255528 12.165615
H 1.018602 0.906810 9.144102
C 1.623889 0.584002 9.993367
H 2.569613 1.575804 13.124349
C 2.490468 0.959636 12.231473
H 4.315671 5.513647 10.295854
H 5.013241 6.864436 9.472633
H 4.084292 5.723264 8.489354
C 2.821600 7.071116 9.712255
C 1.606673 6.148399 9.708449
H 2.751137 7.848916 8.932470
H 2.898234 7.591504 10.677841
H 1.333498 5.804116 8.686419
H 0.721785 6.551636 10.215981

Spin state: triplet

E = -9455.49 kcal mol-1
H = -9092.59 kcal mol-1
TS = -62.11 kcal mol-1
G (298.15 K) = -9154.69 kcal mol-1

H -0.880281 8.530476 13.160038
C -1.476514 3.933048 10.094967
C 0.132677 8.169581 13.341675
C 2.388381 8.555781 14.138190
C 1.770821 6.381921 13.254952
C 0.470902 6.855890 13.013333
H 0.824781 10.047899 14.156745
H -2.069374 3.734762 14.555913
H -0.953801 4.884830 9.987251
H -0.924960 0.701518 11.075534
H -1.904929 2.859629 13.021180
C -1.512984 3.696909 13.610058
H 5.964944 2.483613 16.369410
C -0.022420 3.525735 13.915056
H 3.745530 6.884053 14.002164
H 0.272514 4.337352 14.599977
C 1.696349 1.382547 11.158799
C -0.787405 2.808675 10.579710
C -1.453544 1.578119 10.700071
C 3.081954 -1.053050 11.042839
H 3.615664 -2.003147 11.000109
C -2.803198 1.483005 10.354407
Cr 2.547366 4.511931 10.375036
H -3.320664 0.527814 10.451810
C 2.732342 7.242428 13.814065
C 1.090135 9.020985 13.902715
H -1.711160 4.622950 13.057062
C 3.287475 4.261981 15.232753
C 4.097545 6.261467 9.461996
P 0.937207 3.048629 11.122028
H 3.763005 -0.577405 13.039379
C 4.176300 3.673121 16.133482
H 6.342538 2.237874 13.919682
C 5.484173 2.800974 14.287266
H 2.443290 4.844291 15.604290
C 0.270727 2.182043 14.584715
H -4.546260 2.530961 9.627023
C -3.491280 2.609175 9.892235
H 1.318983 2.116963 14.902829
H 3.135058 9.217088 14.579127
H -0.364930 2.057505 15.472049
H 0.060023 1.352562 13.895567
N 0.848178 3.746977 12.714224
P 2.266227 4.736456 12.640640
C 3.487058 4.112790 13.848663
C 5.271853 2.941063 15.662515
H -0.271318 6.192691 12.568383
H 4.016057 3.788580 17.206028
H -3.361208 4.708396 9.387692
C -2.826416 3.833563 9.758960
H 2.247198 -1.254771 9.056793
C 2.313640 -0.633039 9.950246
C 4.594070 3.384006 13.383917
H 4.755421 3.257346 12.310683
C 3.164467 -0.254675 12.186719
H 1.026915 0.901486 9.148419
C 1.628660 0.581288 10.001171
H 2.551600 1.579276 13.137049
C 2.479586 0.961412 12.244648
H 4.319363 5.533294 10.296794
H 4.999634 6.887421 9.468559
H 4.074506 5.740675 8.489683
C 2.809511 7.076338 9.726516
C 1.599209 6.149619 9.731804
H 2.727074 7.857035 8.950982
H 2.892337 7.594044 10.693181
H 1.313863 5.805938 8.713682
H 0.719300 6.544769 10.252711

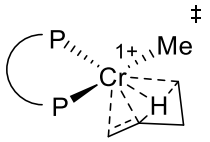
Spin state: quintet

E = -9470.16 kcal mol-1
H = -9106.45 kcal mol-1
TS = -65.53 kcal mol-1

G (298.15 K) = -9171.98 kcal mol-1

H -1.416455 8.003548 13.540257
C -1.287322 4.395157 10.287219
C -0.360852 7.814832 13.739770
C 1.760391 8.523482 14.668532
C 1.575258 6.356909 13.589772
C 0.220145 6.616572 13.321008
H -0.048157 9.704560 14.741220
H -1.634532 3.067454 14.883853
H -0.651968 5.283143 10.245906
H -1.142402 1.055374 11.009280
H -1.439524 2.279172 13.310064
C -1.154194 3.157542 13.900470
H 5.974401 2.620775 16.696370
C 0.360322 3.235913 14.097848
H 3.402771 7.141791 14.462948
H 0.560168 4.055824 14.805731
C 1.628845 1.459840 11.015250
C -0.742021 3.161238 10.680042
C -1.556513 2.017480 10.705808
C 2.840384 -1.020605 10.531287
H 3.301990 -1.991797 10.349517
C -2.903932 2.114386 10.356382
Cr 2.557548 4.762801 10.334726
H -3.533942 1.224639 10.380009
C 2.347226 7.325420 14.256158
C 0.407466 8.769572 14.413552
H -1.552143 4.049160 13.401646
C 3.355340 4.462949 15.526090
C 3.978042 6.092891 8.855142
P 1.000733 3.160910 11.214983
H 3.918467 -0.676104 12.373532
C 4.228643 3.867370 16.437290
H 6.335726 2.305759 14.252581
C 5.496806 2.904579 14.608588
H 2.525303 5.070497 15.888218
C 0.918922 1.937950 14.682891
H -4.501016 3.421080 9.715009
C -3.446618 3.348868 9.984286
H 1.994771 2.018617 14.881426
H 2.362025 9.266179 15.193698
H 0.413409 1.716272 15.633018
H 0.744899 1.094894 14.001225
N 1.093450 3.664408 12.855648
P 2.354539 4.859138 12.886046
C 3.545244 4.275912 14.145564
C 5.294978 3.085042 15.980656
H -0.380532 5.874780 12.793010
H 4.075491 4.011655 17.507419
H -3.057292 5.448941 9.644596
C -2.637516 4.489197 9.947590
H 1.646692 -1.075431 8.728435
C 1.908815 -0.508372 9.622287
C 4.627607 3.501696 13.693466
H 4.782957 3.358030 12.621500
C 3.184915 -0.283259 11.668357
H 0.592172 1.127454 9.134846
C 1.308646 0.730072 9.854846
H 2.872933 1.532366 12.788310
C 2.591239 0.957537 11.906831
H 3.395998 6.645078 9.637839
H 4.651258 6.864498 8.459779
H 4.642842 5.347443 9.342734
C 3.074527 5.455491 7.764013
C 2.202512 4.326256 8.347898
H 3.727257 5.093528 6.954331
H 2.448216 6.250670 7.335821
H 2.611384 3.324388 8.137922
H 1.157903 4.353870 8.011099

Geometry:



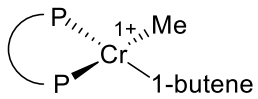
Spin state: triplet

E = -10181.21 kcal mol-1
H = -9786.11 kcal mol-1
TS = -66.26 kcal mol-1
G (298.15 K) = -9852.37 kcal mol-1

H -1.740256 7.427916 13.812862
C -1.384744 4.380724 10.607686
C -0.649881 7.398532 13.811228
C 1.481141 8.477696 14.211266
C 1.413724 6.177015 13.435749
C 0.011092 6.231100 13.420811
H -0.435224 9.431630 14.510971
H -1.297985 2.259450 14.954420
H -0.750329 5.267877 10.673113
H -1.242630 0.976165 10.856200
H -0.987345 1.599686 13.339553
C -0.882977 2.495265 13.965818
H 6.145260 3.138595 16.698467
C 0.584528 2.885933 14.124994
H 3.238145 7.281841 13.844692
H 0.635943 3.752240 14.804542
C 1.526369 1.339650 10.827871
C -0.827437 3.102574 10.789716
C -1.657428 1.973454 10.708241
C 2.680567 -1.110350 10.104995
H 3.123330 -2.067469 9.827503
C -3.021400 2.124730 10.452735
Cr 2.470858 4.781216 10.323377
H -3.660410 1.242962 10.394126
C 2.147029 7.313000 13.826624
C 0.082572 8.522009 14.205155
H -1.484206 3.296701 13.519732
C 3.415498 4.701599 15.383559
C 4.176363 3.654287 10.113815
P 0.959682 3.034643 11.174669
H 3.847034 -0.915222 11.914647
C 4.338455 4.266580 16.336171
H 6.449425 2.517145 14.305095
C 5.596110 3.124676 14.608327
H 2.567552 5.313268 15.692368
C 1.398801 1.743035 14.739006

H -4.635528 3.512980 10.080586
C -3.569444 3.399841 10.280228
H 2.459969 2.005145 14.828293
H 2.055411 9.351335 14.521188
H 1.017495 1.527434 15.746552
H 1.303411 0.828597 14.139451
N 1.183961 3.400730 12.844777
P 2.299186 4.716518 12.780382
C 3.577775 4.343773 14.033404
C 5.426092 3.476313 15.951054
H -0.564812 5.357239 13.116107
H 4.206066 4.543325 17.382747
H -3.171957 5.525811 10.220223
C -2.749480 4.530180 10.359092
H 1.408282 -1.015030 8.358650
C 1.716131 -0.520675 9.280639
C 4.676918 3.556048 13.650144
H 4.812681 3.277023 12.606491
C 3.084746 -0.465638 11.277446
H 0.403738 1.160448 8.975666
C 1.144793 0.702867 9.632355
H 2.856670 1.272792 12.534175
C 2.519740 0.760471 11.633827
H 5.064108 4.167596 10.508425
H 4.323874 3.430605 9.047417
H 4.013352 2.706423 10.649353
C 1.829488 6.856525 9.167018
C 2.912591 6.905972 10.275386
C 1.513342 4.455499 8.349355
C 2.277851 5.638814 8.341990
H 0.445383 4.507090 8.570221
H 1.830046 3.598829 7.753183
H 2.625208 7.339356 11.242509
H 3.816710 7.409840 9.910781
H 1.781828 7.780517 8.570938
H 0.815530 6.705098 9.574771
H 3.075169 5.800578 7.609430
H 3.524305 5.614682 9.448366

Geometry:



Spin state: singlet

E = -10199.35 kcal mol-1
H = -9801.27 kcal mol-1
TS = -67.88 kcal mol-1
G (298.15 K) = -9869.16 kcal mol-1

H -1.556809 7.935697 13.630759
C -1.754147 3.948800 10.637365
C -0.479000 7.773410 13.669959
C 1.751452 8.587379 14.145535
C 1.434529 6.310736 13.363182
C 0.049748 6.535344 13.298757
H -0.044376 9.768409 14.378326
H -1.711495 2.866239 14.922886
H -1.308372 4.933929 10.761856
H -0.964303 0.622753 10.740494
H -1.546330 2.126541 13.319673
C -1.282721 3.004524 13.921622
H 6.124992 2.977110 16.394214
C 0.232486 3.164148 14.054927
H 3.363698 7.188383 13.837399
H 0.421153 4.014868 14.729708
C 1.624243 1.392182 10.983069
C -0.958516 2.794181 10.749027
C -1.556998 1.529066 10.621453
C 3.250754 -0.839608 10.472940
H 3.879540 -1.708328 10.274887
C -2.926853 1.426839 10.371043
Cr 2.441293 4.449291 10.220694
H -3.384484 0.441584 10.275008
C 2.285474 7.349853 13.783523
C 0.369704 8.801367 14.091254
H -1.752149 3.883156 13.463704
C 3.326240 4.572349 15.277831
C 3.038869 3.416124 8.588129
P 0.807259 3.020017 11.149992
H 4.200028 -0.379288 12.360703
C 4.290255 4.097016 16.167629
H 6.349047 2.502904 13.960253
C 5.498442 3.076642 14.329503
H 2.487862 5.163063 15.648805
C 0.876052 1.913839 14.657048
H -4.780825 2.492727 10.064072
C -3.710903 2.578124 10.257014
H 1.950688 2.057578 14.824892
H 2.415339 9.386893 14.476554
H 0.409446 1.691117 15.626420
H 0.729372 1.044628 14.002118
N 0.896213 3.588588 12.772353
P 2.151986 4.771037 12.695810
C 3.438223 4.294395 13.904045
C 5.372938 3.346442 15.695828
H -0.612158 5.735671 12.965487
H 4.197392 4.312597 17.232672
H -3.732496 4.740333 10.316566
C -3.122825 3.839717 10.396031
H 2.130751 -1.035031 8.632640
C 2.266449 -0.463054 9.551213
C 4.536554 3.552190 13.436397
H 4.637592 3.334697 12.370293
C 3.431420 -0.094814 11.640953
H 0.727259 0.953870 9.050464
C 1.463534 0.649967 9.795532
H 2.786498 1.600024 12.799899
C 2.628629 1.019715 11.893033
H 3.785270 3.978128 8.003448
H 2.235560 3.078183 7.916958
H 3.521871 2.520970 9.030792
C 3.113959 7.137535 9.948495
C 4.482693 6.431798 10.057710
C 0.881376 5.869927 9.738138
C 2.127043 6.254910 9.217724
H 0.488246 6.355942 10.635761
H 0.136234 5.437347 9.068732

H 5.195699 7.006068 10.664082
H 4.924302 6.248616 9.070160
H 3.244088 8.091772 9.411322
H 2.732409 7.392777 10.948930
H 2.330860 6.087646 8.155590
H 4.420067 5.443894 10.576862

Spin state: triplet

E = -10210.39 kcal mol-1
H = -9812.26 kcal mol-1
TS = -67.85 kcal mol-1
G (298.15 K) = -9880.11 kcal mol-1

H -1.544599 7.941036 13.675480
C -1.743004 3.937632 10.640808
C -0.466755 7.777431 13.707254
C 1.766993 8.585120 14.177691
C 1.443488 6.316144 13.376569
C 0.058923 6.542460 13.321251
H -0.026512 9.764776 14.433173
H -1.714009 2.882245 14.909189
H -1.302109 4.923075 10.779442
H -0.936892 0.614510 10.705197
H -1.553585 2.147116 13.303286
C -1.283932 3.020962 13.908494
H 6.087058 2.939044 16.428840
C 0.232270 3.169464 14.044074
H 3.376059 7.186986 13.849801
H 0.425407 4.016283 14.722299
C 1.641926 1.389267 10.992792
C -0.941771 2.785747 10.740687
C -1.533427 1.519440 10.596194
C 3.256932 -0.859423 10.519937
H 3.880315 -1.735360 10.337069
C -2.902093 1.413500 10.340434
Cr 2.443722 4.481680 10.207470
H -3.354206 0.427149 10.230690
C 2.297790 7.350271 13.801627
C 0.385166 8.800417 14.133801
H -1.747020 3.904506 13.453896
C 3.310062 4.560482 15.296005
C 2.893877 3.441005 8.517704
P 0.822703 3.018075 11.145042
H 4.192193 -0.386245 12.411673
C 4.262197 4.072913 16.191947
H 6.333914 2.483263 13.993523
C 5.482907 3.059093 14.358554
H 2.471900 5.153990 15.663010
C 0.864410 1.913009 14.645107
H -4.760145 2.473691 10.038833
C -3.691504 2.562059 10.237381
H 1.938977 2.048779 14.819462
H 2.433481 9.380931 14.512409
H 0.391065 1.690961 15.611382
H 0.715225 1.046471 13.987290
N 0.903106 3.595384 12.764480
P 2.159509 4.778226 12.702884
C 3.433198 4.290880 13.921485
C 5.344772 3.318778 15.725594
H -0.605271 5.746593 12.983729
H 4.160135 4.281597 17.257526
H -3.723880 4.723396 10.322868
C -3.110205 3.824820 10.393794
H 2.153467 -1.063875 8.670679
C 2.284760 -0.484192 9.585031
C 4.532876 3.547226 13.459457
H 4.643633 3.337091 12.392881
C 3.432534 -0.103819 11.681699
H 0.761136 0.938781 9.055402
C 1.487855 0.637316 9.810611
H 2.789046 1.606390 12.817680
C 2.635344 1.018742 11.915063
H 3.618889 3.997229 7.901758
H 2.051472 3.130247 7.883451
H 3.382190 2.529300 8.917200
C 3.120631 7.130163 9.879431
C 4.485938 6.408240 9.939156
C 0.866048 5.903763 9.769140
C 2.092579 6.266955 9.182045
H 0.512630 6.414464 10.669264
H 0.091279 5.469535 9.135988
H 5.227322 6.985845 10.506949
H 4.883296 6.211180 8.935770
H 3.246997 8.084789 9.342217
H 2.779606 7.388490 10.894319
H 2.241124 6.107679 8.110546
H 4.441549 5.427216 10.473657

Spin state: quintet

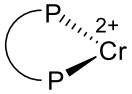
E = -10224.33 kcal mol-1
H = -9826.47 kcal mol-1
TS = -68.77 kcal mol-1
G (298.15 K) = -9895.24 kcal mol-1

H -1.886203 7.628223 13.341621
C -1.675538 3.758212 10.453638
C -0.801910 7.558717 13.436946
C 1.328558 8.580255 13.970385
C 1.238050 6.250940 13.287054
C -0.156849 6.353801 13.150241
H -0.567132 9.613879 14.065096
H -1.472842 2.608003 15.082892
H -1.160823 4.716717 10.350140
H -1.063541 0.485246 11.233805
H -1.260041 1.759323 13.542973
C -1.079012 2.707764 14.062815
H 6.251702 3.315499 16.301794
C 0.413511 3.027956 14.137881
H 3.062603 7.309656 13.803707
H 0.534538 3.924051 14.768205
C 1.627322 1.224482 11.029271
C -0.954429 2.613677 10.834234
C -1.614166 1.378749 10.938118
C 3.121730 -1.089692 10.506262
H 3.697853 -1.994132 10.306995
C -2.981716 1.296541 10.672514
Cr 2.017903 4.670348 10.112532
H -3.491928 0.336181 10.754605

C 1.978687 7.375985 13.693739
C -0.061652 8.673172 13.844387
H -1.645691 3.492273 13.546673
C 3.378006 4.786310 15.203619
C 1.484782 4.015647 8.217460
P 0.815134 2.846735 11.209225
H 4.259401 -0.561870 12.267428
C 4.386722 4.384757 16.081010
H 6.385577 2.688361 13.895164
C 5.541369 3.273166 14.261932
H 2.536621 5.372660 15.574754
C 1.202005 1.877879 14.768699
H -4.766154 2.371595 10.100043
C -3.697711 2.441390 10.307489
H 2.266393 2.125657 14.864174
H 1.908417 9.446262 14.291386
H 0.809175 1.672100 15.773808
H 1.100904 0.962447 14.170931
N 0.983969 3.453742 12.813312
P 2.098759 4.767974 12.657998
C 3.445277 4.429666 13.845846
C 5.465364 3.626686 15.612957
H -0.734222 5.489459 12.819246
H 4.328864 4.660032 17.134742
H -3.599686 4.563997 9.902093
C -3.044710 3.673658 10.199047
H 1.828702 -1.346664 8.791236
C 2.071167 -0.728437 9.656322
C 4.536501 3.675267 13.380840
H 4.592341 3.391026 12.328192
C 3.436886 -0.286210 11.606271
H 0.523499 0.709147 9.229026
C 1.329838 0.427110 9.907257
H 2.959827 1.498506 12.716297
C 2.700186 0.871393 11.864456
H 1.891112 4.692117 7.446641
H 0.392522 3.957610 8.085454
H 1.899399 3.007061 8.047920
C 4.357616 7.016417 10.440299
C 5.417847 5.906011 10.430654
C 1.918232 7.011666 9.726336
C 3.234369 6.778085 9.470849
H 1.594873 7.415780 10.690715
H 1.175945 6.958562 8.926369
H 6.226987 6.128247 11.137578
H 5.858674 5.785662 9.431568
H 4.835663 7.971203 10.157578
H 3.949359 7.165799 11.452164
H 3.525580 6.479364 8.455628
H 4.979148 4.939927 10.723268

6.5 Dicationic Cr^{II}/Cr^{IV} mechanism for complex 1

Geometry:



Spin state: singlet

E = -8004.21 kcal mol-1
H = -7699.95 kcal mol-1
TS = -55.53 kcal mol-1
G (298.15 K) = -7755.48 kcal mol-1

H -1.709255 7.746237 13.396919
C -1.169009 4.369763 10.267861
C -0.624062 7.656389 13.450959
C 1.547285 8.653403 13.896084
C 1.385076 6.317842 13.272094
C -0.014567 6.434707 13.168226
H -0.328080 9.716003 14.033570
H -1.645191 2.475240 14.774329
H -0.526905 5.246724 10.389533
H -1.179501 0.961920 10.690267
H -1.155189 1.731344 13.245738
C -1.121505 2.661959 13.828078
H 6.200628 3.411318 16.646474
C 0.316373 3.066634 14.137352
H 3.254835 7.350568 13.707155
H 0.301282 3.982380 14.749406
C 1.660295 1.308631 11.040077
C -0.691991 3.080393 10.581391
C -1.533081 1.960885 10.435395
C 2.891757 -1.161494 10.604135
H 3.359574 -2.133156 10.441946
C -2.840563 2.140474 9.985341
Cr 2.583662 4.527129 10.518978
H -3.497382 1.276549 9.879938
C 2.169974 7.435850 13.625270
C 0.154087 8.763058 13.813050
H -1.667386 3.438502 13.278461
C 3.409833 4.891283 15.366450
C 2.586877 0.809176 11.978266
P 0.975448 2.963309 11.258373
H 3.882684 -0.831882 12.498327
C 4.373536 4.509312 16.299745
H 6.405970 2.635487 14.290646
C 5.561900 3.257677 14.588782
H 2.576620 5.524826 15.671260
C 1.075917 1.974408 14.888468
H -4.335596 3.553243 9.324775
C -3.312113 3.422115 9.677484
H 2.120140 2.256702 15.071889
H 2.148831 9.516795 14.180807
H 0.595636 1.809296 15.862263
H 1.048234 1.025603 14.337505
N 1.050389 3.498103 12.878425
P 2.202781 4.765661 12.846509
C 3.519522 4.442091 14.035837
C 5.445795 3.697494 15.913049
H -0.621295 5.572880 12.888425
H 4.288306 4.848569 17.332407
H -2.846190 5.532849 9.572132
C -2.476958 4.537010 9.817373
H 1.785605 -1.215836 8.745456
C 2.005126 -0.648515 9.650282
C 4.599437 3.624530 13.649456

H 4.690225 3.268765 12.619520
C 3.186729 -0.430058 11.761478
H 0.705820 0.980659 9.105160
C 1.393164 0.587480 9.854993
H 2.823581 1.378875 12.876420

Spin state: triplet

E = -8011.91 kcal mol-1
H = -7707.69 kcal mol-1
TS = -55.53 kcal mol-1
G (298.15 K) = -7763.22 kcal mol-1

H -1.704686 7.768313 13.415664
C -1.169744 4.362181 10.264898
C -0.620231 7.670396 13.470250
C 1.557982 8.651327 13.918970
C 1.379379 6.319032 13.287272
C -0.019200 6.445577 13.183091
H -0.310171 9.726100 14.059407
H -1.683242 2.493244 14.756004
H -0.531713 5.240750 10.394819
H -1.164253 0.950800 10.662864
H -1.177502 1.740576 13.236598
C -1.148906 2.674104 13.814534
H 6.238390 3.392256 16.588217
C 0.286145 3.079024 14.136487
H 3.256850 7.338261 13.721917
H 0.265939 3.998397 14.742796
C 1.662647 1.305441 11.059367
C -0.688121 3.072939 10.572826
C -1.521456 1.949389 10.411936
C 2.901084 -1.164179 10.642938
H 3.372365 -2.135326 10.487819
C -2.826685 2.125523 9.954098
Cr 2.580745 4.549776 10.512152
H -3.478187 1.258913 9.837952
C 2.172407 7.430723 13.643227
C 0.165616 8.770545 13.836378
H -1.687634 3.448362 13.254720
C 3.429415 4.878041 15.355161
C 2.571581 0.805231 12.013467
P 0.974666 2.959551 11.263148
H 3.857191 -0.836657 12.555506
C 4.406376 4.491570 16.272643
H 6.407618 2.623349 14.227129
C 5.568581 3.245175 14.539826
H 2.600687 5.510329 15.674344
C 1.037260 1.991287 14.902125
H -4.324712 3.534840 9.292948
C -3.303293 3.406929 9.652745
H 2.080418 2.273599 15.091858
H 2.165416 9.509805 14.206053
H 0.548825 1.834609 15.873305
H 1.012605 1.038134 14.358505
N 1.033406 3.501997 12.882283
P 2.188164 4.767016 12.850231
C 3.519071 4.432816 14.021514
C 5.472752 3.681028 15.867099
H -0.631402 5.589220 12.898443
H 4.336085 4.826132 17.308007
H -2.848357 5.521144 9.566715
C -2.475460 4.525576 9.807429
H 1.830502 -1.215498 8.763394
C 2.032385 -0.649846 9.673416
C 4.592708 3.615619 13.616097
H 4.667711 3.263379 12.583816
C 3.174705 -0.434161 11.806562
H 0.745153 0.981104 9.105710
C 1.417215 0.585966 9.868290
H 2.793972 1.374997 12.915095

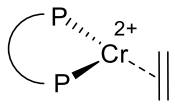
Spin state: quintet

E = -8044.09 kcal mol-1
H = -7739.85 kcal mol-1
TS = -55.42 kcal mol-1
G (298.15 K) = -7795.27 kcal mol-1

H -1.726134 7.740566 13.388841
C -1.165860 4.350544 10.238581
C -0.642013 7.654549 13.465602
C 1.513975 8.653736 13.975736
C 1.377397 6.329739 13.304117
C -0.020204 6.441816 13.172043
H -0.369438 9.704464 14.092520
H -1.621948 2.528621 14.758896
H -0.515008 5.224017 10.334120
H -1.198686 0.951560 10.723845
H -1.154483 1.762593 13.234515
C -1.103561 2.698568 13.806596
H 6.195495 3.371600 16.640991
C 0.341931 3.086376 14.101972
H 3.232336 7.364607 13.794861
H 0.340289 3.999942 14.717521
C 1.648178 1.281909 11.047040
C -0.695049 3.063677 10.570510
C -1.546369 1.948326 10.453018
C 2.860809 -1.204670 10.653020
H 3.322006 -2.182052 10.507171
C -2.856579 2.129350 10.012046
Cr 2.618412 4.571692 10.467968
H -3.520207 1.268340 9.927900
C 2.148705 7.444822 13.694522
C 0.122335 8.758066 13.865175
H -1.643618 3.476522 13.253509
C 3.407992 4.874573 15.380578
C 2.594204 0.805282 11.977346
P 0.980214 2.946776 11.229320
H 3.897027 -0.824970 12.513332
C 4.368234 4.474307 16.309757
H 6.413868 2.648746 14.269898
C 5.567033 3.262555 14.577409
H 2.571184 5.498242 15.695399
C 1.092666 1.983913 14.846901
H -4.347613 3.541281 9.340727
C -3.321953 3.408826 9.686558
H 2.140645 2.253652 15.027471
H 2.104977 9.514593 14.288740
H 0.614015 1.822999 15.822224

H 1.052351 1.036385 14.294903
N 1.074876 3.518357 12.838735
P 2.215381 4.798628 12.849755
C 3.525022 4.454869 14.040708
C 5.443754 3.672913 15.910444
H -0.615817 5.583552 12.859821
H 4.277467 4.790391 17.349292
H -2.841584 5.513756 9.539882
C -2.477430 4.519659 9.799557
H 1.715020 -1.304387 8.820353
C 1.955788 -0.714022 9.704716
C 4.608689 3.648392 13.641482
H 4.706352 3.317520 12.604145
C 3.184832 -0.441784 11.781969
H 0.656730 0.907146 9.138844
C 1.354172 0.530337 9.887631
H 2.854997 1.399159 12.852792

Geometry:



Spin state: singlet

E = -8775.20 kcal mol-1
H = -8435.99 kcal mol-1
TS = -64.21 kcal mol-1
G (298.15 K) = -8500.20 kcal mol-1

H -1.823320 7.650472 12.935412
C -1.325176 4.897517 10.409269
C -0.743891 7.557886 12.811850
C 1.380602 8.545653 12.156083
C 1.287258 6.245280 13.014485
C -0.116982 6.357340 13.133930
H -0.511881 9.572896 12.054682
H -0.987183 2.134530 15.091534
H -0.685157 5.781659 10.357074
H -1.201527 1.522650 10.981592
H -1.335113 2.878561 13.515381
C -0.608969 2.837582 14.337832
H 5.758349 4.201038 17.442100
C 0.762389 2.375340 13.843827
H 3.134672 7.323292 12.516727
H 1.485806 2.457020 14.670229
C 1.660024 2.069784 10.243679
C -0.779463 3.641241 10.727949
C -1.614407 2.507465 10.765253
C 2.873444 0.003242 8.802437
H 3.343423 -0.806536 8.243405
C -2.978254 2.642760 10.509126
Cr 2.210275 5.582392 10.916254
H -3.623117 1.764265 10.542027
C 2.034631 7.349181 12.502739
C -0.002639 8.644176 12.314818
H -0.546423 3.824796 14.815833
C 3.315159 5.522594 15.469114
C 2.886708 1.532701 10.677628
P 0.993746 3.528737 11.080454
H 4.427157 0.071030 10.305609
C 4.195719 5.388126 16.541893
H 5.766423 2.488240 15.637111
C 5.079642 3.333130 15.584062
H 2.621326 6.362724 15.430603
C 0.769637 0.934564 13.341555
H -4.582283 3.996088 9.994189
C -3.516339 3.898309 10.202261
H 1.771983 0.614517 13.035331
H 1.958287 9.392993 11.786090
H 0.427706 0.275385 14.149368
H 0.090118 0.795043 12.491170
N 1.304657 3.316829 12.795488
P 2.234498 4.692511 13.042527
C 3.322774 4.548740 14.451138
C 5.073290 4.299376 16.599272
H -0.703585 5.504954 13.473623
H 4.191308 6.130269 17.340599
H -3.106988 5.997778 9.887039
C -2.689405 5.024537 10.146017
H 1.191891 0.164744 7.452719
C 1.665575 0.548251 8.356744
C 4.212648 3.454600 14.501796
H 4.220853 2.705169 13.708846
C 3.484039 0.496781 9.962147
H 0.120923 2.010612 8.707097
C 1.057714 1.585376 9.067291
H 3.365053 1.915701 11.579657
C 2.306037 4.986985 8.777504
C 3.387004 5.764870 9.192709
H 2.427467 3.920707 8.591784
H 1.428883 5.448243 8.311213
H 3.383443 6.854933 9.047617
H 4.369177 5.313111 9.369356

Spin state: triplet

E = -8785.94 kcal mol-1
H = -8447.34 kcal mol-1
TS = -62.86 kcal mol-1
G (298.15 K) = -8510.20 kcal mol-1

H -1.831874 7.630425 12.949841
C -1.343593 4.878860 10.415825
C -0.750759 7.550627 12.832255
C 1.371015 8.572185 12.218109
C 1.290144 6.249994 13.007087
C -0.114685 6.345942 13.123746
H -0.530517 9.586475 12.132789
H -0.933613 2.144486 15.113298
H -0.709801 5.766995 10.359417
H -1.197940 1.505075 10.991311
H -1.307206 2.878649 13.538306
C -0.568099 2.843639 14.349681
H 5.709649 4.213169 17.478694
C 0.795615 2.379559 13.837545
H 3.131072 7.350802 12.540594
H 1.530116 2.461483 14.653818
C 1.651923 2.059822 10.235276

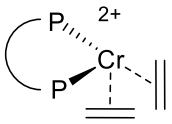
C -0.789046 3.625765 10.732572
C -1.617548 2.487338 10.776483
C 2.870796 0.006457 8.780779
H 3.343235 -0.797936 8.216113
C -2.983763 2.614987 10.529296
Cr 2.194794 5.594697 10.882834
H -3.623689 1.733105 10.567765
C 2.031746 7.373872 12.535810
C -0.015525 8.655069 12.371410
H -0.499320 3.833564 14.821131
C 3.281206 5.520689 15.478424
C 2.880309 1.523358 10.666176
P 0.987173 3.518912 11.069680
H 4.424739 0.068773 10.284137
C 4.144748 5.386802 16.565053
H 5.777897 2.524280 15.652477
C 5.078249 3.358466 15.597849
H 2.575622 6.350901 15.437854
C 0.793855 0.937885 13.338121
H -4.598533 3.959036 10.023955
C -3.530611 3.867172 10.224494
H 1.792623 0.612234 13.026553
H 1.942831 9.434136 11.873751
H 0.454296 0.282370 14.149895
H 0.108254 0.798821 12.492644
N 1.322930 3.322560 12.780744
P 2.252219 4.701870 13.025021
C 3.321719 4.559887 14.448876
C 5.038180 4.311243 16.624942
H -0.695649 5.478806 13.434425
H 4.114088 6.118638 17.372623
H -3.134530 5.968261 9.903112
C -2.710068 4.997673 10.160858
H 1.188880 0.172221 7.431935
C 1.661122 0.550822 8.338751
C 4.228156 3.479447 14.502276
H 4.263672 2.741157 13.699615
C 3.480202 0.493919 9.943871
H 0.113959 2.008618 8.697162
C 1.050936 1.582163 9.055330
H 3.357956 1.902728 11.570058
C 2.406213 4.928335 8.776107
C 3.418913 5.798343 9.191210
H 2.609208 3.866412 8.643275
H 1.520320 5.303497 8.253245
H 3.345032 6.878008 8.995473
H 4.425240 5.425183 9.407396

Spin state: quintet

E = -8801.77 kcal mol-1
H = -8462.77 kcal mol-1
TS = -61.91 kcal mol-1
G (298.15 K) = -8524.68 kcal mol-1

H -1.958039 7.796330 13.762575
C -1.307938 4.884225 10.250740
C -0.868565 7.765831 13.794575
C 1.248070 8.835518 14.311838
C 1.209498 6.570057 13.450886
C -0.194729 6.616595 13.379611
H -0.681087 9.769570 14.579884
H -1.567425 2.454318 14.557372
H -0.686519 5.761596 10.450795
H -1.226035 1.454522 10.352911
H -1.104856 1.916514 12.937357
C -1.084566 2.773127 13.624973
H 6.249943 3.518278 16.354452
C 0.347261 3.199131 13.933447
H 3.023185 7.661415 13.966304
H 0.319314 4.031914 14.654182
C 1.629821 1.865865 10.612655
C -0.793177 3.584949 10.436020
C -1.608669 2.462986 10.195929
C 3.004852 -0.421121 9.777487
H 3.532115 -1.320295 9.457622
C -2.926284 2.648476 9.777664
Cr 2.428000 5.189699 10.370620
H -3.562618 1.781202 9.599120
C 1.933659 7.689348 13.908676
C -0.149738 8.873685 14.257578
H -1.679681 3.585198 13.189652
C 3.377192 5.033155 15.318589
C 2.634348 1.311214 11.429585
P 0.897945 3.453983 11.057819
H 4.066686 -0.282864 11.655947
C 4.384461 4.592484 16.177588
H 6.392899 2.985805 13.928743
C 5.544553 3.552026 14.313633
H 2.536880 5.606518 15.710721
C 1.174766 2.056063 14.521255
H -4.464133 4.076058 9.263490
C -3.433648 3.939923 9.593291
H 2.212113 2.360265 14.707521
H 1.806235 9.698594 14.675127
H 0.734877 1.750009 15.479765
H 1.166723 1.182360 13.856620
N 1.020800 3.807475 12.718470
P 2.113528 5.137285 12.809630
C 3.454429 4.726625 13.947464
C 5.463269 3.854484 15.678105
H -0.758118 5.755961 13.018001
H 4.327556 4.826024 17.241105
H -3.023621 6.062740 9.684990
C -2.625581 5.058367 9.830350
H 1.798509 -0.307659 7.984669
C 2.030385 0.147369 8.947984
C 4.543551 3.987556 13.446789
H 4.608460 3.746608 12.382209
C 3.306479 0.162083 11.013528
H 0.586891 1.727175 8.702121
C 1.345361 1.292127 9.354258
H 2.879609 1.770006 12.387087
C 2.921985 4.575524 8.047034
C 1.874133 5.433364 7.978246
H 3.948339 4.919438 7.883285
H 2.771009 3.495186 8.141307
H 0.839788 5.077446 8.017325
H 2.021892 6.495751 7.759973

Geometry:



Spin state: singlet

E = -9536.02 kcal mol-1
H = -9161.57 kcal mol-1
TS = -66.96 kcal mol-1
G (298.15 K) = -9228.52 kcal mol-1

H -0.826258 8.734267 12.742738
C -1.744319 4.223548 11.003552
C 0.214259 8.427008 12.851085
C 2.552510 9.005435 13.175111
C 1.884052 6.680938 13.012130
C 0.544518 7.072689 12.844143
H 0.955278 10.450882 13.011014
H -0.906423 3.758846 15.679411
H -1.507799 5.113656 11.586663
H -0.281964 1.418017 9.669791
H -1.379836 4.441843 14.108285
C -0.521904 4.205025 14.752972
H 5.728588 3.409899 17.146939
C 0.418019 3.223674 14.057860
H 3.932543 7.352429 13.316617
H 1.269190 3.002416 14.722514
C 2.099005 2.370641 10.547729
C -0.736737 3.299737 10.662416
C -1.051993 2.148666 9.916687
C 4.169163 0.800294 9.485440
H 4.965987 0.177856 9.077169
C -2.372120 1.928038 9.521287
Cr 2.838994 4.766576 10.528316
H -2.622726 1.031978 8.953217
C 2.893206 7.653152 13.174590
C 1.217176 9.392271 13.008296
H -0.008489 5.138858 15.017190
C 3.351780 5.135360 15.417770
C 2.906717 1.583289 11.404489
P 0.950530 3.615753 11.184411
H 4.515979 0.160710 11.525999
C 4.151766 4.728740 16.486907
H 6.005935 2.323696 14.925541
C 5.256353 3.103489 15.060964
H 2.618536 5.930159 15.557462
C -0.267873 1.913806 13.678793
H -4.401991 2.663711 9.554672
C -3.371863 2.843878 9.863530
H 0.404768 1.236631 13.134206
H 3.327338 9.759661 13.313754
H -0.582323 1.400432 14.596030
H -1.163182 2.087968 13.068953
N 1.048878 3.876606 12.851550
P 2.396302 4.959261 12.807143
C 3.502543 4.514950 14.162653
C 5.101099 3.717404 16.309776
H -0.233458 6.317021 12.742736
H 4.035022 5.206472 17.460037
H -3.841890 4.698722 10.873612
C -3.058495 3.989263 10.606326
H 3.580816 1.576741 7.556457
C 3.394007 1.584929 8.630545
C 4.458783 3.496867 13.987308
H 4.588406 3.021517 13.013860
C 3.918982 0.794606 10.869152
H 1.705446 2.921647 8.466082
C 2.359683 2.376378 9.148958
H 2.713727 1.580434 12.477762
C 1.029818 5.727068 9.451775
C 2.261760 6.383178 9.350436
H 0.648002 5.114448 8.633143
H 0.271427 6.107030 10.135849
H 2.471531 7.250873 9.987344
H 2.871962 6.293739 8.444320
C 4.890369 4.356396 9.990818
C 4.954392 5.329801 10.974493
H 4.870547 4.625503 8.928966
H 5.141079 3.313266 10.202778
H 4.957649 6.390703 10.705256
H 5.290411 5.097843 11.984848

Spin state: triplet

E = -9545.57 kcal mol-1
H = -9171.56 kcal mol-1
TS = -65.40 kcal mol-1
G (298.15 K) = -9236.95 kcal mol-1

H -0.935663 8.682299 13.507153
C -1.654181 4.434237 10.422541
C 0.119389 8.416574 13.436940
C 2.459015 9.061516 13.536775
C 1.849200 6.755467 13.117348
C 0.487250 7.095064 13.180137
H 0.809189 10.430633 13.802065
H -1.688172 3.339586 14.815127
H -1.290427 5.440845 10.633031
H -0.601954 1.160490 10.395569
H -1.495137 2.697976 13.174039
C -1.215590 3.522979 13.841828
H 5.922411 3.327184 16.798351
C 0.297413 3.598767 14.036974
H 3.897564 7.478413 13.258685
H 0.518753 4.409045 14.749603
C 1.966541 2.221629 10.695733
C -0.803712 3.319955 10.566598
C -1.264098 2.019887 10.284617
C 3.972593 0.482251 9.778371
H 4.745160 -0.202728 9.427392
C -2.585329 1.840637 9.875132
Cr 2.792371 4.664085 10.349503
H -2.954238 0.837151 9.662197
C 2.838677 7.741740 13.293776
C 1.101937 9.398231 13.608115
H -1.625802 4.454027 13.431362
C 3.414026 5.067356 15.284146

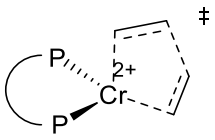
C 2.797211 1.546382 11.616206
P 0.867157 3.597938 11.140768
H 4.404981 0.136104 11.869486
C 4.255312 4.604896 16.295893
H 6.228810 2.498525 14.472211
C 5.431760 3.207471 14.697552
H 2.643661 5.804254 15.512024
C 0.883272 2.292687 14.567098
H -4.468104 2.796266 9.425610
C -3.435888 2.944259 9.744730
H 1.963752 2.378773 14.741819
H 3.221547 9.827567 13.678221
H 0.408459 2.037265 15.523499
H 0.687014 1.465471 13.869907
N 0.989636 4.050907 12.771197
P 2.374214 5.076848 12.704263
C 3.568297 4.578780 13.970806
C 5.261345 3.677597 16.004898
H -0.276188 6.329386 13.040160
H 4.129605 4.976342 17.313178
H -3.638750 5.092822 9.901500
C -2.971472 4.238204 10.014825
H 3.308739 0.996500 7.783646
C 3.168968 1.157140 8.852927
C 4.586708 3.652078 13.681544
H 4.721482 3.275374 12.668234
C 3.782993 0.675030 11.153943
H 1.514717 2.516947 8.574178
C 2.177221 2.034703 9.299854
H 2.659235 1.699107 12.684859
C 2.808031 6.749711 9.645782
C 1.485856 6.314896 9.775677
H 3.235083 7.440400 10.374322
H 3.304020 6.727002 8.671898
H 0.942637 5.931393 8.905184
H 0.860834 6.693856 10.583368
C 4.855453 4.027267 9.903952
C 5.102551 5.303193 10.351243
H 4.864426 3.806649 8.831201
H 4.919047 3.153517 10.560114
H 5.339351 6.111546 9.662699
H 5.298913 5.501153 11.407776

Spin state: quintet

E = -9556.25 kcal mol-1
H = -9182.19 kcal mol-1
TS = -66.38 kcal mol-1
G (298.15 K) = -9248.57 kcal mol-1

H -1.212330 8.408901 13.015431
C -1.029062 4.883752 10.123663
C -0.197214 8.172510 13.335634
C 1.848751 8.809490 14.473275
C 1.652805 6.609376 13.472882
C 0.352337 6.926259 13.035719
H 0.117065 10.087133 14.287968
H -1.395483 3.333246 14.942717
H -0.361254 5.748654 10.102462
H -1.045890 1.526752 10.824352
H -1.489858 3.661029 13.199506
C -0.879853 3.812334 14.099978
H 6.423818 3.260808 16.509736
C 0.508040 3.190172 13.933368
H 3.419983 7.333798 14.517154
H 1.123307 3.434721 14.813851
C 1.857050 1.894591 10.676710
C -0.544640 3.620498 10.513802
C -1.410932 2.511277 10.531270
C 3.219143 -0.402029 9.840754
H 3.742632 -1.303276 9.520685
C -2.749246 2.675381 10.173064
Cr 2.870869 5.158073 10.477745
H -3.421517 1.817151 10.189947
C 2.407818 7.563415 14.182606
C 0.549716 9.114188 14.053090
H -0.817459 4.885826 14.310321
C 3.526142 4.714567 15.454235
C 2.953022 1.414572 11.419987
P 1.163285 3.514614 11.100680
H 4.456657 -0.120181 11.592154
C 4.504451 4.234730 16.326396
H 6.748000 3.021487 14.054487
C 5.842783 3.489397 14.442308
H 2.635602 5.203680 15.851130
C 0.454795 1.670062 13.797137
H -4.275625 4.055936 9.516514
C -3.228323 3.934913 9.795234
H 1.454520 1.226246 13.734746
H 2.427381 9.542056 15.036714
H -0.053716 1.251036 14.674664
H -0.118887 1.365525 12.911433
N 1.255452 3.817464 12.781917
P 2.417285 5.071213 12.895250
C 3.704401 4.575123 14.064132
C 5.659468 3.626295 15.823061
H -0.236604 6.192604 12.483849
H 4.367141 4.340780 17.402811
H -2.742650 6.015771 9.460371
C -2.368435 5.038284 9.765754
H 1.827850 -0.438309 8.185637
C 2.144106 0.083868 9.088964
C 4.866480 3.958103 13.563364
H 5.010600 3.842280 12.485750
C 3.622067 0.263466 11.004739
H 0.626776 1.604440 8.904086
C 1.463496 1.233463 9.496981
H 3.267157 1.928679 12.329889
C 3.257699 4.216802 8.194226
C 2.182017 5.031624 8.070908
H 4.262654 4.562998 7.941660
H 3.141813 3.154065 8.428125
H 1.163231 4.652218 8.187914
H 2.284960 6.062683 7.721336
C 4.460930 6.954274 11.242402
C 4.725959 6.701526 9.937149
H 5.041447 6.483932 12.039918
H 3.750375 7.728309 11.545917
H 5.535250 6.026891 9.644536
H 4.252164 7.280287 9.139418

Geometry:

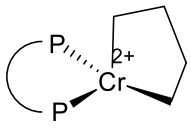


Spin state: triplet

E = -9535.29 kcal mol-1
H = -9161.18 kcal mol-1
TS = -66.80 kcal mol-1
G (298.15 K) = -9227.97 kcal mol-1

H -1.072963 8.606648 13.259431
C -1.656823 4.468686 10.435873
C -0.010928 8.360359 13.279623
C 2.299332 9.048764 13.571481
C 1.768744 6.728887 13.122092
C 0.400793 7.044286 13.066068
H 0.609124 10.388682 13.689398
H -1.656106 3.223041 14.858798
H -1.255393 5.469437 10.604713
H -0.693740 1.166511 10.471504
H -1.470001 2.605643 13.207827
C -1.195595 3.425903 13.883592
H 5.977039 3.415880 16.796365
C 0.318492 3.521053 14.065339
H 3.784924 7.490265 13.427317
H 0.532828 4.324175 14.788185
C 1.937323 2.218293 10.672439
C -0.837139 3.334136 10.594967
C -1.335381 2.040412 10.352718
C 3.908546 0.473973 9.695272
H 4.665207 -0.215675 9.319844
C -2.668242 1.888262 9.971447
Cr 2.819097 4.610350 10.393065
H -3.067739 0.890758 9.787722
C 2.722527 7.734617 13.369843
C 0.935737 9.361260 13.526055
H -1.621553 4.357215 13.490275
C 3.382883 5.061859 15.322679
C 2.837449 1.592184 11.562899
P 0.840216 3.584313 11.161645
H 4.480904 0.214026 11.764398
C 4.250408 4.623363 16.322693
H 6.312437 2.641956 14.455561
C 5.484116 3.308936 14.695726
H 2.579545 5.758247 15.564962
C 0.932103 2.216210 14.566965
H -4.533442 2.884216 9.536130
C -3.491544 3.011823 9.831844
H 2.010871 2.321772 14.741621
H 3.033214 9.829277 13.773242
H 0.464393 1.929512 15.517958
H 0.754463 1.401065 13.850905
N 0.990953 4.000239 12.801143
P 2.347471 5.061451 12.736751
C 3.555011 4.602960 14.001189
C 5.297099 3.748672 16.011313
H -0.334788 6.262860 12.874104
H 4.113237 4.971360 17.346763
H -3.632854 5.168442 9.934034
C -2.987381 4.298857 10.059236
H 3.117738 0.913275 7.729107
C 3.040699 1.108102 8.799000
C 4.614630 3.730584 13.690341
H 4.762461 3.380379 12.668318
C 3.807053 0.717312 11.070462
H 1.362320 2.448065 8.574442
C 2.065385 1.987463 9.273863
H 2.758547 1.775800 12.633082
C 3.524034 6.716787 9.708806
C 2.092920 6.375606 9.747772
H 3.828923 7.488463 10.420065
H 3.909736 6.897004 8.704308
H 1.606970 6.182228 8.781328
H 1.460387 6.925992 10.446628
C 4.693257 4.082043 9.777417
C 4.928736 5.462045 10.187343
H 4.781525 3.861055 8.707859
H 4.998739 3.252434 10.423366
H 5.626870 6.039036 9.578346
H 5.144051 5.614435 11.251763

Geometry:



Spin state: singlet

E = -9530.26 kcal mol-1
H = -9156.04 kcal mol-1
TS = -64.38 kcal mol-1
G (298.15 K) = -9220.42 kcal mol-1

H -1.309671 8.170055 13.291707
C -1.211683 4.908975 10.816514
C -0.249254 7.949283 13.162979
C 1.984256 8.702212 12.580789
C 1.600253 6.384199 13.313715
C 0.220052 6.665969 13.429201
H 0.238783 9.965272 12.537906
H -1.134522 2.574344 15.226790
H -0.689272 5.833530 11.067155
H -0.675157 1.547250 10.417357
H -1.309825 3.403301 13.662324
C -0.626565 3.226620 14.504740
H 5.936062 3.929524 17.609489
C 0.664652 2.563956 14.023411
H 3.569294 7.255147 12.877955
H 1.378405 2.500298 14.860535
C 2.041303 2.258824 10.472823
C -0.522775 3.681888 10.801969
C -1.203611 2.499755 10.455661
C 3.512009 0.296378 9.124745

H 4.080877 -0.472668 8.601396
C -2.564712 2.549559 10.151703
Cr 2.492535 5.644000 11.166496
H -3.091792 1.633084 9.885409
C 2.482961 7.412702 12.850908
C 0.625612 8.965620 12.737079
H -0.420485 4.178458 15.013262
C 3.429589 5.342042 15.785960
C 3.061577 1.559569 11.139476
P 1.221247 3.654132 11.289295
H 4.565745 0.021645 10.992561
C 4.310386 5.126400 16.845666
H 6.060705 2.464825 15.603063
C 5.320244 3.263675 15.649281
H 2.692472 6.144113 15.838295
C 0.430152 1.162103 13.468832
H -4.311700 3.802286 9.942289
C -3.248482 3.769340 10.182851
H 1.356328 0.693741 13.118575
H 2.668577 9.491657 12.268821
H 0.008667 0.533694 14.263264
H -0.294631 1.177367 12.645167
N 1.366399 3.434727 13.013323
P 2.377495 4.745999 13.286467
C 3.495967 4.502677 14.656715
C 5.249652 4.091537 16.777702
H -0.470818 5.880624 13.732118
H 4.260977 5.764133 17.728443
H -3.103907 5.900494 10.517041
C -2.571133 4.949323 10.510034
H 2.280604 0.769908 7.411362
C 2.503193 0.995665 8.454624
C 4.449866 3.466848 14.581592
H 4.514444 2.834795 13.695184
C 3.787756 0.576556 10.467473
H 0.971370 2.502406 8.592285
C 1.767412 1.977311 9.120909
H 3.272336 1.771627 12.187345
C 3.346198 5.346935 8.655262
C 1.955511 5.404306 9.261421
H 1.162960 4.858348 8.742876
H 1.600340 6.465046 9.443002
C 4.393316 4.998912 10.943252
C 4.385457 5.862261 9.683640
H 4.473255 3.921594 10.751848
H 5.098247 5.319028 11.721437
H 5.395472 5.925572 9.243488
H 4.160893 6.927121 9.943008
H 3.386857 5.940903 7.726951
H 3.580821 4.304716 8.390007

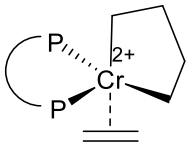
Spin state: triplet

E = -9540.73 kcal mol-1
H = -9166.53 kcal mol-1
TS = -65.32 kcal mol-1
G (298.15 K) = -9231.85 kcal mol-1

H -1.278764 8.213304 13.138200
C -1.265783 4.842720 10.746007
C -0.206939 8.010781 13.143306
C 2.078117 8.812429 12.969501
C 1.631999 6.444901 13.400491
C 0.246150 6.704753 13.344784
H 0.334887 10.075432 12.798521
H -1.175828 2.730953 15.275759
H -0.769351 5.784591 10.987617
H -0.644977 1.487609 10.407626
H -1.369564 3.505881 13.687297
C -0.674792 3.356763 14.525947
H 5.990043 3.710395 17.500621
C 0.604402 2.670082 14.047991
H 3.629831 7.335166 13.274005
H 1.326161 2.617046 14.879313
C 2.053895 2.249088 10.538028
C -0.549943 3.630696 10.762554
C -1.196128 2.427818 10.420594
C 3.597542 0.279439 9.293212
H 4.196388 -0.492349 8.808928
C -2.552862 2.442546 10.094935
Cr 2.373917 5.707724 11.128707
H -3.054676 1.510460 9.833977
C 2.553647 7.510884 13.183037
C 0.702001 9.060650 12.954073
H -0.459228 4.325080 14.997356
C 3.347393 5.106771 15.866394
C 3.050934 1.575131 11.263320
P 1.181435 3.645516 11.284673
H 4.575569 0.052021 11.208537
C 4.235643 4.816029 16.901394
H 6.321902 2.648865 15.276050
C 5.483485 3.326889 15.436420
H 2.520378 5.798778 16.029372
C 0.348994 1.260085 13.525938
H -4.324612 3.651339 9.841141
C -3.264646 3.646705 10.097734
H 1.264225 0.776496 13.167873
H 2.786655 9.629927 12.832951
H -0.060765 0.650854 14.341320
H -0.393312 1.264800 12.717762
N 1.306981 3.518300 13.015528
P 2.379391 4.790627 13.280967
C 3.528543 4.488116 14.613249
C 5.297053 3.929187 16.687403
H -0.465528 5.890304 13.473584
H 4.099034 5.281667 17.877747
H -3.174272 5.786148 10.399562
C -2.620340 4.847381 10.416789
H 2.439047 0.710180 7.518366
C 2.612139 0.955974 8.566415
C 4.603389 3.602726 14.392450
H 4.757816 3.151600 13.411238
C 3.814211 0.587556 10.640735
H 1.070323 2.460816 8.607679
C 1.840337 1.943362 9.180742
H 3.216111 1.808200 12.315273
C 3.363367 5.216818 8.476541
C 2.031161 5.420131 9.161554
H 1.156621 4.957207 8.690280
H 1.793516 6.524635 9.315823

C 4.297302 5.107087 10.775140
C 4.467265 5.749993 9.402639
H 4.358958 4.010469 10.740172
H 4.960066 5.502325 11.560601
H 5.476860 5.551078 9.003218
H 4.404275 6.854327 9.467841
H 3.380513 5.697996 7.484108
H 3.506700 4.137353 8.304267

Geometry:



Spin state: singlet

E = -10282.75 kcal mol-1
H = -9873.51 kcal mol-1
TS = -68.12 kcal mol-1
G (298.15 K) = -9941.63 kcal mol-1

H -2.543007 7.901154 13.905997
C -1.617827 4.786194 10.583519
C -1.600516 7.573750 14.345224
C -0.126603 7.399867 16.265958
C 0.554427 6.477377 14.132128
C -0.662460 6.901723 13.564484
H -2.064675 8.350723 16.307537
H -0.911276 2.778609 15.572170
H -1.050500 5.694437 10.350147
H -1.208059 1.558186 11.645824
H -1.368923 2.879103 13.860697
C -0.697993 3.289965 14.624348
H 6.934321 5.753239 15.317257
C 0.769653 3.065481 14.254049
H 1.756176 6.397513 15.941097
H 1.405103 3.469343 15.059163
C 1.594194 2.207923 10.749197
C -0.961860 3.632671 11.046271
C -1.704681 2.466180 11.302748
C 2.978275 0.073522 9.579652
H 3.514952 -0.760955 9.127107
C -3.086416 2.468769 11.108585
Cr 1.681218 5.854800 10.705241
H -3.661251 1.563563 11.306631
C 0.821154 6.728999 15.489884
C -1.330824 7.824089 15.696623
H -0.926262 4.353866 14.752536
C 4.073354 4.388819 14.063519
C 2.888577 1.876028 11.189886
P 0.820307 3.717246 11.376641
H 4.572169 0.550376 10.962569
C 5.366037 4.460002 14.584721
H 5.608904 7.838249 15.011851
C 5.179225 6.873644 14.740622
H 3.638752 3.420906 13.815963
C 1.104622 1.588307 14.065692
H -4.812743 3.619619 10.506224
C -3.732893 3.625138 10.657823
H 2.170636 1.425060 13.869124
H 0.077571 7.590855 17.319887
H 0.836049 1.042519 14.978794
H 0.534283 1.147732 13.236647
N 1.176295 3.879034 13.046394
P 1.692934 5.505870 13.105510
C 3.323108 5.563798 13.890646
C 5.922139 5.700100 14.915029
H -0.891003 6.684996 12.518540
H 5.940120 3.545585 14.737535
H -3.502337 5.679814 10.022041
C -2.998877 4.785186 10.388822
H 1.231590 -0.170909 8.329665
C 1.697015 0.405844 9.129268
C 3.883151 6.811494 14.229396
H 3.303189 7.729040 14.122790
C 3.573284 0.809470 10.610845
H 0.007441 1.724670 9.339918
C 1.004082 1.473949 9.702878
H 3.357451 2.449643 11.988184
C 2.817827 4.412774 8.428938
C 1.468924 4.800376 8.982044
H 0.622981 4.175015 8.673071
H 1.206112 5.886664 8.754569
C 3.647265 5.387990 10.539739
C 3.877811 5.343821 9.034758
H 3.835013 4.414286 11.014523
H 4.203953 6.168025 11.083017
H 4.901045 5.001852 8.807471
H 3.795770 6.350207 8.588608
H 2.803303 4.446403 7.325827
H 3.017988 3.362983 8.699615
C 1.388315 8.127758 10.304857
C 2.011788 8.226158 11.511140
H 0.300402 8.225479 10.225064
H 1.956098 8.187708 9.371140
H 3.098712 8.298098 11.582892
H 1.439712 8.364893 12.429499

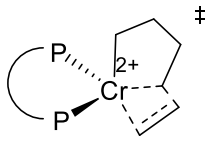
Spin state: triplet

E = -10294.52 kcal mol-1
H = -9885.22 kcal mol-1
TS = -68.27 kcal mol-1
G (298.15 K) = -9953.49 kcal mol-1

H -2.539126 7.924006 13.892545
C -1.646669 4.761624 10.609553
C -1.605299 7.582694 14.339627
C -0.162333 7.362274 16.278911
C 0.545235 6.474511 14.138310
C -0.659686 6.918902 13.560687
H -2.094172 8.326438 16.308885
H -0.882150 2.770152 15.581436
H -1.092022 5.676337 10.370842
H -1.191370 1.533615 11.652012
H -1.354016 2.860321 13.873394
C -0.679676 3.278743 14.629789
H 6.904553 5.742414 15.394265

C 0.786548 3.061998 14.248998
H 1.715894 6.349241 15.965337
H 1.425991 3.466865 15.050508
C 1.585089 2.210504 10.731076
C -0.973616 3.613667 11.060946
C -1.701434 2.437801 11.318840
C 2.969633 0.101828 9.516425
H 3.507191 -0.721744 9.045346
C -3.085073 2.426650 11.140360
Cr 1.663237 5.873475 10.690240
H -3.647840 1.514269 11.340201
C 0.791801 6.698442 15.505167
C -1.354798 7.805848 15.699446
H -0.914112 4.341633 14.755485
C 4.077056 4.393019 14.052045
C 2.882150 1.874083 11.160043
P 0.811361 3.712706 11.372795
H 4.568372 0.557652 10.900884
C 5.362001 4.459554 14.591948
H 5.558792 7.822058 15.147003
C 5.144474 6.863339 14.834097
H 3.655532 3.430030 13.765807
C 1.127288 1.586753 14.056035
H -4.830128 3.561872 10.562763
C -3.748815 3.578276 10.702637
H 2.193333 1.428667 13.855422
H 0.026987 7.531785 17.339251
H 0.864668 1.037770 14.969004
H 0.555529 1.145333 13.228464
N 1.182369 3.879978 13.039766
P 1.691353 5.510787 13.113174
C 3.314501 5.564529 13.912469
C 5.898929 5.692829 14.975457
H -0.875048 6.723168 12.507765
H 5.944913 3.546805 14.718552
H -3.546553 5.637580 10.072391
C -3.029961 4.746903 10.430320
H 1.217493 -0.125402 8.270697
C 1.684954 0.437909 9.078687
C 3.855625 6.805318 14.304253
H 3.264381 7.718740 14.227789
C 3.567071 0.820121 10.558646
H -0.006591 1.749169 9.320013
C 0.991683 1.493344 9.674772
H 3.353848 2.435493 11.965186
C 2.786614 4.411040 8.418070
C 1.444889 4.844818 8.946220
H 0.577645 4.260857 8.616556
H 1.234738 5.948435 8.737627
C 3.647231 5.386863 10.535614
C 3.882788 5.293416 9.033819
H 3.799531 4.422514 11.041209
H 4.227038 6.164170 11.055719
H 4.886459 4.887927 8.823787
H 3.865353 6.292736 8.566449
H 2.791215 4.449184 7.314409
H 2.941937 3.352183 8.681604
C 1.701728 8.234243 10.217827
C 2.073606 8.257051 11.521544
H 0.667323 8.434206 9.920588
H 2.447142 8.200050 9.417704
H 3.124872 8.201164 11.810592
H 1.347942 8.447367 12.314481

Geometry:



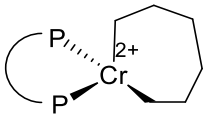
Spin state: triplet

E = -10279.30 kcal mol-1
H = -9870.61 kcal mol-1
TS = -65.54 kcal mol-1
G (298.15 K) = -9936.15 kcal mol-1

H -2.483493 7.066151 14.754610
C -1.746644 4.932815 10.930457
C -1.405588 7.230083 14.753181
C 0.518090 8.576883 15.376686
C 0.831422 6.497807 14.169426
C -0.562749 6.298236 14.145620
H -1.529631 9.095129 15.836166
H -0.876865 1.725707 14.889715
H -1.270654 5.901572 11.108671
H -1.042900 1.582499 10.773286
H -0.610567 1.583326 13.147150
C -0.617604 2.291388 13.985855
H 6.469036 4.065968 16.428200
C 0.754883 2.928475 14.177780
H 2.449739 7.808674 14.807202
H 0.716643 3.577966 15.067520
C 1.697428 2.566250 10.561805
C -0.989916 3.746570 10.974363
C -1.616619 2.508611 10.742502
C 3.360732 0.778010 9.189717
H 4.002420 0.072663 8.660800
C -2.984993 2.466158 10.476632
Cr 1.817886 6.106001 10.960364
H -3.470552 1.506467 10.297877
C 1.370075 7.650337 14.779690
C -0.868385 8.368068 15.363715
H -1.402763 3.036512 13.808580
C 3.318264 5.131135 15.682946
C 2.952906 2.215794 11.094248
P 0.771825 3.902461 11.363196
H 4.738335 1.035243 10.836931
C 4.425282 4.763654 16.448415
H 6.613523 3.987573 13.945069
C 5.688343 4.303186 14.427755
H 2.399460 5.448799 16.176061
C 1.855119 1.883930 14.366245
H -4.801838 3.607705 10.227148
C -3.732795 3.648556 10.439054
H 2.837259 2.352437 14.507648
H 0.932527 9.460495 15.862916
H 1.635275 1.281227 15.257495
H 1.901765 1.206716 13.503693

N 1.085228 3.882989 13.053562
P 1.913999 5.352560 13.276367
C 3.394610 5.076886 14.277061
C 5.606623 4.349861 15.824217
H -0.981872 5.409621 13.672526
H 4.364522 4.800037 17.536505
H -3.697855 5.803432 10.627715
C -3.114961 4.883107 10.665279
H 1.798022 0.713647 7.696770
C 2.122324 1.137224 8.647681
C 4.586471 4.663539 13.652757
H 4.655368 4.615797 12.566631
C 3.775578 1.319719 10.411403
H 0.334873 2.314281 8.883027
C 1.292074 2.034490 9.322459
H 3.276165 2.624546 12.052033
C 2.763364 5.103851 8.226640
C 1.549215 5.456914 9.039841
H 0.635626 4.904494 8.790100
H 1.338795 6.567945 9.000006
C 3.975680 5.896395 10.244359
C 3.964092 5.904290 8.727626
H 3.737905 4.891091 10.638543
H 4.936864 6.172482 10.682573
H 4.908898 5.477640 8.353976
H 3.928360 6.935160 8.338371
H 2.571388 5.278668 7.153716
H 2.955528 4.024493 8.319860
C 3.505929 7.844814 11.038456
C 2.157551 8.198147 11.245124
H 4.012165 8.198714 10.140523
H 4.148905 7.727778 11.912408
H 1.622712 8.734438 10.455996
H 1.822205 8.415418 12.260051

Geometry:



Spin state: singlet

E = -10294.74 kcal mol-1
H = -9884.56 kcal mol-1
TS = -69.21 kcal mol-1
G (298.15 K) = -9953.77 kcal mol-1

H -1.724500 8.682315 13.493526
C -1.921011 4.145069 11.780105
C -0.975518 8.113039 14.044562
C 0.112178 7.550596 16.141920
C 0.860840 6.530416 14.077532
C -0.116413 7.248952 13.366065
H -1.535864 8.935129 15.961299
H -0.877028 3.074946 16.006800
H -1.527680 5.149955 11.943652
H -0.884578 0.901476 11.339073
H -1.393779 2.944194 14.313597
C -0.675373 3.427172 14.986655
H 7.028283 5.375435 15.639677
C 0.764761 3.066091 14.610564
H 1.750679 6.150968 16.025426
H 1.447990 3.487237 15.365073
C 1.673417 2.008259 11.010129
C -1.046306 3.055157 11.605674
C -1.555863 1.752577 11.454299
C 3.278901 0.107928 9.733003
H 3.898909 -0.642432 9.241487
C -2.936625 1.550928 11.471108
Cr 1.868304 5.246124 10.807935
H -3.335527 0.542527 11.358666
C 0.982046 6.690885 15.471268
C -0.864665 8.258086 15.431964
H -0.839585 4.510982 14.960149
C 4.132326 4.088941 14.385397
C 2.904919 1.631654 11.575786
P 0.723248 3.380424 11.711943
H 4.642364 0.369826 11.391027
C 5.399586 4.125240 14.969419
H 5.904872 7.503053 14.997271
C 5.408653 6.548267 14.821562
H 3.631565 3.133129 14.235361
C 0.980469 1.557406 14.529489
H -4.882217 2.469715 11.649413
C -3.804347 2.635132 11.637714
H 2.027828 1.294050 14.339655
H 0.201091 7.674646 17.221528
H 0.680271 1.097522 15.479566
H 0.359752 1.111784 13.738897
N 1.188534 3.737475 13.322544
P 1.881127 5.311128 13.213464
C 3.493499 5.289586 14.033444
C 6.038162 5.351467 15.183247
H -0.193649 7.150647 12.282062
H 5.886888 3.196162 15.266044
H -3.977610 4.770846 11.936459
C -3.296993 3.930915 11.796356
H 1.745493 0.060272 8.207347
C 2.068544 0.502920 9.149856
C 4.137846 6.524186 14.248133
H 3.640806 7.460962 13.989473
C 3.697343 0.675744 10.941656
H 0.326153 1.759601 9.313834
C 1.267306 1.457153 9.775330
H 3.237280 2.085815 12.507223
C 3.692509 6.638846 8.322765
C 2.240461 6.706538 7.797488
C 3.728652 4.909142 10.219746
C 3.857176 6.363362 9.830118
H 3.911030 4.171037 9.430699
H 4.197523 4.619369 11.175605
H 4.805198 6.772520 10.216180
H 3.111095 6.984015 10.420284
H 4.194517 7.582532 8.073933
H 4.245510 5.851945 7.788352
C 1.208095 5.816073 8.518884
C 0.630174 6.411506 9.787048
H 0.735190 7.497950 9.891748

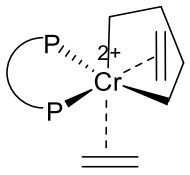
H -0.378922 6.061254 10.054408
H 0.390491 5.513666 7.845582
H 1.670070 4.799669 8.741684
H 2.246230 6.451452 6.729858
H 1.871024 7.740998 7.858987

Spin state: triplet

E = -10306.15 kcal mol-1
H = -9895.39 kcal mol-1
TS = -70.95 kcal mol-1
G (298.15 K) = -9966.34 kcal mol-1

H -1.761284 8.655171 13.497306
C -1.882382 4.184375 11.810999
C -1.027845 8.078336 14.061223
C -0.024969 7.458048 16.184678
C 0.832535 6.524007 14.121905
C -0.122634 7.254368 13.392331
H -1.691088 8.817317 15.978764
H -0.790704 3.000699 16.001459
H -1.484211 5.187845 11.971514
H -0.862327 0.938123 11.352405
H -1.311508 2.856598 14.311273
C -0.606146 3.362364 14.981375
H 6.990072 5.426695 15.803214
C 0.843727 3.050667 14.599035
H 1.641037 6.089541 16.093372
H 1.516378 3.482036 15.357093
C 1.686990 2.035087 10.986417
C -1.013216 3.092106 11.624444
C -1.529375 1.791299 11.475821
C 3.260885 0.144774 9.657107
H 3.868984 -0.602022 9.145636
C -2.910395 1.594441 11.506610
Cr 1.863482 5.331479 10.818959
H -3.314005 0.587673 11.396067
C 0.888912 6.637217 15.524394
C -0.983052 8.173028 15.456500
H -0.808545 4.439583 14.958706
C 4.177536 4.137562 14.375472
C 2.926663 1.647566 11.524450
P 0.758835 3.406379 11.715047
H 4.654233 0.380108 11.294274
C 5.429559 4.174153 14.989927
H 5.791209 7.554354 15.318027
C 5.338881 6.599132 15.050773
H 3.720755 3.179812 14.129738
C 1.103599 1.550227 14.500704
H -4.850765 2.519677 11.707769
C -3.772507 2.681352 11.684810
H 2.159709 1.318599 14.319633
H 0.013282 7.544700 17.270926
H 0.806990 1.071028 15.442418
H 0.503741 1.096035 13.698984
N 1.250314 3.752857 13.318335
P 1.902366 5.349104 13.257591
C 3.494224 5.337488 14.113633
C 6.011145 5.402271 15.323295
H -0.147472 7.197953 12.301880
H 5.949869 3.243289 15.216985
H -3.935110 4.816913 11.989747
C -3.258828 3.975007 11.840853
H 1.701471 0.123914 8.157715
C 2.042928 0.552675 9.100206
C 4.081636 6.574060 14.447695
H 3.552484 7.509397 14.257322
C 3.702888 0.695623 10.865310
H 0.308204 1.812928 9.311762
C 1.256248 1.501523 9.752814
H 3.278923 2.090873 12.453633
C 3.642607 6.292044 8.059955
C 2.169878 6.428886 7.624770
C 3.726987 4.923021 10.232164
C 3.903303 6.281550 9.579837
H 3.863104 4.053574 9.578234
H 4.237971 4.792095 11.200915
H 4.912231 6.663250 9.809133
H 3.256576 7.051738 10.088043
H 4.211815 7.112377 7.603571
H 4.066274 5.363353 7.647652
C 1.134150 5.679191 8.488744
C 0.639151 6.442403 9.700344
H 0.789494 7.527877 9.680975
H -0.365463 6.160117 10.052984
H 0.275510 5.335329 7.890450
H 1.569596 4.676120 8.807961
H 2.082451 6.083988 6.586247
H 1.881688 7.490766 7.616700

Geometry:



Spin state: singlet

E = -11019.64 kcal mol-1
H = -10573.72 kcal mol-1
TS = -73.75 kcal mol-1
G (298.15 K) = -10647.47 kcal mol-1

H -2.619412 6.644591 14.890303
C -1.667146 4.937672 11.037912
C -1.566875 6.928024 14.860728
C 0.216896 8.449349 15.477750
C 0.714313 6.462545 14.173068
C -0.647944 6.113156 14.197176
H -1.859057 8.738264 16.004793
H -0.758309 1.653120 14.668013
H -1.198653 5.879363 11.317285
H -0.921724 1.640452 10.511617
H -0.360309 1.538431 12.947963
C -0.489442 2.241461 13.781659
H 6.403117 4.255515 16.445981
C 0.806425 2.993993 14.067846
H 2.202294 7.895628 14.857665

H 0.637439 3.668395 14.922985
C 1.750791 2.499749 10.539182
C -0.879829 3.781601 10.897823
C -1.502103 2.558540 10.586585
C 3.253708 0.438316 9.377894
H 3.833427 -0.369455 8.930191
C -2.884303 2.510307 10.401081
Cr 1.940154 6.132921 10.824264
H -3.360651 1.559166 10.161786
C 1.143330 7.634659 14.826215
C -1.138754 8.101414 15.490467
H -1.325133 2.912047 13.548035
C 3.252739 5.277737 15.637151
C 2.924014 2.038148 11.163990
P 0.900447 3.932664 11.252301
H 4.567971 0.647737 11.082670
C 4.349422 4.924523 16.425011
H 6.594083 4.180254 13.964633
C 5.657139 4.485779 14.431019
H 2.319005 5.571099 16.116076
C 1.949227 2.038923 14.417436
H -4.736961 3.621832 10.379841
C -3.657752 3.668505 10.528595
H 2.898601 2.570123 14.556887
H 0.554679 9.350880 15.989534
H 1.708256 1.528298 15.359448
H 2.073893 1.270924 13.644174
N 1.172297 3.940205 12.942980
P 1.885792 5.469084 13.191911
C 3.356748 5.232987 14.233300
C 5.549180 4.529364 15.825489
H -0.991229 5.206320 13.700525
H 4.264083 4.955482 17.511640
H -3.648470 5.788103 10.964905
C -3.048143 4.884502 10.854631
H 1.782768 0.470124 7.793016
C 2.101437 0.907986 8.739237
C 4.565933 4.833465 13.634692
H 4.654830 4.779976 12.551193
C 3.666166 1.007927 10.587069
H 0.471385 2.310031 8.786195
C 1.355527 1.942381 9.306530
H 3.254987 2.482345 12.102135
C 2.490642 4.921677 8.132488
C 1.404806 5.532035 8.970910
H 0.366778 5.308164 8.691127
H 1.535075 6.672420 9.016642
C 3.746175 5.342525 10.213418
C 3.831028 5.406593 8.690668
H 3.750386 4.297475 10.556423
H 4.555673 5.890225 10.718466
H 4.672843 4.802723 8.316077
H 4.019611 6.437096 8.347753
H 2.347039 5.176143 7.067362
H 2.413812 3.823812 8.184023
C 3.154334 8.355541 10.651195
C 3.216824 8.049446 11.968242
H 2.372441 9.007320 10.259137
H 3.961622 8.091769 9.966797
H 2.480027 8.444726 12.668986
H 4.073868 7.525939 12.396206
C -0.329490 8.105379 10.120273
C -0.181443 8.317229 11.436292
H -1.012541 7.349914 9.728414
H 0.165883 8.735379 9.378634
H -0.736799 7.753474 12.186847
H 0.440744 9.128796 11.816335

Spin state: triplet

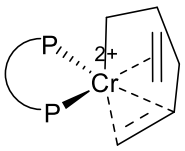
E = -11032.97 kcal mol-1
H = -10587.09 kcal mol-1
TS = -73.99 kcal mol-1
G (298.15 K) = -10661.08 kcal mol-1

H -2.621969 6.633929 14.877859
C -1.666717 4.936610 11.036873
C -1.570080 6.919861 14.849647
C 0.207997 8.450020 15.462570
C 0.714242 6.456024 14.172416
C -0.647187 6.103201 14.194006
H -1.870388 8.736489 15.981407
H -0.739085 1.641089 14.671960
H -1.195036 5.879295 11.307691
H -0.931401 1.634014 10.530765
H -0.343752 1.528476 12.951132
C -0.473634 2.230730 13.785383
H 6.404160 4.267720 16.468178
C 0.820402 2.986814 14.069705
H 2.196534 7.898289 14.850371
H 0.650216 3.661188 14.924648
C 1.742449 2.492620 10.533326
C -0.883221 3.776817 10.905802
C -1.509537 2.553839 10.601708
C 3.233407 0.431391 9.356866
H 3.808588 -0.376321 8.903210
C -2.891831 2.508789 10.416556
Cr 1.944090 6.142106 10.818990
H -3.371317 1.557852 10.182782
C 1.138393 7.633999 14.818796
C -1.146815 8.098247 15.473437
H -1.311940 2.898659 13.553794
C 3.254534 5.284869 15.650800
C 2.916685 2.024612 11.151175
P 0.898464 3.925933 11.252232
H 4.555352 0.628691 11.057056
C 4.350409 4.936080 16.441595
H 6.598361 4.179778 13.987551
C 5.660731 4.487499 14.451058
H 2.319855 5.580102 16.126733
C 1.966208 2.035354 14.418512
H -4.740819 3.626201 10.388254
C -3.661493 3.670322 10.536977
H 2.914714 2.568854 14.555092
H 0.541613 9.355798 15.969553
H 1.728345 1.525781 15.361906
H 2.091132 1.266190 13.646465
N 1.183373 3.933813 12.942581
P 1.893142 5.462439 13.202425
C 3.360476 5.232153 14.247220

C 5.550925 4.538276 15.845263
H -0.986290 5.192165 13.702327
H 4.263840 4.972215 17.527963
H -3.645355 5.792882 10.958114
C -3.047980 4.886560 10.854627
H 1.755372 0.474108 7.778850
C 2.079864 0.907487 8.725163
C 4.570533 4.830361 13.651522
H 4.659791 4.771026 12.568347
C 3.652798 0.994255 10.566743
H 0.453884 2.313985 8.785940
C 1.339593 1.941569 9.300218
H 3.253145 2.464304 12.089480
C 2.501509 4.928548 8.135091
C 1.401119 5.547605 8.945922
H 0.366666 5.313297 8.664443
H 1.525585 6.684907 8.986367
C 3.764576 5.328322 10.229891
C 3.838664 5.409132 8.707316
H 3.771578 4.282512 10.566185
H 4.571881 5.879287 10.733870
H 4.681000 4.810822 8.324096
H 4.027438 6.443036 8.373941
H 2.380105 5.177711 7.065591
H 2.420265 3.831225 8.189807
C 3.165743 8.370380 10.643983
C 3.213544 8.073867 11.962999
H 2.385715 9.015329 10.236642
H 3.980071 8.098903 9.970856
H 2.466895 8.469514 12.653088
H 4.064173 7.549572 12.402925
C -0.342584 8.116801 10.112863
C -0.188448 8.329015 11.427902
H -1.020427 7.355405 9.723457
H 0.145971 8.750180 9.369507
H -0.734039 7.759471 12.181455
H 0.430737 9.144665 11.804103

Geometry:

‡



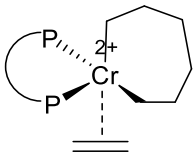
Spin state: triplet

E = -11021.96 kcal mol-1
H = -10577.59 kcal mol-1
TS = -67.85 kcal mol-1
G (298.15 K) = -10645.44 kcal mol-1

H -2.570449 6.497677 15.225345
C -1.886682 4.789511 11.471701
C -1.563620 6.860496 15.016973
C 0.098682 8.622252 15.116567
C 0.667936 6.467237 14.149491
C -0.636604 6.012938 14.406182
H -1.929244 8.825523 15.837614
H -0.730303 1.635453 14.708096
H -1.466404 5.711746 11.866848
H -0.983502 1.703215 10.306741
H -0.497329 1.569738 12.954331
C -0.509495 2.242928 13.821061
H 6.481617 4.689888 16.481712
C 0.849641 2.909652 14.016976
H 2.044370 8.146246 14.336153
H 0.809645 3.537806 14.921246
C 1.572767 2.623868 10.344992
C -1.040481 3.749892 11.045227
C -1.611647 2.542955 10.599225
C 3.025443 0.773550 8.814489
H 3.583007 0.045702 8.224349
C -2.998846 2.397262 10.565615
Cr 1.973824 6.232657 10.868906
H -3.431278 1.456654 10.223263
C 1.030586 7.781568 14.510166
C -1.201755 8.165263 15.364760
H -1.327001 2.960836 13.684689
C 3.388655 5.797216 15.566523
C 2.758938 2.062232 10.847481
P 0.761834 3.986221 11.231619
H 4.387444 0.693738 10.490585
C 4.528032 5.601164 16.349437
H 6.339557 3.639742 14.226445
C 5.516982 4.252407 14.596312
H 2.558067 6.373046 15.970960
C 1.951387 1.866748 14.202341
H -4.914559 3.321057 10.949016
C -3.831256 3.441850 10.979458
H 2.937765 2.329851 14.320527
H 0.386327 9.635060 15.400607
H 1.742550 1.288637 15.112720
H 1.975183 1.162665 13.361220
N 1.174002 3.905442 12.909678
P 1.847023 5.435393 13.222530
C 3.312105 5.227421 14.280994
C 5.593922 4.838391 15.865900
H -0.933287 5.003124 14.129347
H 4.576263 6.039953 17.346444
H -3.914996 5.452446 11.775040
C -3.272126 4.637612 11.441016
H 1.505002 1.068149 7.304094
C 1.856829 1.344457 8.298461
C 4.386629 4.446850 13.806076
H 4.329698 3.964072 12.832111
C 3.477081 1.137382 10.086117
H 0.246155 2.731312 8.619998
C 1.138672 2.275576 9.049338
H 3.109960 2.329271 11.842837
C 3.156945 4.959300 8.349123
C 1.943904 5.648701 8.909020
H 0.987238 5.367305 8.453264
H 2.060398 6.773611 8.872614
C 4.091513 5.422704 10.604527
C 4.399081 5.404139 9.119050
H 3.507857 4.531775 10.901638
H 4.979427 5.426936 11.239920
H 5.245952 4.724576 8.931533

H 4.731237 6.396671 8.772668
H 3.249215 5.162526 7.268012
H 3.021779 3.870718 8.434027
C 4.019244 7.433711 11.361537
C 2.806418 8.150966 11.302981
H 4.779163 7.620396 10.602823
H 4.409530 7.160576 12.343386
H 2.615998 8.801679 10.444635
H 2.342489 8.471786 12.236638
C -0.319273 7.378084 9.998492
C -0.192049 7.938939 11.216357
H -0.867414 6.447411 9.845046
H 0.014612 7.905690 9.103152
H -0.612038 7.485897 12.115325
H 0.239592 8.931108 11.341352

Geometry:



Spin state: singlet

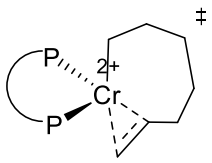
E = -11035.34 kcal mol-1
H = -10589.70 kcal mol-1
TS = -72.07 kcal mol-1
G (298.15 K) = -10661.76 kcal mol-1

H 0.779778 9.964500 14.773570
C -0.690539 3.146343 9.852566
C 0.533848 8.902395 14.791690
C -0.951073 7.101392 15.439335
C 1.091299 6.608114 14.224036
C 1.399381 7.982010 14.200243
H -1.315896 9.185949 15.872919
H -0.391734 1.642643 15.184601
H 0.030833 2.570619 9.272397
H -0.996152 4.950000 12.744908
H -0.248419 1.672488 13.420208
C -0.194541 2.294082 14.323773
H 6.848262 4.952283 16.772752
C 1.189497 2.920780 14.475363
H -0.343603 5.114945 14.886237
H 1.205325 3.552364 15.377564
C 2.130448 2.103732 11.228863
C -0.331410 3.716531 11.089415
C -1.276163 4.469588 11.808658
C 3.336127 -0.405434 10.933904
H 3.805107 -1.383340 10.820268
C -2.572903 4.618783 11.316445
Cr 2.559609 5.746532 11.066074
H -3.304800 5.194030 11.884045
C -0.092684 6.173542 14.846025
C -0.642450 8.464224 15.409828
H -0.993242 3.043760 14.268946
C 4.756537 4.472437 14.129502
C 3.532160 1.991116 11.181899
P 1.394417 3.711272 11.648539
H 5.217711 0.659525 10.993431
C 5.892088 4.358363 14.927319
H 4.938032 6.355917 17.529268
C 4.887208 5.832508 16.574222
H 4.696822 3.920364 13.189293
C 2.292431 1.867847 14.607758
H -3.943867 4.158530 9.710493
C -2.930792 4.038442 10.095243
H 3.279454 2.334144 14.704581
H -1.861048 6.756531 15.931130
H 2.108737 1.269932 15.510263
H 2.302828 1.187538 13.748221
N 1.470770 3.890331 13.349817
P 2.230872 5.403985 13.468666
C 3.674809 5.269577 14.554379
C 5.957607 5.040765 16.149836
H 2.316504 8.341017 13.735649
H 6.727243 3.736786 14.603757
H -2.266835 2.851463 8.413630
C -1.988589 3.306023 9.364777
H 1.324014 -1.195335 10.900826
C 1.943081 -0.301054 10.976759
C 3.745111 5.956202 15.779205
H 2.912959 6.574656 16.114845
C 4.131381 0.742127 11.032827
H 0.249442 1.014219 11.168697
C 1.335943 0.947666 11.122478
H 4.163127 2.877453 11.267304
C 1.173074 5.663594 7.371089
C 0.348535 6.842609 7.911564
C 2.545728 4.733193 9.311641
C 2.575043 5.487685 7.991309
H 2.040389 3.769754 9.179117
H 3.576778 4.502662 9.721619
H 3.192664 4.884927 7.299433
H 3.086852 6.460741 8.068023
H 1.293616 5.805510 6.287920
H 0.604233 4.727298 7.495540
C 0.000727 6.776865 9.408423
C 1.211825 6.871295 10.279388
H 1.952367 7.622477 9.924541
H 1.019296 7.024072 11.388363
H -0.673431 7.617374 9.657785
H -0.562246 5.863211 9.648208
H -0.592521 6.900387 7.346706
H 0.882758 7.785398 7.706594
C 4.602404 6.531906 11.003205
C 4.031543 7.395398 11.918118
H 4.707259 6.803597 9.948714
H 5.232703 5.705630 11.349156
H 3.617702 8.355398 11.603222
H 4.228142 7.269723 12.982474

Spin state: triplet
E = -11053.34 kcal mol-1
H = -10606.94 kcal mol-1
TS = -73.88 kcal mol-1
G (298.15 K) = -10680.82 kcal mol-1

H 0.906126 9.954663 14.920079
C -0.660437 3.083029 9.756400
C 0.611122 8.906251 14.869866
C -0.989939 7.150858 15.341810
C 1.092655 6.617624 14.216522
C 1.463857 7.974332 14.278531
H -1.279085 9.226219 15.867517
H -0.388001 1.674711 15.222904
H 0.089398 2.522088 9.197667
H -1.108728 4.796467 12.684018
H -0.241843 1.658540 13.459070
C -0.209913 2.307656 14.344233
H 6.970842 4.999481 16.495254
C 1.152775 2.982072 14.479934
H -0.445439 5.167352 14.713673
H 1.138458 3.653909 15.352819
C 2.071212 2.000168 11.291612
C -0.359816 3.627475 11.020894
C -1.343895 4.343090 11.722764
C 3.236661 -0.534896 11.067665
H 3.689757 -1.522821 10.979296
C -2.620216 4.490362 11.181018
Cr 2.473436 5.673402 10.962911
H -3.383444 5.038134 11.734312
C -0.144488 6.213019 14.745282
C -0.616231 8.496176 15.402287
H -1.032560 3.029023 14.269145
C 4.790597 4.577972 13.915219
C 3.470529 1.858822 11.299154
P 1.351253 3.634765 11.620352
H 5.135922 0.493590 11.189353
C 5.962117 4.464449 14.659779
H 5.041917 6.284345 17.399274
C 4.971287 5.809926 16.420082
H 4.712981 4.070969 12.950824
C 2.285289 1.969909 14.670060
H -3.915763 4.064259 9.504926
C -2.918430 3.943217 9.928584
H 3.260728 2.467616 14.721271
H -1.940315 6.827070 15.767027
H 2.127823 1.430112 15.613185
H 2.304766 1.233823 13.857665
N 1.420759 3.908383 13.314468
P 2.197394 5.422416 13.404857
C 3.696526 5.307389 14.421605
C 6.052926 5.085000 15.912901
H 2.419821 8.311790 13.878580
H 6.804735 3.891951 14.271470
H -2.172238 2.808174 8.245612
C -1.938830 3.240826 9.218709
H 1.211699 -1.285481 10.972642
C 1.845408 -0.402584 11.060848
C 3.791551 5.926222 15.680515
H 2.950666 6.490118 16.083523
C 4.050746 0.597791 11.185455
H 0.171810 0.948988 11.173206
C 1.257810 0.859351 11.170418
H 4.113253 2.733780 11.405654
C 1.445287 5.927376 7.707563
C 0.562309 7.084043 8.192387
C 2.801156 4.442841 9.344429
C 2.711273 5.714383 8.562332
H 2.141746 3.638930 9.009925
H 3.814886 4.059777 9.535470
H 3.644353 5.885566 7.999241
H 2.781959 6.620068 9.265565
H 1.756849 6.109900 6.670649
H 0.854061 4.999168 7.701567
C -0.093606 6.823036 9.553640
C 0.805406 6.832526 10.776406
H 1.367299 7.787239 10.888537
H 0.224013 6.659762 11.693520
H -0.861952 7.599380 9.725609
H -0.649628 5.873467 9.518293
H -0.231584 7.253417 7.451764
H 1.150538 8.017301 8.223484
C 4.798874 6.793677 10.951310
C 4.200029 7.675054 11.776879
H 4.951968 7.010563 9.892902
H 5.288874 5.900887 11.353408
H 3.790525 8.619210 11.412288
H 4.199204 7.505323 12.855055

Geometry:



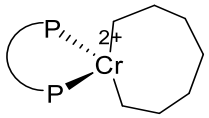
Spin state: triplet

E = -11042.13 kcal mol-1
H = -10596.05 kcal mol-1
TS = -70.14 kcal mol-1
G (298.15 K) = -10666.19 kcal mol-1

Cr -0.957164 -2.745579 -1.957466
P -3.326093 -2.371405 -1.995171
N -3.338292 -0.836638 -1.216717
P -1.711267 -0.738378 -0.675650
C -4.594974 -0.190798 -0.647200
C -4.291189 1.037079 0.211212
H -5.057570 -0.959784 -0.006310
C -5.559169 0.167857 -1.778302
C -4.004806 -2.241081 -3.667921
C -3.844634 -1.049425 -4.398307
C -4.270166 -0.987953 -5.723556
C -4.831619 -2.117322 -6.333060
C -4.972787 -3.309661 -5.615189
C -4.559117 -3.379256 -4.283498
H -3.405906 -0.173249 -3.920854
H -4.168094 -0.058806 -6.284793
H -5.162207 -2.065680 -7.370944
C -4.350436 -3.552475 -1.072912
C -5.755875 -3.525418 -1.157445
C -6.512440 -4.410095 -0.387856
C -5.879436 -5.327769 0.458085
C -4.483537 -5.364920 0.540429

C -3.721161 -4.479094 -0.221462
H -0.917123 -0.432304 -3.479392
H -7.600671 -4.387300 -0.452630
H -6.476898 -6.022066 1.050070
H -3.993177 -6.087285 1.193449
H -2.631565 -4.508280 -0.154905
C -0.932006 0.789401 -1.267735
C 0.443405 0.972448 -1.028126
C 1.091939 2.102097 -1.529433
C 0.381435 3.038644 -2.288247
C -0.977200 2.840729 -2.554883
C -1.634788 1.715051 -2.054306
H 2.152720 2.252712 -1.327018
H 0.889861 3.921325 -2.676891
H -1.528004 3.567274 -3.152947
H -2.689780 1.555770 -2.276505
C -1.725984 -0.709032 1.143191
C -0.971803 0.208128 1.894186
C -1.038427 0.181180 3.289455
C -1.850871 -0.750766 3.940236
C -2.607155 -1.663873 3.194597
C -2.543396 -1.649839 1.803004
H 0.797736 -2.365605 0.073885
H -0.461459 0.902546 3.868787
H -1.903287 -0.761439 5.029383
H -3.253183 -2.381833 3.700469
H -3.153966 -2.352102 1.232314
H -6.256540 -2.828270 -1.829103
H 2.488713 -2.971859 -4.043267
H -1.135644 -1.955206 -4.419132
H 1.606056 -2.110977 -5.302385
H -4.685332 -4.307371 -3.724030
C 0.259318 -4.347389 -0.618982
H 1.010063 0.243639 -0.444861
H 1.238547 -4.548942 -1.053235
H -0.362959 0.965546 1.402866
H -0.289225 -5.228806 -0.287635
H -0.748811 -3.069904 0.788162
H -5.416397 -4.185435 -6.089711
C 0.014823 -3.122293 0.011450
H 1.381181 -0.918156 -3.138320
H 0.939606 -2.360753 -2.332692
C 0.730807 -4.004576 -4.775108
C 1.476607 -2.717497 -4.393606
C 0.481032 -5.025562 -3.649536
C -0.623537 -4.691652 -2.657321
H -1.127049 -5.582092 -2.266752
H -1.479815 -4.108238 -3.160075
H 0.205405 -5.986136 -4.116395
H 1.418544 -5.242343 -3.110383
H 1.321515 -4.508003 -5.553359
H -0.232842 -3.763134 -5.253538
C -0.655333 -1.489510 -3.549281
C 0.797197 -1.827448 -3.339657
H -3.692602 0.802532 1.095655
H -5.247305 1.447665 0.560275
H -3.786517 1.823258 -0.363698
H -5.138623 0.954649 -2.419062
H -6.492500 0.547170 -1.342388
H -5.811013 -0.687515 -2.415163

Geometry:



Spin state: singlet

E = -11049.72 kcal mol-1
H = -10603.40 kcal mol-1
TS = -68.82 kcal mol-1
G (298.15 K) = -10672.22 kcal mol-1

H -1.751071 8.197994 14.945198
C -1.081222 3.312771 10.182335
C -0.871097 7.648617 15.280178
C 0.567346 6.882316 17.079849
C 1.105297 6.336776 14.781943
C -0.036526 7.034053 14.346827
H -1.223867 8.052839 17.372497
H -0.182874 2.425713 16.180763
H -0.418551 2.812987 9.474745
H -1.109379 4.680254 13.328224
H -0.855837 2.600121 14.548418
C -0.116727 3.007044 15.251559
H 7.554795 5.253427 15.147948
C 1.297674 2.891612 14.684465
H 2.300533 5.737767 16.497615
H 2.014993 3.293619 15.417963
C 1.837270 2.059520 11.154131
C -0.611427 3.699875 11.455729
C -1.471232 4.362268 12.351468
C 2.990129 -0.308726 10.225055
H 3.439030 -1.234009 9.862234
C -2.796289 4.603208 11.989423
Cr 2.016127 5.715685 11.183666
H -3.467546 5.098326 12.691405
C 1.411526 6.267770 16.155149
C -0.571312 7.569488 16.644723
H -0.374465 4.047665 15.485380
C 4.532792 4.128932 14.044061
C 3.219636 2.003855 10.893352
P 1.153577 3.587088 11.828362
H 4.862187 0.775477 10.227115
C 5.883233 4.110448 14.395028
H 6.241457 7.352930 15.406446
C 5.761621 6.452097 15.023106
H 4.055402 3.225970 13.661426
C 1.679789 1.445400 14.378634
H -4.303173 4.389491 10.454650
C -3.265363 4.203151 10.732964
H 2.672946 1.364071 13.919667
H 0.800252 6.826887 18.143615
H 1.687162 0.877346 15.317366
H 0.949658 0.969696 13.711595
N 1.493424 3.791268 13.483195
P 2.089480 5.407557 13.584031
C 3.788434 5.311144 14.202732

C 6.498236 5.270737 14.878507
H -0.271916 7.097628 13.284713
H 6.457425 3.188764 14.296520
H -2.777641 3.243177 8.856204
C -2.407843 3.559133 9.832138
H 0.995154 -1.138750 10.324660
C 1.615615 -0.255858 10.481140
C 4.407920 6.479259 14.686513
H 3.835383 7.400109 14.810388
C 3.792097 0.819894 10.431000
C 1.032645 0.923625 10.943354
H 3.851372 2.878576 11.056623
C 4.356936 5.533092 8.284325
C 3.367939 6.098311 7.235755
C 3.956518 5.981647 10.853189
C 4.575566 6.417114 9.539794
H 4.235387 4.948607 11.159671
H 4.219399 6.659650 11.687486
H 5.660992 6.482524 9.744057
H 4.286479 7.459612 9.327235
H 5.331233 5.413993 7.793416
H 4.059489 4.512120 8.583306
C 1.916689 5.602912 7.342499
C 1.275664 5.727403 8.728284
H 1.285414 6.150536 6.624722
H 1.874094 4.543439 7.046134
H 3.721823 5.829219 6.230944
H 3.400000 7.198741 7.265142
C 0.726447 7.161138 10.753340
C 1.155019 7.165242 9.287553
H 0.877000 8.099262 11.303610
H -0.280094 6.743998 10.917559
H -0.036293 0.953737 11.155449
H 1.912463 5.028884 9.366093
H 0.283762 5.251132 8.745789
H 2.095024 7.719459 9.154830
H 0.409885 7.700159 8.671619

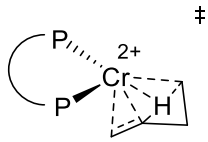
Spin state: triplet

E = -11061.47 kcal mol-1
H = -10614.18 kcal mol-1
TS = -73.60 kcal mol-1
G (298.15 K) = -10687.78 kcal mol-1

H -1.469980 8.557543 14.771362
C -1.628790 4.628341 11.862597
C -0.656978 7.936256 15.147671
C 0.631050 7.067624 17.013899
C 1.219711 6.456002 14.745926
C 0.164769 7.246761 14.256827
H -1.070288 8.381261 17.220629
H -0.718595 2.903424 15.972890
H -1.201926 5.604309 12.098924
H -0.701521 1.394383 11.181145
H -1.194872 3.059978 14.269988
C -0.475513 3.400859 15.024762
H 7.405594 4.842383 15.769000
C 0.958175 3.041289 14.625662
H 2.290558 5.781861 16.513286
H 1.639489 3.324721 15.443371
C 1.872582 2.453278 10.912596
C -0.790711 3.522657 11.624382
C -1.345003 2.256730 11.356552
C 3.405126 0.755781 9.305098
H 3.998967 0.085842 8.682360
C -2.731822 2.106451 11.335267
Cr 2.109308 5.777930 11.192981
H -3.164854 1.125510 11.137785
C 1.461157 6.377226 16.130752
C -0.427608 7.840617 16.525024
H -0.595856 4.481365 15.165352
C 4.377539 3.924499 14.503901
C 3.087680 1.937874 11.393962
P 0.987647 3.746842 11.814298
H 4.778311 0.668816 10.973192
C 5.666606 3.800425 15.025305
H 6.407915 7.104220 15.465830
C 5.839050 6.215103 15.193031
H 3.805262 3.032295 14.253074
C 1.124232 1.553212 14.331720
H -4.645840 3.082326 11.551171
C -3.562664 3.206976 11.570995
H 2.166023 1.281451 14.123698
H 0.813645 7.005797 18.087056
H 0.788648 0.973455 15.200875
H 0.505646 1.246589 13.476056
N 1.436504 3.873310 13.453016
P 2.175171 5.429392 13.603677
C 3.811241 5.198378 14.340873
C 6.398140 4.943013 15.364169
H -0.005016 7.337574 13.183507
H 6.098485 2.810573 15.174671
H -3.664524 5.320994 12.018316
C -3.011886 4.467647 11.833388
H 1.867280 1.032337 7.808503
C 2.207935 1.287531 8.812284
C 4.547402 6.349154 14.684202
H 4.108881 7.342828 14.571895
C 3.843884 1.082694 10.593259
C 1.442123 2.140812 9.605904
H 3.441331 2.209911 12.387127
C 4.239575 4.887769 8.265807
C 3.362683 5.540580 7.168653
C 4.067841 5.586655 10.796538
C 4.658714 5.832625 9.424434
H 4.179782 4.541903 11.150177
H 4.475125 6.266965 11.569381
H 5.754640 5.763901 9.562704
H 4.501613 6.885243 9.136213
H 5.156295 4.520531 7.787669
H 3.744110 3.986032 8.668128
C 1.842871 5.377207 7.342291
C 1.299995 5.755401 8.725480
H 1.312894 5.976598 6.585408
H 1.572198 4.326581 7.154655
H 3.621147 5.101707 6.195105
H 3.625429 6.606209 7.081415
C 1.142231 7.428682 10.615897
C 1.457905 7.238889 9.136406

H 1.504492 8.353777 11.084421
H 0.082272 7.241688 10.860487
H 0.511597 2.554711 9.214302
H 1.852278 5.032093 9.399250
H 0.243367 5.460385 8.824774
H 2.468647 7.602123 8.904754
H 0.774759 7.839592 8.510282

Geometry:

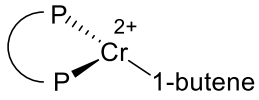


Spin state: triplet

E = -9509.10 kcal mol-1
H = -9138.22 kcal mol-1
TS = -63.93 kcal mol-1
G (298.15 K) = -9202.15 kcal mol-1

Cr -4.832116 2.126524 0.925377
H -1.916566 1.632443 1.024100
H -5.779732 2.444163 3.544408
H -5.260596 4.051890 2.835853
C -2.586768 3.352108 2.211359
H -2.348143 3.000362 -0.034041
C -3.680883 2.537530 2.949199
C -5.065280 2.981543 2.915583
H -3.464007 1.719968 1.952786
C -2.590047 2.496856 0.914162
H -2.899434 4.390686 2.041369
H -3.375651 1.870845 3.766984
H -1.622943 3.371646 2.736719
H -9.586040 0.748277 4.675152
C -9.180671 3.603508 0.774557
C -8.617224 0.308450 4.437224
C -6.678176 -0.989999 5.110014
C -6.851817 -0.146325 2.846632
C -8.085156 0.451280 3.155879
H -8.335603 -0.521033 6.412688
H -10.129403 -1.280099 -0.526286
H -8.918092 3.245144 1.770990
H -8.079359 3.500609 -2.481663
H -10.029000 0.374618 0.119650
C -9.489577 -0.578489 0.025123
H -3.786083 -4.839790 -0.440430
C -8.174661 -0.376351 -0.726172
H -5.182934 -1.328660 3.591427
H -7.626310 -1.330323 -0.773624
C -5.647896 2.533756 -1.298913
C -8.389023 3.263877 -0.340371
C -8.697342 3.761466 -1.621854
C -3.250652 3.077049 -2.679628
H -2.338926 3.292107 -3.237600
C -9.810462 4.584908 -1.781610
H -5.163961 0.439901 -1.667957
H -10.059007 4.971529 -2.770209
C -6.138463 -0.858933 3.830216
C -7.914424 -0.408904 5.413130
H -9.320696 -0.988796 1.028665
C -6.010829 -2.688829 0.986285
C -4.829435 1.473611 -1.769064
P -6.968278 2.205478 -0.087720
H -3.050282 0.934109 -2.865653
C -5.453674 -3.891001 0.551047
H -2.563969 -2.710287 -0.836154
C -3.533352 -2.697456 -0.337363
H -6.962410 -2.688292 1.519472
C -8.377867 0.143400 -2.146872
H -11.476543 5.556862 -0.810417
C -10.608119 4.910620 -0.677728
H -7.424643 0.326266 -2.660129
H -6.138020 -1.556142 5.869243
H -8.931011 -0.606129 -2.726868
H -8.974207 1.065242 -2.153669
N -7.269072 0.541450 0.058501
P -6.077377 0.088916 1.232297
C -5.330185 -1.478967 0.740598
C -4.219723 -3.895409 -0.109708
H -8.641138 0.992288 2.390067
H -5.979531 -4.828431 0.734656
H -10.913034 4.691749 1.452639
C -10.294945 4.421811 0.596244
H -3.715465 5.164828 -2.340038
C -4.028277 4.132925 -2.177498
C -4.084891 -1.487691 0.084606
H -3.541685 -0.555250 -0.082996
C -3.647554 1.756382 -2.470930
H -5.814057 4.703646 -1.109073
C -5.206031 3.875327 -1.477823

Geometry:



Spin state: singlet

E = -9541.73 kcal mol-1
H = -9166.55 kcal mol-1
TS = -65.89 kcal mol-1
G (298.15 K) = -9232.44 kcal mol-1

H -1.404693 8.075808 13.522742
C -2.119796 3.970136 10.920368
C -0.339877 7.853433 13.447926
C 1.969140 8.601109 13.493136
C 1.456926 6.253382 13.180649
C 0.082955 6.538589 13.245712
H 0.265106 9.909376 13.720561
H -1.688134 2.544920 15.325485
H -1.724853 4.969068 11.112141
H -1.123135 0.680894 10.792607
H -1.613178 1.972753 13.649843
C -1.328085 2.794907 14.319589
H 6.061601 3.352182 16.656005
C 0.186900 2.979513 14.367016

H 3.472234 7.068309 13.273526
H 0.421026 3.782222 15.083260
C 1.535524 1.813429 10.775824
C -1.279718 2.841927 10.996376
C -1.776499 1.552071 10.730079
C 3.741419 0.653280 9.438596
H 4.582203 0.187045 8.924365
C -3.122998 1.397767 10.399437
Cr 2.286313 3.993953 10.513867
H -3.519466 0.402558 10.197499
C 2.403255 7.288879 13.302487
C 0.600136 8.883599 13.564453
H -1.840334 3.706788 13.988203
C 3.209422 4.669594 15.335949
H 3.948046 6.902748 8.887699
P 0.430983 3.092441 11.444344
H 4.666264 0.549687 11.388784
C 4.176583 4.339440 16.284762
H 6.363729 2.634001 14.293232
C 5.472390 3.190091 14.584418
H 2.347577 5.271692 15.625680
C 0.928094 1.705035 14.767105
H -5.014700 2.386549 10.078257
C -3.962718 2.515361 10.334900
H 2.008514 1.882351 14.850756
H 2.699639 9.403707 13.597324
H 0.567618 1.348986 15.741091
H 0.747117 0.906996 14.031933
N 0.712205 3.501664 13.056177
P 2.047933 4.584356 12.802429
C 3.360402 4.234729 14.003906
C 5.303816 3.598855 15.911658
H -0.647822 5.733361 13.162905
H 4.055286 4.670120 17.316597
H -4.122259 4.664409 10.530783
C -3.462893 3.798464 10.592301
H 2.566444 0.886170 7.632816
C 2.605726 1.044882 8.711209
C 4.503215 3.504051 13.631346
H 4.644585 3.186768 12.597394
C 3.790607 0.861478 10.818519
H 0.624577 1.908408 8.791192
C 1.513534 1.629147 9.361141
H 2.744424 1.586898 12.571084
C 2.710192 1.460888 11.488691
H 3.413126 6.701957 10.553838
H 2.335739 5.032309 8.146454
H 4.338083 4.214033 10.477380
C 3.575719 6.158324 9.610233
C 4.634838 5.043653 9.774984
C 1.043604 5.696567 9.729397
C 2.284981 5.544017 9.120022
H 0.894687 6.416963 10.535993
H 0.141971 5.357055 9.218643
H 5.555925 5.420098 10.238001
H 4.889359 4.579052 8.813857

Spin state: triplet

E = -9551.18 kcal mol-1
H = -9175.40 kcal mol-1
TS = -67.81 kcal mol-1
G (298.15 K) = -9243.21 kcal mol-1

H -1.508847 7.997246 13.557015
C -2.098941 3.968732 10.894526
C -0.437548 7.807899 13.484308
C 1.847664 8.624368 13.545436
C 1.407598 6.266274 13.204646
C 0.025468 6.508906 13.268281
H 0.104116 9.878046 13.780652
H -1.623188 2.499942 15.304860
H -1.689782 4.967799 11.054058
H -1.137626 0.666961 10.832558
H -1.559699 1.927612 13.629246
C -1.277975 2.754104 14.294662
H 6.082292 3.406311 16.631055
C 0.234820 2.958485 14.328221
H 3.397217 7.141230 13.310012
H 0.463965 3.758886 15.048792
C 1.530995 1.778448 10.754646
C -1.268335 2.834476 10.984245
C -1.782578 1.543424 10.758817
C 3.614834 0.397347 9.450446
H 4.408859 -0.156306 8.948685
C -3.135561 1.394987 10.454473
Cr 2.304269 4.051513 10.479463
H -3.545135 0.399315 10.283249
C 2.322072 7.328379 13.340677
C 0.470502 8.864532 13.615272
H -1.806434 3.658603 13.968871
C 3.222702 4.717608 15.321203
H 4.122795 6.969343 8.940462
P 0.450006 3.086657 11.404876
H 4.651626 0.483023 11.343673
C 4.194102 4.389673 16.266467
H 6.374964 2.684276 14.268120
C 5.484666 3.240503 14.562032
H 2.359822 5.316493 15.614230
C 0.996958 1.691835 14.712196
H -5.022728 2.394756 10.139370
C -3.965645 2.519227 10.376543
H 2.075052 1.884233 14.791728
H 2.553095 9.447699 13.660080
H 0.646903 1.322975 15.685253
H 0.825047 0.897332 13.971459
N 0.745013 3.500979 13.016413
P 2.046801 4.623210 12.797355
C 3.369396 4.282474 13.988555
C 5.321082 3.651001 15.889565
H -0.680604 5.683876 13.170283
H 4.075730 4.720345 17.298644
H -4.101583 4.673630 10.522821
C -3.449490 3.802983 10.594548
H 2.336983 0.445877 7.701247
C 2.446227 0.734499 8.747339
C 4.511623 3.551681 13.612394
H 4.650501 3.230082 12.579450
C 3.754129 0.760861 10.790232
H 0.506489 1.680869 8.828514

C 1.415002 1.430178 9.379589
H 2.815211 1.683258 12.509747
C 2.729195 1.464777 11.445197
H 3.542183 6.798417 10.597731
H 2.452569 5.184033 8.163694
H 4.373510 4.284726 10.560222
C 3.710231 6.245709 9.661011
C 4.725020 5.098477 9.864803
C 1.168939 5.829286 9.766819
C 2.412227 5.662091 9.155769
H 1.035234 6.537520 10.585978
H 0.259919 5.532046 9.241734
H 5.644399 5.441007 10.357148
H 4.994550 4.617951 8.915219

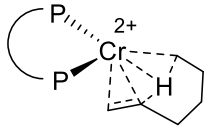
Spin state: quintet

E = -9567.94 kcal mol-1
H = -9192.86 kcal mol-1
TS = -65.61 kcal mol-1
G (298.15 K) = -9258.46 kcal mol-1

H -1.969614 7.389285 14.135887
C -1.524240 4.368531 10.623802
C -0.879407 7.370507 14.126219
C 1.243981 8.451335 14.588012
C 1.196693 6.205757 13.677158
C -0.209554 6.238270 13.660913
H -0.683194 9.357443 14.951050
H -1.409983 2.110112 15.025118
H -0.924136 5.277582 10.716920
H -1.278116 0.956863 10.874249
H -1.092826 1.541428 13.380407
C -1.006942 2.408241 14.048871
H 6.446021 3.214622 16.253843
C 0.449312 2.828316 14.224683
H 3.016556 7.303640 14.150643
H 0.487455 3.657556 14.949652
C 1.564004 1.494375 10.854970
C -0.936488 3.103619 10.820031
C -1.719329 1.940079 10.709688
C 2.963142 -0.776993 10.012646
H 3.499169 -1.670536 9.691648
C -3.076884 2.048982 10.408230
Cr 2.244452 4.860109 10.529165
H -3.685823 1.148151 10.328516
C 1.925448 7.322170 14.132714
C -0.155219 8.475462 14.587376
H -1.630830 3.218040 13.651185
C 3.484753 4.673711 15.403728
H 4.378848 5.980657 7.496442
P 0.806018 3.074688 11.304501
H 4.176297 -0.497386 11.781165
C 4.545772 4.239847 16.199403
H 6.483431 2.757663 13.808354
C 5.640516 3.288727 14.251272
H 2.648941 5.209702 15.854425
C 1.321035 1.680402 14.733748
H -4.720013 3.385473 9.982926
C -3.657891 3.307746 10.217632
H 2.367731 1.987467 14.851131
H 1.806384 9.311268 14.952407
H 0.951910 1.355463 15.715743
H 1.271477 0.818753 14.055327
N 1.012505 3.442780 12.960989
P 2.079809 4.790045 12.969783
C 3.500662 4.409032 14.021915
C 5.618817 3.548389 15.626547
H -0.776069 5.378110 13.302601
H 4.534802 4.440963 17.271072
H -3.337340 5.446975 10.173122
C -2.882346 4.467886 10.324964
H 1.600878 -0.805780 8.332817
C 1.896208 -0.291988 9.247922
C 4.584677 3.718170 13.448168
H 4.600516 3.506218 12.375651
C 3.344356 -0.118311 11.187141
H 0.367558 1.213028 9.054980
C 1.199029 0.845331 9.657293
H 2.959416 1.532748 12.519164
C 2.657600 1.021094 11.605651
H 2.950591 6.987418 7.800672
H 3.174177 3.914997 8.029396
H 3.220884 6.765837 10.275572
C 3.518876 6.121011 8.165583
C 4.034630 6.407746 9.592847
C 1.301112 4.880140 8.217584
C 2.656057 4.877233 8.138651
H 0.732387 5.815794 8.220767
H 0.723369 3.956579 8.148864
H 4.745807 7.244291 9.615202
H 4.573704 5.548600 10.038412

Geometry:

‡



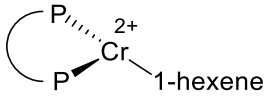
Spin state: triplet

E = -10296.51 kcal mol-1
H = -9887.89 kcal mol-1
TS = -67.30 kcal mol-1
G (298.15 K) = -9955.19 kcal mol-1

H -1.543530 7.871092 13.715908
C -1.171233 3.986409 10.193573
C -0.512127 7.614955 13.960062
C 1.615641 8.202842 14.965732
C 1.319024 6.028206 13.939083
C -0.001335 6.368613 13.596740
H -0.105998 9.506325 14.922424
H -0.649331 4.923971 10.387109
H -0.897302 0.606125 10.724328
C -1.716927 2.911414 13.701069
H 5.315276 2.316912 17.510674
C -0.285346 2.982104 14.230427
H 3.158178 6.696919 14.890274

C 1.733680 1.186735 11.485905
C -0.622547 2.762963 10.622986
C -1.305345 1.555726 10.378262
C 3.320223 -1.104657 11.242631
H 3.930428 -2.003639 11.149219
C -2.530036 1.583389 9.711833
Cr 2.742362 4.215260 11.037556
H -3.064758 0.650988 9.528340
C 2.132782 6.953093 14.619136
C 0.295865 8.532453 14.641231
C 2.741825 4.024053 16.068030
H 5.733837 3.402934 8.481266
P 0.912090 2.797453 11.565604
H 3.853227 -0.770230 13.312067
C 3.539583 3.464435 17.065729
H 5.962312 2.040023 15.123134
C 5.055232 2.585591 15.383944
H 1.853497 4.595890 16.338146
C 0.134960 1.693580 14.934756
H -4.030497 2.813906 8.763656
C -3.073503 2.800462 9.286339
H 1.143143 1.776851 15.359446
H 2.243190 8.917647 15.498568
H -0.561155 1.484182 15.757795
H 0.103743 0.839319 14.244782
N 0.696393 3.374480 13.146749
P 2.028970 4.457620 13.377783
C 3.093567 3.852121 14.715355
C 4.692011 2.745837 16.725310
H -0.631605 5.654300 13.065556
H 3.266179 3.593741 18.113277
H -2.822604 4.947375 9.194577
C -2.395536 4.001419 9.528183
H 2.606832 -1.195894 9.201313
C 2.576887 -0.649584 10.144368
C 4.257944 3.136987 14.380804
H 4.545383 3.002643 13.334380
C 3.279029 -0.412501 12.457214
H 1.223433 0.847902 9.393890
C 1.792406 0.495669 10.255152
H 2.469190 1.271428 13.528414
C 2.495934 0.735149 12.581722
H 5.569775 4.541542 9.808695
H 5.339105 5.640159 7.546508
H 3.917155 4.657120 7.203041
C 3.616713 6.177612 8.738671
C 4.486866 5.133306 8.017762
C 1.948094 6.092072 10.705782
C 2.344142 5.620853 9.393897
H 2.573878 6.845013 11.199363
H 0.891093 6.193828 10.959100
H 3.297454 6.959424 8.031012
H 4.223075 6.688653 9.504523
H 1.528042 5.383132 8.697322
H 2.804480 4.269721 9.387377
C 5.006908 4.055386 8.991876
C 3.874251 3.189705 9.545712
H 4.170047 2.534719 10.397160
H 3.417461 2.548481 8.779810
H -1.995387 3.809934 13.137088
H -2.402361 2.813988 14.552616
H -1.866199 2.037360 13.054559
H -0.220049 3.821789 14.940222

Geometry:



Spin state: singlet

E = -10298.17 kcal mol-1
H = -9886.66 kcal mol-1
TS = -70.07 kcal mol-1
G (298.15 K) = -9956.73 kcal mol-1

H -1.760638 7.873068 13.766026
C -2.195478 3.837965 10.993705
C -0.682798 7.736486 13.674535
C 1.562108 8.659097 13.726863
C 1.229125 6.291489 13.333980
C -0.161562 6.466225 13.421948
H -0.235267 9.822971 14.011274
H -1.553483 2.211459 15.325562
H -1.881122 4.856127 11.229681
H -0.927407 0.655080 10.689901
H -1.477823 1.756392 13.614323
C -1.239354 2.553243 14.331184
H 6.125209 3.641090 16.592024
C 0.257796 2.852071 14.358814
H 3.176360 7.256086 13.438590
H 0.448495 3.623048 15.121108
C 1.629397 2.031118 10.678309
C -1.263461 2.781657 11.005381
C -1.653158 1.469392 10.678772
C 3.939936 1.275284 9.223015
H 4.822161 0.967018 8.662299
C -2.987056 1.218700 10.355787
Cr 2.200484 4.255357 10.545831
H -3.302370 0.204737 10.108506
C 2.094119 7.392045 13.485892
C 0.176241 8.831869 13.818169
H -1.827273 3.442272 14.070901
C 3.139282 4.753334 15.383328
H 3.695146 7.305369 9.071212
P 0.425972 3.159592 11.444425
H 4.889199 1.065933 11.152694
C 4.151597 4.468656 16.299403
H 6.440685 3.061087 14.193584
C 5.509087 3.520163 14.525315
H 2.233691 5.262358 15.715006
C 1.105398 1.617231 14.659612
H -4.959434 2.059621 10.105080
C -3.918082 2.263595 10.356846
H 2.170367 1.874392 14.734275
H 2.229434 9.512020 13.853183
H 0.797980 1.171584 15.614610
H 0.969406 0.856540 13.876769
N 0.706149 3.495264 13.074003

P 1.945563 4.696884 12.861715
C 3.300910 4.395910 14.029709
C 5.332848 3.851466 15.873034
H -0.828567 5.610131 13.314675
H 4.023038 4.739610 17.347714
H -4.254923 4.379399 10.661052
C -3.524394 3.570231 10.672689
H 2.726414 1.575059 7.452520
C 2.759376 1.615432 8.541929
C 4.496417 3.789456 13.604250
H 4.644472 3.538486 12.553249
C 3.978502 1.335713 10.616895
H 0.692940 2.230401 8.712524
C 1.614347 1.995621 9.250365
H 2.883912 1.769096 12.436240
C 2.846000 1.741727 11.346793
H 3.183895 6.980605 10.720635
H 2.137761 5.414986 8.231797
H 4.176824 4.529677 10.464384
C 3.360974 6.500378 9.745841
C 4.486613 5.432213 9.848754
C 0.857591 5.929535 9.874842
C 2.090245 5.866495 9.232534
H 0.694324 6.597937 10.722034
H -0.039308 5.575110 9.365828
H 5.297533 5.832194 10.477161
C 5.053752 4.923919 8.513803
H 5.749147 4.099160 8.731490
C 5.782032 6.015358 7.723181
H 4.250729 4.485071 7.899482
H 6.235124 5.594525 6.816666
H 6.586650 6.466924 8.320524
H 5.104867 6.818802 7.402928

Spin state: triplet

E = -10311.93 kcal mol-1
H = -9900.43 kcal mol-1
TS = -68.78 kcal mol-1
G (298.15 K) = -9969.21 kcal mol-1

H -2.105775 7.532123 14.125546
C -1.809858 4.034261 10.541224
C -1.016017 7.496942 14.139270
C 1.111042 8.525277 14.692169
C 1.052910 6.321179 13.686640
C -0.350896 6.375377 13.642635
H -0.810292 9.447783 15.044241
H -1.574599 2.188094 14.936100
H -1.445293 5.048800 10.711122
H -0.746042 0.767193 10.599800
H -1.316072 1.721070 13.248001
C -1.184959 2.536173 13.970957
H 6.281120 3.528714 16.346637
C 0.286981 2.907730 14.138610
H 2.875623 7.366375 14.250200
H 0.362946 3.673131 14.926951
C 1.880473 1.968961 10.717795
C -0.946977 2.932305 10.695233
C -1.410381 1.622373 10.470375
C 3.957009 0.403823 9.668671
H 4.757181 -0.215397 9.261846
C -2.739862 1.423699 10.099440
Cr 2.371510 4.767698 10.569128
H -3.108320 0.411900 9.929352
C 1.785810 7.403766 14.207604
C -0.286734 8.572216 14.659337
H -1.790359 3.390560 13.644352
C 3.192029 4.637705 15.424575
H 3.361393 6.848084 7.744058
P 0.722877 3.261402 11.263210
H 4.955905 0.729336 11.558288
C 4.248906 4.256608 16.251470
H 6.563331 3.444143 13.875749
C 5.614688 3.765658 14.306295
H 2.261155 4.997502 15.863966
C 1.156522 1.707254 14.507284
H -4.638658 2.354914 9.662952
C -3.600228 2.518283 9.953185
H 2.197950 2.005536 14.682991
H 1.677721 9.361060 15.103175
H 0.778250 1.242063 15.427081
H 1.129669 0.948634 13.712026
N 0.826729 3.609603 12.916602
P 1.937963 4.937042 12.925164
C 3.336186 4.563059 14.025562
C 5.456154 3.818746 15.695048
H -0.919803 5.537834 13.237281
H 4.132952 4.307528 17.334433
H -3.811105 4.669128 10.049740
C -3.137021 3.821203 10.172361
H 2.711038 0.211588 7.907667
C 2.805433 0.646102 8.903486
C 4.557339 4.134159 13.474114
H 4.689600 4.083002 12.390027
C 4.072393 0.937830 10.954178
H 0.889165 1.626507 8.806141
C 1.774990 1.431466 9.412589
H 3.117550 2.095717 12.503882
C 3.041149 1.719726 11.484385
H 3.642298 7.689915 9.273906
H 1.196058 6.023933 8.549181
H 4.326953 5.581038 10.408707
C 3.323470 6.734066 8.834794
C 4.291509 5.613005 9.278943
C 1.456222 6.732709 10.573167
C 1.916071 6.378915 9.295119
H 2.032772 7.417549 11.201715
H 0.393523 6.693185 10.817670
H 5.338748 5.856276 9.045502
C 3.947181 4.227944 8.686535
H 4.489698 3.428724 9.215557
C 4.204257 4.125290 7.177589
H 2.847367 3.980066 8.786719
H 3.954063 3.122498 6.811316
H 5.267199 4.309787 6.971203
H 3.612095 4.853268 6.609975

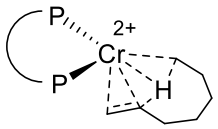
Spin state: quintet

E = -10326.95 kcal mol-1
H = -9914.87 kcal mol-1
TS = -70.18 kcal mol-1
G (298.15 K) = -9985.05 kcal mol-1

H -1.659439 7.608234 13.826643
C -1.359207 4.384144 10.507907
C -0.572862 7.520137 13.850122
C 1.602750 8.485044 14.325049
C 1.434849 6.202909 13.523626
C 0.034839 6.324889 13.462519
H -0.270319 9.530165 14.583000
H -1.406753 2.276250 14.956989
H -0.726188 5.272310 10.588980
H -1.244687 0.974463 10.835699
H -1.085800 1.635811 13.339139
C -0.973730 2.521064 13.978861
H 6.558334 3.073474 16.190898
C 0.496419 2.882984 14.167321
H 3.307081 7.200557 14.008224
H 0.558354 3.734655 14.864469
C 1.602912 1.390474 10.858163
C -0.820679 3.103643 10.740638
C -1.646384 1.969633 10.644664
C 2.895279 -0.973592 10.106789
H 3.390619 -1.901801 9.820467
C -2.995085 2.122515 10.321382
Cr 2.365464 4.803355 10.454468
H -3.635928 1.243175 10.251887
C 2.221075 7.291905 13.948507
C 0.208638 8.599266 14.277992
H -1.553613 3.342718 13.540638
C 3.639210 4.600083 15.315299
H 2.524800 7.488186 7.544526
P 0.918679 3.020083 11.242101
H 4.083334 -0.711079 11.894328
C 4.688677 4.152177 16.118207
H 6.577051 2.563518 13.755620
C 5.751000 3.128047 14.188631
H 2.820401 5.170017 15.755508
C 1.308611 1.717154 14.731993
H -4.581393 3.508940 9.843316
C -3.526357 3.396917 10.095123
H 2.365586 1.983444 14.856983
H 2.208886 9.323690 14.668763
H 0.909922 1.442600 15.717716
H 1.233519 0.835800 14.081965
N 1.107107 3.427936 12.895458
P 2.242068 4.713661 12.877445
C 3.645488 4.305448 13.939182
C 5.739667 3.417504 15.557896
H -0.575217 5.483628 13.131148
H 4.686242 4.375677 17.185492
H -3.124340 5.520964 10.009726
C -2.708545 4.529122 10.188394
H 1.572062 -0.973813 8.396024
C 1.873137 -0.453253 9.305393
C 4.706491 3.570526 13.377523
H 4.713857 3.339283 12.309274
C 3.285138 -0.304852 11.272574
H 0.434581 1.127617 9.037817
C 1.229229 0.729714 9.669908
H 2.965070 1.402786 12.549542
C 2.652302 0.880864 11.645611
H 0.895861 6.941267 7.967430
H 3.485000 5.267644 7.876879
H 1.372078 6.934066 10.351946
C 1.956458 6.855998 8.241476
C 2.141283 7.389566 9.686291
C 1.606596 4.337713 8.122257
C 2.417907 5.425869 8.081892
H 0.520905 4.439475 8.214877
H 1.994611 3.333554 7.933867
H 1.894275 8.461545 9.707009
C 3.546540 7.219343 10.295680
H 3.525051 7.584411 11.332846
C 4.660081 7.906801 9.501154
H 3.882813 6.138495 10.390167
H 5.625477 7.817614 10.013387
H 4.428312 8.975996 9.396270
H 4.771021 7.485242 8.493688

Geometry:

‡



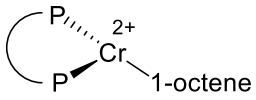
Spin state: triplet

E = -11047.47 kcal mol-1
H = -10602.82 kcal mol-1
TS = -67.12 kcal mol-1
G (298.15 K) = -10669.94 kcal mol-1

H -1.748193 8.112238 14.888255
C -1.818769 4.384890 11.628678
C -0.744024 7.776431 15.148189
C 1.131640 7.761857 16.687363
C 1.245430 6.490645 14.627977
C -0.049645 6.928735 14.289122
H -0.694358 8.865431 17.015191
H -0.963992 2.942805 16.003177
H -1.443509 5.406238 11.691129
H -0.718768 1.137019 11.524401
H -1.378824 3.063267 14.280899
C -0.691307 3.425175 15.055317
H 7.442121 4.690342 15.374942
C 0.759331 3.077509 14.714369
H 2.832504 6.568694 16.112611
H 1.407421 3.437542 15.529033
C 1.798239 2.290800 11.091938
C -0.921958 3.301469 11.619744
C -1.406884 1.982502 11.535970
C 3.449710 0.473707 9.747839
H 4.086400 -0.244992 9.230919
C -2.782287 1.758693 11.474974
Cr 2.118544 5.562228 11.117108

H -3.160670 0.738006 11.413261
C 1.836085 6.909909 15.833772
C -0.151379 8.197162 16.346080
H -0.824765 4.506841 15.171007
C 4.220309 3.842150 14.649329
C 3.038779 1.920914 11.644711
P 0.837447 3.638129 11.844384
H 4.804656 0.706110 11.417728
C 5.541204 3.708139 15.084290
H 6.638023 6.893985 14.533382
C 5.961868 6.039051 14.560623
H 3.548116 2.986567 14.701592
C 0.971807 1.577086 14.526657
H -4.746277 2.656005 11.446804
C -3.672154 2.838237 11.494576
H 2.018598 1.324070 14.318782
H 1.587931 8.082114 17.624306
H 0.665156 1.049778 15.438739
H 0.355452 1.192871 13.702264
N 1.237450 3.841314 13.499503
P 2.088089 5.326684 13.523748
C 3.765217 5.081804 14.173051
C 6.411676 4.800862 15.036020
H -0.518451 6.590999 13.365105
H 5.888814 2.749016 15.469358
H -3.888474 4.988654 11.575197
C -3.191356 4.150526 11.568818
H 1.916153 0.443051 8.222812
C 2.230294 0.860431 9.179899
C 4.643807 6.183287 14.128877
H 4.294980 7.155991 13.773463
C 3.853885 1.007255 10.977047
C 1.405670 1.772147 9.840240
H 3.362929 2.346112 12.593746
C 4.411806 5.633410 7.930714
C 3.597576 6.849296 7.417838
C 4.143425 5.523583 10.508938
C 5.038901 5.827407 9.323140
H 3.874576 4.434732 10.516205
H 4.612956 5.783376 11.470445
H 5.911041 5.156442 9.427944
H 5.449366 6.845803 9.414879
H 5.230731 5.438349 7.226283
H 3.795079 4.718142 7.923792
C 2.071761 6.692064 7.372000
C 1.354522 6.406933 8.699905
H 1.639448 7.620636 6.967169
H 1.803824 5.896175 6.661434
H 3.917381 7.083593 6.393392
H 3.867254 7.744442 8.002045
C 0.883625 7.229704 11.041495
C 1.776090 7.263131 9.892689
H 1.037663 7.961169 11.838291
H -0.163926 6.970726 10.866532
H 0.454639 2.064193 9.392453
H 1.498137 5.314812 8.958405
H 0.263538 6.483144 8.572130
H 3.053322 6.642533 10.191284
H 2.331731 8.185833 9.682590

Geometry:



Spin state: singlet

E = -11057.51 kcal mol-1
H = -10610.09 kcal mol-1
TS = -70.46 kcal mol-1
G (298.15 K) = -10680.55 kcal mol-1

H -2.431070 7.102298 14.298342
C -1.724024 4.003649 10.399477
C -1.345804 7.142744 14.395863
C 0.644864 8.220299 15.267289
C 0.839713 6.199669 13.943014
C -0.557191 6.161383 13.794054
H -1.365773 8.936584 15.599980
H -1.420741 1.681826 14.540894
H -1.530315 5.024734 10.731769
H -0.173185 0.953774 10.080542
H -1.115999 1.540577 12.802077
C -1.051892 2.221938 13.659776
H 6.105979 3.615308 16.655271
C 0.385736 2.667535 13.919985
H 2.525545 7.273882 14.800223
H 0.392628 3.293972 14.825110
C 2.230076 2.499463 10.480587
C -0.708762 3.029910 10.456834
C -0.954314 1.712908 10.024534
C 4.556403 1.407783 9.352098
H 5.453783 0.971414 8.911829
C -2.218938 1.378243 9.541400
Cr 2.405097 5.177821 10.737261
H -2.418480 0.358756 9.210485
C 1.442210 7.239099 14.675455
C -0.746323 8.172361 15.129746
H -1.716588 3.075304 13.477226
C 2.977183 4.460088 15.598711
H 3.540350 8.015266 8.665714
P 0.872819 3.509324 11.156439
H 5.435404 1.629956 11.315302
C 4.007649 4.093900 16.464148
H 6.586336 3.925045 14.233195
C 5.572863 4.062293 14.610729
H 1.977925 4.642820 15.994356
C 1.344856 1.492787 14.103768
H -4.216535 2.075906 9.108973
C -3.230289 2.344730 9.488861
H 2.355279 1.838703 14.357102
H 1.110638 9.018923 15.845109
H 0.993965 0.846410 14.918805
H 1.393471 0.884320 13.189434
N 0.882170 3.597390 12.844530
P 1.880350 4.996497 13.069707
C 3.236451 4.607215 14.221521
C 5.302266 3.892830 15.972404
H -1.025485 5.356454 13.226463

H 3.801829 3.974025 17.528161
H -3.774969 4.403850 9.867791
C -2.984320 3.654743 9.916941
H 3.411540 1.268011 7.519891
C 3.404276 1.572880 8.566398
C 4.543415 4.416304 13.737884
H 4.765952 4.543528 12.676098
C 4.550445 1.782011 10.696627
H 1.368663 2.274313 8.489758
C 2.252374 2.128773 9.112473
H 3.369202 2.536586 12.335516
C 3.392507 2.322773 11.267779
H 3.516345 8.309712 10.410221
H 1.468134 6.678998 8.780169
H 4.298807 6.038080 10.934641
C 3.360340 7.542378 9.639882
C 4.352901 6.375650 9.853619
C 1.193406 7.015372 10.886732
C 1.951209 6.979191 9.717538
H 1.520284 7.605653 11.745212
H 0.127048 6.787619 10.870598
H 5.399502 6.709339 9.796649
C 4.136986 5.194120 8.888925
H 4.774004 4.342774 9.172817
C 4.348537 5.547077 7.408561
H 3.077799 4.786012 8.911201
C 4.148478 4.350899 6.472305
H 5.370978 5.944971 7.300378
H 3.667271 6.359445 7.112780
H 3.125314 3.957810 6.603563
H 4.830726 3.538768 6.773063
C 4.382010 4.714067 5.003664
H 4.229778 3.845003 4.351087
H 5.407264 5.075605 4.843503
H 3.692587 5.504602 4.674404

Spin state: triplet

E = -11067.87 kcal mol-1
H = -10620.54 kcal mol-1
TS = -70.64 kcal mol-1
G (298.15 K) = -10691.18 kcal mol-1

H -2.525063 6.976029 14.319547
C -1.627710 4.043248 10.316699
C -1.442699 7.048115 14.429823
C 0.504474 8.170734 15.341858
C 0.776303 6.182572 13.982116
C -0.617753 6.104069 13.817541
H -1.530806 8.817104 15.667442
H -1.401606 1.667213 14.472121
H -1.410244 5.063770 10.637116
H -0.155728 0.948056 10.069637
H -1.025390 1.487661 12.751288
C -1.013501 2.193841 13.591064
H 6.142180 3.681625 16.617531
C 0.400868 2.684080 13.894407
H 2.418693 7.294862 14.874564
H 0.358049 3.326793 14.787461
C 2.281338 2.438694 10.509047
C -0.641395 3.042533 10.407916
C -0.914766 1.726916 9.988813
C 4.600768 1.277403 9.444059
H 5.496325 0.813862 9.028722
C -2.178576 1.420675 9.485276
Cr 2.419533 5.267970 10.761028
H -2.399623 0.402743 9.163164
C 1.338198 7.227003 14.739591
C -0.883168 8.081473 15.189700
H -1.693982 3.022266 13.358692
C 2.990810 4.504848 15.612463
H 3.325760 7.959787 8.442557
P 0.937150 3.495112 11.131601
H 5.447858 1.515690 11.419601
C 4.037404 4.143914 16.460556
H 6.584087 4.004277 14.190145
C 5.575371 4.132665 14.583182
H 1.994532 4.673197 16.021850
C 1.379528 1.536512 14.138231
H -4.147223 2.166634 9.004039
C -3.161542 2.413769 9.399684
H 2.373365 1.909791 14.416497
H 0.939125 8.973277 15.938101
H 1.014239 0.903950 14.957885
H 1.471336 0.905827 13.242613
N 0.912753 3.612357 12.821259
P 1.861682 5.034482 13.093134
C 3.229491 4.662548 14.232862
C 5.326089 3.955834 15.948146
H -1.054939 5.297575 13.227660
H 3.848896 4.016818 17.526941
H -3.656256 4.492268 9.738959
C -2.887889 3.722645 9.814284
H 3.486885 1.130685 7.594320
C 3.468466 1.454954 8.634870
C 4.530229 4.482995 13.727903
H 4.734822 4.614645 12.662368
C 4.577594 1.675389 10.782357
H 1.449327 2.195616 8.509010
C 2.317973 2.044102 9.151143
H 3.392217 2.508028 12.379181
C 3.423628 2.253369 11.320717
H 3.434532 8.447584 10.138840
H 1.243758 6.721732 8.875167
H 4.301043 6.232889 10.831065
C 3.238131 7.595083 9.473602
C 4.286691 6.486098 9.727973
C 1.260445 7.095378 11.002103
C 1.853779 7.021306 9.734517
H 1.697543 7.722086 11.784217
H 0.197740 6.888302 11.137329
H 5.314140 6.854066 9.589962
C 4.075260 5.227320 8.860673
H 4.706554 4.394546 9.209137
C 4.305769 5.467793 7.358749
H 3.009666 4.839678 8.901239
C 4.094769 4.212489 6.506062
H 5.336359 5.838190 7.234540
H 3.642108 6.268915 7.000325
H 3.063262 3.847304 6.649736

H 4.758440 3.412138 6.871523
C 4.353592 4.467826 5.018660
H 4.196890 3.556583 4.427224
H 5.386170 4.802574 4.847805
H 3.680607 5.242162 4.623730

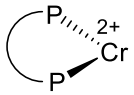
Spin state: quintet

E = -11082.02 kcal mol-1
H = -10633.56 kcal mol-1
TS = -74.76 kcal mol-1
G (298.15 K) = -10708.32 kcal mol-1

H -2.211682 6.698628 14.791593
C -1.822004 4.137496 10.985072
C -1.157274 6.900897 14.601264
C 0.768251 8.365260 14.790955
C 0.989845 6.199568 13.724736
C -0.376895 5.949742 13.942438
H -1.199787 8.845704 15.541010
H -0.584763 1.543855 15.018816
H -1.372366 5.127755 11.095016
H -0.975313 0.819174 10.801917
H -0.404441 1.181113 13.296474
C -0.400659 1.994065 14.035070
H 7.051134 4.241190 15.267464
C 0.948477 2.705526 14.064862
H 2.620961 7.619011 13.978353
H 0.918877 3.476788 14.851833
C 1.694433 1.851553 10.451035
C -1.008793 2.988400 10.948508
C -1.594273 1.716295 10.816072
C 3.302571 -0.061071 9.191312
H 3.922272 -0.817142 8.708275
C -2.981586 1.603085 10.723827
Cr 1.805901 5.262240 10.357570
H -3.436978 0.617470 10.623553
C 1.560711 7.418216 14.141270
C -0.586967 8.106132 15.024772
H -1.229367 2.675801 13.807556
C 3.759530 5.076644 14.968689
H 2.935584 7.359497 7.257873
P 0.769997 3.237455 11.162338
H 4.708618 0.287406 10.797199
C 4.999841 4.847566 15.566005
H 6.780798 3.869997 12.819980
C 5.932993 4.202643 13.419201
H 2.917665 5.414595 15.573364
C 2.099047 1.741677 14.355884
H -4.870836 2.649710 10.694746
C -3.787043 2.746574 10.766672
H 3.068670 2.255009 14.350057
H 1.211303 9.303880 15.124694
H 1.956783 1.299763 15.351136
H 2.119754 0.922705 13.625004
N 1.189675 3.499986 12.800408
P 1.989807 5.018601 12.778991
C 3.604361 4.864549 13.586061
C 6.083483 4.413267 14.794901
H -0.824323 5.011521 13.613077
H 5.121270 5.009294 16.637416
H -3.837954 4.903365 10.929595
C -3.208178 4.014016 10.899335
H 1.722790 -0.197851 7.720712
C 2.066187 0.285906 8.635456
C 4.697195 4.426752 12.814233
H 4.585803 4.255040 11.741661
C 3.745260 0.559325 10.364858
H 0.298453 1.503630 8.814741
C 1.262307 1.244195 9.254372
H 3.303907 2.007575 11.900552
C 2.953274 1.522608 10.989854
H 1.326945 7.763465 7.879128
H 2.588256 4.964626 7.614278
H 2.012578 7.453174 10.208364
C 2.207403 7.127794 8.046968
C 2.820449 7.481319 9.426936
C 0.574360 5.187619 8.211891
C 1.817241 5.669636 7.949519
H -0.261583 5.856791 8.440578
H 0.331537 4.133566 8.063540
H 3.101416 8.544942 9.434624
C 4.043308 6.648102 9.861393
H 4.344529 6.947685 10.876998
C 5.248225 6.723550 8.916968
H 3.817225 5.545861 9.943073
C 6.435860 5.890525 9.415620
H 5.543361 7.781133 8.817492
H 4.962551 6.385354 7.908080
H 6.116762 4.838205 9.523829
H 6.717657 6.232894 10.425117
C 7.644688 5.968104 8.479167
H 8.479955 5.365639 8.858254
H 7.999914 7.002907 8.376809
H 7.394761 5.598576 7.474414

6.6 Dicationic Cr^{II}/Cr^{IV} mechanism for complex 2

Geometry:



Spin state: singlet

E = -9369.04 kcal mol-1
H = -9014.44 kcal mol-1
TS = -68.75 kcal mol-1
G (298.15 K) = -9083.19 kcal mol-1

Cr -0.563423 -2.318738 -2.418821
P -2.808995 -2.752012 -1.897246
N -2.997477 -1.161444 -1.259384
P -1.379225 -0.661098 -0.995293
C -4.176652 -0.278529 -1.263643
H -4.206347 0.287418 -0.322831
H -5.078340 -0.891005 -1.329917

H -4.141590 0.413997 -2.116162
C -3.588372 -2.810867 -3.533339
C -4.960410 -3.026308 -3.739783
C -5.482316 -3.068409 -5.032109
C -4.629673 -2.906325 -6.124987
C -3.254999 -2.704254 -5.946137
C -2.746017 -2.661661 -4.652030
H -5.610451 -3.161350 -2.875271
H -6.547863 -3.235082 -5.187367
H -5.026642 -2.946488 -7.139567
H -2.618221 -2.599773 -6.821439
C -3.477037 -4.075821 -0.868081
C -4.735405 -4.048148 -0.223487
C -5.132602 -5.141791 0.557049
C -4.300497 -6.258491 0.669982
C -3.063534 -6.305446 0.021354
C -2.654676 -5.208646 -0.734868
H -6.671640 -2.885816 1.320150
H -6.092636 -5.136697 1.069255
H -4.630382 -7.104045 1.274362
H -2.423124 -7.182030 0.109990
H -1.680343 -5.227026 -1.228569
C -0.973315 0.756560 -2.069921
C 0.075321 0.581812 -2.993775
C 0.469237 1.602298 -3.853431
C -0.207348 2.825764 -3.803321
C -1.265228 3.021093 -2.910986
C -1.643229 1.993677 -2.046729
H 2.433664 -0.504409 -4.245879
H 1.285863 1.459433 -4.559741
H 0.097066 3.629344 -4.474332
H -1.788070 3.976844 -2.882623
H -2.447706 2.157134 -1.329468
C -1.139221 -0.152713 0.709334
C -1.397513 -1.105578 1.733826
C -1.221823 -0.739308 3.073647
C -0.759674 0.540551 3.387788
C -0.463047 1.471376 2.385989
C -0.646994 1.122607 1.051834
H -2.938411 -2.985578 2.954235
H -1.425940 -1.448006 3.873510
H -0.619295 0.808595 4.435579
H -0.091544 2.462108 2.644806
H -0.411496 1.842346 0.269115
O -5.492623 -2.929342 -0.425161
C -6.784961 -2.853927 0.227744
H -7.206092 -1.889266 -0.070443
H -7.442792 -3.665472 -0.113207
O -1.352004 -2.483377 -4.392697
C -0.489032 -2.284810 -5.561512
O 0.702801 -0.694323 -3.045138
C 2.166756 -0.699585 -3.200463
H 2.605177 0.053514 -2.536016
H 2.503333 -1.701599 -2.912204
O -1.794602 -2.339749 1.311263
C -2.112572 -3.332540 2.317844
H -2.422131 -4.219501 1.759584
H -1.229521 -3.564225 2.929436
H -0.519916 -3.175882 -6.198977
H -0.803769 -1.387888 -6.108028
H 0.519963 -2.142839 -5.166635

Spin state: triplet

E = -9378.95 kcal mol-1
H = -9024.35 kcal mol-1
TS = -68.12 kcal mol-1
G (298.15 K) = -9092.47 kcal mol-1

Cr -0.575491 -2.308425 -2.490118
P -2.823342 -2.752962 -1.913700
N -3.002189 -1.184417 -1.208818
P -1.385796 -0.693681 -1.018961
C -4.204041 -0.466940 -0.748667
H -4.527588 -0.839783 0.230105
H -5.011472 -0.600393 -1.477275
H -3.974042 0.601712 -0.671035
C -3.642410 -2.759630 -3.535337
C -5.007399 -3.026656 -3.731055
C -5.556224 -3.016561 -5.013114
C -4.740063 -2.745511 -6.111472
C -3.372886 -2.489991 -5.946711
C -2.836269 -2.503834 -4.663872
H -5.632370 -3.238906 -2.865189
H -6.616154 -3.225669 -5.155226
H -5.158775 -2.740906 -7.118087
H -2.759590 -2.302203 -6.824924
C -3.451843 -4.096829 -0.881754
C -4.736697 -4.125766 -0.289019
C -5.106066 -5.217278 0.506843
C -4.216641 -6.279536 0.690423
C -2.951529 -6.271238 0.097266
C -2.573687 -5.175837 -0.677598
H -6.808978 -3.031522 1.128212
H -6.087645 -5.253605 0.975467
H -4.524220 -7.126031 1.305246
H -2.266135 -7.105517 0.240876
H -1.580450 -5.153299 -1.130921
C -0.944381 0.687736 -2.137956
C 0.144536 0.462628 -3.000493
C 0.540742 1.388118 -3.957407
C -0.171322 2.587775 -4.062904
C -1.260037 2.840784 -3.221618
C -1.646075 1.899547 -2.265751
H 2.754280 0.079506 -2.664196
H 1.388073 1.173575 -4.609361
H 0.126290 3.325065 -4.808897
H -1.809382 3.778172 -3.309832
H -2.489281 2.112749 -1.609116
C -1.083302 -0.149159 0.661942
C -1.356748 -1.058700 1.720470
C -1.148750 -0.655588 3.044749
C -0.648421 0.621834 3.308431
C -0.347761 1.513771 2.272538
C -0.561875 1.127264 0.953167
H -2.957615 -2.830963 3.014976
H -1.360495 -1.331669 3.870704
H -0.485629 0.920991 4.344468
H 0.045387 2.505062 2.494619
H -0.335103 1.818735 0.141930

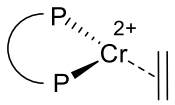
O -5.542147 -3.055748 -0.555540
C -6.867188 -3.030539 0.030767
H -7.318203 -2.095467 -0.313958
H -7.466612 -3.882154 -0.319800
O -1.445244 -2.285170 -4.431663
C -0.630248 -1.899393 -5.590544
O 0.851435 -0.784983 -2.922856
C 2.130169 -0.681472 -2.182877
H 1.923649 -0.412552 -1.138379
H 2.607056 -1.664612 -2.254904
O -1.808142 -2.287231 1.338761
C -2.161862 -3.236805 2.374888
H -2.525467 -4.119573 1.842449
H -1.282570 -3.499777 2.979007
H -0.606308 -2.721078 -6.315560
H -1.033724 -0.981090 -6.033463
H 0.373518 -1.713416 -5.197948

Spin state: quintet

E = -9404.40 kcal mol-1
H = -9050.32 kcal mol-1
TS = -67.17 kcal mol-1
G (298.15 K) = -9117.49 kcal mol-1

Cr -0.554793 -2.239554 -2.547339
P -2.798748 -2.721180 -1.920015
N -2.938108 -1.133311 -1.274172
P -1.319848 -0.646511 -0.943880
C -4.113557 -0.247719 -1.195937
H -4.136855 0.238812 -0.211173
H -5.020626 -0.845108 -1.308594
H -4.075485 0.512482 -1.988263
C -3.589897 -2.798369 -3.551954
C -4.982625 -2.871138 -3.726084
C -5.535224 -2.950674 -5.002790
C -4.694038 -2.972412 -6.116289
C -3.302690 -2.918885 -5.970910
C -2.758826 -2.834315 -4.692254
H -5.624427 -2.874336 -2.845339
H -6.616085 -3.004290 -5.129479
H -5.115262 -3.043635 -7.119321
H -2.677160 -2.953348 -6.859819
C -3.453451 -4.045681 -0.884614
C -4.713605 -4.022924 -0.243064
C -5.115386 -5.125298 0.522030
C -4.283910 -6.243513 0.626251
C -3.043137 -6.282623 -0.015404
C -2.630149 -5.178461 -0.759073
H -6.654854 -2.879416 1.309656
H -6.077533 -5.125351 1.030337
H -4.616702 -7.095432 1.219982
H -2.401990 -7.159037 0.069434
H -1.653052 -5.189598 -1.246399
C -0.917680 0.800775 -1.986282
C 0.094609 0.663489 -2.958083
C 0.456733 1.719376 -3.788863
C -0.214316 2.940069 -3.664407
C -1.238679 3.099004 -2.727529
C -1.584784 2.037241 -1.892721
H 2.273443 -0.433900 -4.507740
H 1.244433 1.606605 -4.531983
H 0.067395 3.769488 -4.313466
H -1.759637 4.052315 -2.641019
H -2.361799 2.171730 -1.140146
C -1.144905 -0.154330 0.774700
C -1.458595 -1.108897 1.781929
C -1.318029 -0.757714 3.130306
C -0.837462 0.507775 3.471993
C -0.485995 1.438910 2.488943
C -0.633802 1.105495 1.146366
H -3.034908 -3.002558 2.956780
H -1.564963 -1.468013 3.916515
H -0.726404 0.763603 4.526324
H -0.098021 2.417697 2.768211
H -0.350269 1.825118 0.379937
O -5.466209 -2.898101 -0.429584
C -6.762006 -2.829467 0.217326
H -7.178622 -1.858637 -0.067015
H -7.420172 -3.633479 -0.140391
O -1.350504 -2.799625 -4.478738
C -0.490682 -2.892933 -5.659737
O 0.717281 -0.610227 -3.087636
C 2.146734 -0.620683 -3.435103
H 2.668457 0.135722 -2.838045
H 2.515193 -1.620089 -3.180605
O -1.872529 -2.329527 1.337641
C -2.196827 -3.335441 2.328779
H -2.490300 -4.219271 1.757550
H -1.320922 -3.566021 2.950936
H -0.671471 -3.841761 -6.178845
H -0.664181 -2.035525 -6.321470
H 0.537703 -2.871456 -5.283818

Geometry:



Spin state: singlet

E = -10135.71 kcal mol-1
H = -9746.21 kcal mol-1
TS = -71.80 kcal mol-1
G (298.15 K) = -9818.02 kcal mol-1

Cr -0.739404 -2.528168 -1.967989
P -3.081380 -2.750938 -2.042078
N -3.488742 -1.119342 -1.676272
P -1.898643 -0.595587 -1.418125
C -4.789688 -0.515228 -1.355397
H -4.719922 0.037521 -0.409394
H -5.530072 -1.313925 -1.226485
H -5.121245 0.150819 -2.161968
C -3.484242 -3.030293 -3.779492
C -4.744115 -3.434111 -4.253066
C -4.986599 -3.517073 -5.622965
C -3.968442 -3.191216 -6.521680
C -2.713774 -2.762117 -6.072676

C -2.478695 -2.672320 -4.701462
H -5.531848 -3.685683 -3.542394
H -5.961883 -3.837897 -5.987793
H -4.144406 -3.265956 -7.595109
H -1.946897 -2.512050 -6.801750
C -3.980096 -3.921397 -1.008033
C -4.251482 -3.645121 0.361242
C -4.903997 -4.607410 1.141861
C -5.234376 -5.847467 0.591052
C -4.921371 -6.152592 -0.737538
C -4.297269 -5.194482 -1.529744
H -3.729833 -2.756378 2.916541
H -5.149678 -4.400611 2.181739
H -5.736882 -6.587070 1.215281
H -5.169849 -7.127579 -1.154922
H -4.055082 -5.429332 -2.566101
C -1.345144 0.812592 -2.386635
C 0.028346 0.724074 -2.702589
C 0.658926 1.739701 -3.414528
C -0.101159 2.842122 -3.830706
C -1.465871 2.931098 -3.546276
C -2.091423 1.915725 -2.818543
H 1.718921 1.689294 -3.658340
H 0.389086 3.637158 -4.393144
H -2.040615 3.792733 -3.884327
H -3.154081 1.984163 -2.584322
C -1.536477 -0.263179 0.315694
C -0.970330 -1.343283 1.013828
C -0.627723 -1.221797 2.358434
C -0.869621 -0.004606 3.007828
C -1.429020 1.081285 2.327257
C -1.750613 0.956418 0.975069
H -1.601141 -3.622514 1.851548
H -0.160190 -2.042185 2.900650
H -0.595354 0.095908 4.058339
H -1.596771 2.025511 2.844741
H -2.158179 1.805290 0.424138
O -3.823343 -2.437269 0.832963
C -4.167961 -2.060780 2.186008
H -3.730882 -1.066972 2.323067
H -5.258152 -2.017534 2.315214
O -1.266560 -2.208486 -4.164375
C -0.284221 -1.703723 -5.119576
O 0.670874 -0.454147 -2.283217
C 2.122844 -0.408862 -2.150301
O -0.741092 -2.527553 0.283711
C -0.866826 -3.771906 1.054416
H -1.236191 -4.534630 0.365534
H 0.109362 -4.056096 1.462701
H 0.083540 -2.518770 -5.754785
H -0.737102 -0.904835 -5.718361
H 0.528057 -1.297112 -4.517550
C 0.700550 -4.147333 -1.620605
C 0.796786 -3.760723 -2.947638
H 0.135194 -5.042776 -1.350610
H 1.422356 -3.802312 -0.875850
H 0.299302 -4.332482 -3.733510
H 1.599985 -3.098315 -3.280238
H 2.400664 -1.318042 -1.609266
H 2.418064 0.475746 -1.572985
H 2.603535 -0.402671 -3.137886

Spin state: triplet

E = -10154.87 kcal mol-1
H = -9766.10 kcal mol-1
TS = -69.51 kcal mol-1
G (298.15 K) = -9835.61 kcal mol-1

Cr -0.760469 -2.464960 -1.929769
P -3.053395 -2.790476 -2.012222
N -3.517561 -1.158165 -1.634634
P -1.955506 -0.541189 -1.407242
C -4.836649 -0.604763 -1.299473
H -4.774422 -0.027454 -0.367378
H -5.536939 -1.433687 -1.137562
H -5.216836 0.028871 -2.111189
C -3.366465 -3.000709 -3.784662
C -4.613494 -3.316500 -4.347398
C -4.774814 -3.348500 -5.732303
C -3.690497 -3.053456 -6.560551
C -2.443879 -2.710036 -6.023426
C -2.295236 -2.677699 -4.639872
H -5.457497 -3.540376 -3.694511
H -5.742661 -3.602289 -6.163650
H -3.805823 -3.083607 -7.644174
H -1.622165 -2.476318 -6.696128
C -4.017284 -3.963951 -1.049517
C -4.219447 -3.742625 0.340186
C -4.921443 -4.688666 1.095436
C -5.366350 -5.868189 0.493374
C -5.116655 -6.126414 -0.857892
C -4.444381 -5.178365 -1.624249
H -3.581039 -2.969725 2.927513
H -5.113130 -4.520526 2.153491
H -5.904993 -6.599826 1.096436
H -5.449914 -7.058105 -1.313437
H -4.246964 -5.378888 -2.676720
C -1.426354 0.860366 -2.397036
C -0.044310 0.795337 -2.702413
C 0.556368 1.801714 -3.453779
C -0.230692 2.865249 -3.917164
C -1.598655 2.927851 -3.642706
C -2.198683 1.924661 -2.878245
H 1.619302 1.775462 -3.688225
H 0.241542 3.651492 -4.506695
H -2.195021 3.759770 -4.015940
H -3.264668 1.970787 -2.653610
C -1.572367 -0.213595 0.323787
C -0.873949 -1.246545 0.970759
C -0.483439 -1.123851 2.300725
C -0.809838 0.050717 2.991634
C -1.504107 1.089259 2.365760
C -1.873246 0.962396 1.025464
H -1.333013 -3.670481 1.692284
H 0.078851 -1.905936 2.806822
H -0.499402 0.152849 4.031764
H -1.742650 1.999376 2.915502
H -2.388333 1.778374 0.516441
O -3.673222 -2.596802 0.853038

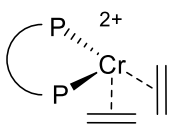
C -3.989255 -2.235753 2.217366
H -3.506299 -1.266390 2.374177
H -5.075177 -2.142996 2.356298
O -1.080177 -2.293689 -4.020061
C 0.035994 -1.941914 -4.899369
O 0.640258 -0.333361 -2.222956
C 2.093075 -0.243110 -2.130434
O -0.570005 -2.407360 0.204790
C -0.494430 -3.651182 0.988716
H -0.585771 -4.474302 0.280146
H 0.470741 -3.702863 1.504030
H 0.310117 -2.806644 -5.515030
H -0.243566 -1.077639 -5.512818
H 0.858302 -1.673515 -4.234801
C 0.710222 -4.015473 -2.152294
C -0.550612 -4.614951 -2.318746
H 1.274758 -4.148050 -1.225470
H 1.325902 -3.798473 -3.029930
H -1.000341 -5.228912 -1.535201
H -0.929514 -4.837282 -3.318462
H 2.405664 -1.137896 -1.585346
H 2.378562 0.659201 -1.575617
H 2.551405 -0.237392 -3.129224

Spin state: quintet

E = -10155.58 kcal mol-1
H = -9766.20 kcal mol-1
TS = -73.69 kcal mol-1
G (298.15 K) = -9839.89 kcal mol-1

Cr -0.469893 -2.396398 -2.482729
P -2.792216 -2.794460 -1.970234
N -2.987749 -1.191743 -1.379076
P -1.384062 -0.684312 -1.066027
C -4.214543 -0.385718 -1.265360
H -4.499660 -0.261508 -0.213237
H -5.024402 -0.893800 -1.798456
H -4.057930 0.593396 -1.734378
C -3.641225 -2.846853 -3.565966
C -4.978806 -3.245817 -3.714160
C -5.594067 -3.196737 -4.964732
C -4.866376 -2.757447 -6.071806
C -3.524749 -2.372885 -5.951246
C -2.916311 -2.423591 -4.699222
H -5.532884 -3.585733 -2.839381
H -6.633944 -3.502150 -5.076450
H -5.337627 -2.719670 -7.054278
H -2.983853 -2.053119 -6.838825
C -3.438954 -4.116863 -0.922814
C -4.653404 -4.048780 -0.201064
C -5.049698 -5.138385 0.587032
C -4.258729 -6.288573 0.635618
C -3.067544 -6.376333 -0.091192
C -2.662304 -5.286570 -0.859436
H -6.452028 -2.830600 1.459054
H -5.977175 -5.102076 1.154875
H -4.585112 -7.129494 1.248244
H -2.462928 -7.281478 -0.056537
H -1.732566 -5.343082 -1.427773
C -0.927912 0.729812 -2.126849
C 0.174823 0.550250 -2.985822
C 0.608038 1.562520 -3.836813
C -0.077764 2.782526 -3.842641
C -1.178435 2.986355 -3.007555
C -1.595003 1.967874 -2.150061
H 1.465287 1.421293 -4.493126
H 0.259466 3.577948 -4.507668
H -1.703160 3.941432 -3.014575
H -2.427457 2.143643 -1.468844
C -1.194829 -0.159211 0.642891
C -1.457371 -1.114878 1.662455
C -1.312165 -0.749356 3.005804
C -0.878586 0.538282 3.330584
C -0.580882 1.474622 2.335270
C -0.733827 1.123602 0.997075
H -2.954595 -3.061671 2.862281
H -1.520045 -1.462040 3.801118
H -0.762864 0.807285 4.381102
H -0.231915 2.471738 2.601182
H -0.494465 1.848311 0.220224
O -5.369220 -2.897900 -0.346045
C -6.619336 -2.774695 0.374245
H -7.008656 -1.786612 0.112204
H -7.332199 -3.549015 0.057551
O -1.565052 -2.078621 -4.490164
C -0.835825 -1.563842 -5.643532
O 0.818926 -0.719130 -2.967600
C 2.264180 -0.731456 -3.223418
O -1.829884 -2.356334 1.230911
C -2.107609 -3.365158 2.231262
H -2.370312 -4.265062 1.669286
H -1.220461 -3.555364 2.851557
H -0.777294 -2.328338 -6.428308
H -1.317131 -0.650753 -6.015216
H 0.165856 -1.327962 -5.276923
C 0.997383 -4.118891 -1.744598
C 0.806379 -4.393662 -3.065274
H 0.371326 -4.561233 -0.965757
H 1.884566 -3.582852 -1.396644
H 0.004425 -5.056811 -3.400441
H 1.526566 -4.080502 -3.825437
H 2.621540 -1.709559 -2.887919
H 2.742835 0.066247 -2.644126
H 2.463253 -0.610863 -4.295360

Geometry:



Spin state: singlet

E = -10884.36 kcal mol-1
H = -10459.53 kcal mol-1
TS = -76.27 kcal mol-1
G (298.15 K) = -10535.80 kcal mol-1

Cr -0.304608 -2.542613 -2.234415
P -2.687515 -2.891148 -1.966718
N -2.911355 -1.274874 -1.422652
P -1.329590 -0.783619 -1.045466
C -4.102657 -0.419076 -1.525383
H -4.319870 0.036834 -0.550319
H -4.953310 -1.036026 -1.825905
H -3.944476 0.359906 -2.283718
C -3.597454 -3.024366 -3.522464
C -4.597990 -3.985674 -3.739049
C -5.265833 -4.046869 -4.960873
C -4.929064 -3.148000 -5.975469
C -3.922248 -2.193358 -5.790599
C -3.249526 -2.134737 -4.568131
H -4.849483 -4.686508 -2.943439
H -6.042685 -4.793363 -5.122121
H -5.445747 -3.190159 -6.934855
H -3.673550 -1.515342 -6.604226
C -3.333001 -4.152176 -0.845560
C -4.653512 -4.121718 -0.331572
C -5.100407 -5.175183 0.478658
C -4.243944 -6.238490 0.776682
C -2.936973 -6.274207 0.281721
C -2.490804 -5.228984 -0.525025
H -6.841773 -2.961716 0.853114
H -6.112726 -5.174437 0.878235
H -4.608819 -7.050649 1.406355
H -2.278017 -7.108704 0.517998
H -1.476812 -5.248683 -0.926094
C -0.733803 0.578958 -2.107742
C 0.469012 0.365720 -2.809731
C 1.039149 1.367922 -3.591650
C 0.377009 2.596710 -3.703128
C -0.832678 2.822559 -3.043433
C -1.375753 1.821564 -2.236740
H 1.977924 1.217254 -4.120298
H 0.820430 3.380717 -4.317242
H -1.339488 3.782624 -3.138201
H -2.290690 2.013629 -1.675897
C -1.242467 -0.150598 0.641032
C -1.739755 -0.937480 1.717302
C -1.625680 -0.464568 3.030412
C -1.005981 0.761048 3.280678
C -0.489578 1.532254 2.235934
C -0.605940 1.074534 0.926746
H -3.557196 -2.563682 3.015049
H -2.012011 -1.048088 3.863303
H -0.922136 1.111728 4.309857
H -0.001953 2.484732 2.440011
H -0.198650 1.674512 0.114748
O -5.406706 -3.045473 -0.686495
C -6.785042 -2.997079 -0.243844
H -7.192025 -2.072549 -0.663540
H -7.349513 -3.857744 -0.629033
O -2.216651 -1.258269 -4.289315
C -1.822588 -0.348105 -5.344192
O 1.046297 -0.923937 -2.699557
C 2.408767 -1.102782 -3.204857
O -2.298794 -2.137505 1.382089
C -2.723507 -3.010479 2.455857
H -3.056320 -3.928439 1.965086
H -1.886869 -3.232341 3.133367
H -1.451788 -0.901326 -6.218699
H -2.664039 0.296620 -5.631449
H -1.024575 0.265376 -4.919975
C 0.508765 -4.431652 -3.596272
C -0.075117 -3.433751 -4.323618
H -0.073500 -5.293678 -3.267617
H 1.590776 -4.526010 -3.511826
H -1.120126 -3.510675 -4.626242
H 0.529646 -2.687195 -4.844551
C 1.011330 -3.865619 -1.027072
C 0.395960 -2.935200 -0.193007
H 2.043671 -3.708670 -1.347290
H 0.693687 -4.908067 -1.025380
H 0.941287 -2.049805 0.140456
H -0.453441 -3.219011 0.429290
H 2.694388 -2.120914 -2.928393
H 3.075692 -0.380552 -2.720004
H 2.428277 -0.990144 -4.296001

Spin state: triplet

E = -10896.53 kcal mol-1
H = -10471.76 kcal mol-1
TS = -75.49 kcal mol-1
G (298.15 K) = -10547.25 kcal mol-1

Cr -0.299315 -2.541214 -2.243859
P -2.701245 -2.899359 -1.975233
N -2.910679 -1.283945 -1.412941
P -1.328527 -0.786621 -1.040084
C -4.082241 -0.407397 -1.565858
H -4.155252 0.250846 -0.689608
H -4.982197 -1.024505 -1.618398
H -3.996044 0.192746 -2.483012
C -3.623109 -3.011934 -3.524225
C -4.641497 -3.954551 -3.738635
C -5.317709 -3.997738 -4.956720
C -4.970871 -3.100471 -5.969242
C -3.946140 -2.164499 -5.786207
C -3.266871 -2.122730 -4.566849
H -4.900149 -4.654802 -2.944824
H -6.109001 -4.729215 -5.116655
H -5.493754 -3.129323 -6.925721
H -3.690724 -1.486503 -6.597773
C -3.343998 -4.159031 -0.851884
C -4.657892 -4.131608 -0.320642
C -5.089897 -5.185386 0.497385
C -4.227939 -6.247481 0.783176
C -2.928864 -6.282125 0.268184
C -2.496273 -5.235570 -0.544000
H -6.839658 -2.983984 0.889950
H -6.096054 -5.186539 0.912165
H -4.582457 -7.059572 1.418864
H -2.265558 -7.116262 0.493219
H -1.488711 -5.254290 -0.960943
C -0.726106 0.561226 -2.117190
C 0.497120 0.352737 -2.786278
C 1.064971 1.346318 -3.580991

C 0.383129 2.559408 -3.737645
C -0.846699 2.777545 -3.113195
C -1.390821 1.785492 -2.296315
H 2.018292 1.200357 -4.084341
H 0.826702 3.336897 -4.359904
H -1.369560 3.724593 -3.244823
H -2.327436 1.969447 -1.769919
C -1.252489 -0.142920 0.641009
C -1.732678 -0.937573 1.719629
C -1.630649 -0.456847 3.030726
C -1.041893 0.785275 3.275342
C -0.546032 1.566134 2.227515
C -0.649201 1.100130 0.920043
H -3.521914 -2.594468 3.015231
H -2.002094 -1.046774 3.865965
H -0.966383 1.142209 4.303048
H -0.083979 2.531969 2.428231
H -0.258048 1.706257 0.104468
O -5.422981 -3.060869 -0.667581
C -6.796521 -3.022848 -0.207479
H -7.217296 -2.103532 -0.625172
H -7.358040 -3.889705 -0.582830
O -2.222685 -1.259912 -4.285303
C -1.805489 -0.363475 -5.342804
O 1.096498 -0.919556 -2.624751
C 2.468354 -1.092469 -3.102481
O -2.264426 -2.150148 1.386625
C -2.679051 -3.028512 2.459838
H -2.995795 -3.951943 1.968283
H -1.841587 -3.236329 3.140789
H -1.448136 -0.928878 -6.215033
H -2.630486 0.301112 -5.632695
H -0.992784 0.231823 -4.920332
C 0.572289 -4.374877 -3.619117
C -0.078170 -3.403419 -4.331414
H 0.047678 -5.277956 -3.305099
H 1.659269 -4.407993 -3.553222
H -1.118169 -3.538386 -4.631445
H 0.480276 -2.617607 -4.847594
C 1.010504 -3.895439 -1.037285
C 0.404855 -2.952498 -0.207300
H 2.047630 -3.758455 -1.349098
H 0.673378 -4.931687 -1.039617
H 0.963845 -2.075332 0.125144
H -0.449513 -3.224059 0.413276
H 2.769047 -2.091296 -2.776328
H 3.115190 -0.338417 -2.639160
H 2.503002 -1.026062 -4.197139

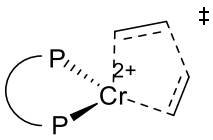
Spin state: quintet

E = -10903.13 kcal mol-1
H = -10478.61 kcal mol-1
TS = -78.08 kcal mol-1
G (298.15 K) = -10556.69 kcal mol-1

Cr -0.258717 -2.686166 -2.065041
P -2.715705 -2.833688 -2.037504
N -2.916084 -1.243826 -1.413637
P -1.326734 -0.784626 -1.034230
C -4.084553 -0.356873 -1.510336
H -4.088844 0.324958 -0.649334
H -4.993439 -0.962508 -1.481718
H -4.053275 0.218226 -2.446666
C -3.669342 -2.945612 -3.568264
C -4.612693 -3.966015 -3.782659
C -5.311908 -4.044166 -4.984588
C -5.068779 -3.099619 -5.985827
C -4.122945 -2.086305 -5.806132
C -3.410887 -2.010778 -4.604202
H -4.796654 -4.700105 -2.998936
H -6.044026 -4.835764 -5.140007
H -5.616400 -3.150840 -6.927448
H -3.947686 -1.369273 -6.605426
C -3.347007 -4.113638 -0.915380
C -4.665323 -4.123847 -0.395677
C -5.073931 -5.183244 0.428017
C -4.185209 -6.217973 0.731042
C -2.880961 -6.218170 0.228296
C -2.474237 -5.164003 -0.588055
H -6.936857 -3.056255 0.744653
H -6.083765 -5.210760 0.832845
H -4.522182 -7.034980 1.369942
H -2.196110 -7.031623 0.464630
H -1.460022 -5.158484 -0.995857
C -0.700863 0.521102 -2.143242
C 0.510804 0.284113 -2.822857
C 1.062905 1.251620 -3.661645
C 0.389760 2.466993 -3.835455
C -0.821635 2.715499 -3.187181
C -1.360289 1.745515 -2.340604
H 2.003079 1.084011 -4.183044
H 0.825339 3.222424 -4.489741
H -1.337260 3.664930 -3.329057
H -2.290076 1.947372 -1.808705
C -1.247863 -0.116365 0.636378
C -1.689372 -0.931895 1.714828
C -1.620692 -0.444556 3.025047
C -1.091347 0.825666 3.266259
C -0.625070 1.624955 2.218132
C -0.700619 1.152409 0.910670
H -3.517888 -2.565087 2.918912
H -1.967339 -1.048534 3.861057
H -1.037976 1.189936 4.292815
H -0.209598 2.611773 2.418718
H -0.336754 1.772468 0.092606
O -5.460715 -3.081399 -0.759064
C -6.850120 -3.105538 -0.349845
H -7.299360 -2.213147 -0.795227
H -7.353548 -4.003574 -0.734281
O -2.433114 -1.084777 -4.338601
C -2.119999 -0.124292 -5.372123
O 1.119635 -0.969822 -2.610366
C 2.496312 -1.130903 -3.066310
O -2.145277 -2.174181 1.373951
C -2.649948 -3.027392 2.428633
H -2.953044 -3.951359 1.929560
H -1.866357 -3.242437 3.169169
H -1.773849 -0.628358 -6.286118
H -2.991333 0.506411 -5.598054

H -1.318728 0.493977 -4.959280
C 0.580436 -4.273218 -3.761959
C -0.210884 -3.389077 -4.421726
H 0.193297 -5.241330 -3.435009
H 1.658635 -4.122179 -3.673270
H -1.254419 -3.616366 -4.644699
H 0.193920 -2.474832 -4.862011
C 1.415132 -3.998291 -0.604147
C 0.799542 -3.108373 0.205657
H 2.403310 -3.799917 -1.024867
H 1.018739 -5.005075 -0.754675
H 1.258674 -2.148007 0.451138
H -0.134069 -3.346983 0.720376
H 2.832384 -2.088460 -2.658789
H 3.120259 -0.322143 -2.666952
H 2.539743 -1.153440 -4.163094

Geometry:

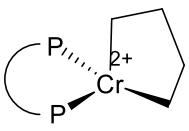


Spin state: triplet

E = -10886.19 kcal mol-1
H = -10462.08 kcal mol-1
TS = -75.51 kcal mol-1
G (298.15 K) = -10537.58 kcal mol-1

Cr -0.302408 -2.520883 -2.165967
P -2.711014 -2.852562 -1.984475
N -2.967376 -1.231394 -1.464390
P -1.405340 -0.696104 -1.073228
C -4.184960 -0.412609 -1.573716
H -4.499017 -0.063155 -0.581561
H -4.982614 -1.025420 -2.003257
H -4.003505 0.440339 -2.240804
C -3.591436 -3.008961 -3.550147
C -4.641016 -3.921939 -3.744678
C -5.289675 -3.997505 -4.975693
C -4.880643 -3.165459 -6.020725
C -3.827315 -2.259026 -5.855756
C -3.177229 -2.180402 -4.621816
H -4.945558 -4.571695 -2.924408
H -6.105962 -4.704112 -5.121307
H -5.379394 -3.222623 -6.988849
H -3.526039 -1.632280 -6.692336
C -3.360759 -4.124674 -0.875856
C -4.637339 -4.048011 -0.267176
C -5.083325 -5.110085 0.533154
C -4.275189 -6.234862 0.714592
C -3.017103 -6.324833 0.111194
C -2.567541 -5.266378 -0.676050
H -6.681313 -2.825153 1.106434
H -6.060144 -5.069842 1.011191
H -4.639299 -7.053247 1.336542
H -2.397608 -7.209758 0.251517
H -1.588907 -5.327515 -1.153609
C -0.816576 0.665345 -2.128439
C 0.405183 0.454973 -2.799410
C 0.989706 1.461190 -3.564783
C 0.324954 2.687264 -3.693141
C -0.901410 2.908906 -3.064569
C -1.460080 1.905475 -2.271735
H 1.941920 1.316177 -4.070247
H 0.780443 3.472623 -4.296609
H -1.409913 3.866598 -3.172752
H -2.390161 2.093979 -1.735183
C -1.292632 -0.108378 0.622811
C -1.671662 -0.981472 1.681646
C -1.554049 -0.548978 3.008399
C -1.041191 0.719813 3.284598
C -0.637212 1.575413 2.254544
C -0.758096 1.159092 0.932811
H -3.288025 -2.813882 2.959567
H -1.851568 -1.196640 3.830389
H -0.950218 1.038574 4.323589
H -0.231194 2.560395 2.481414
H -0.434981 1.820960 0.131016
O -5.355399 -2.921919 -0.527939
C -6.697776 -2.826871 0.007459
H -7.087987 -1.871883 -0.356224
H -7.325490 -3.648715 -0.364501
O -2.119754 -1.336464 -4.350970
C -1.645784 -0.502680 -5.434145
O 0.985761 -0.833281 -2.678204
C 2.339722 -1.014955 -3.204021
O -2.124037 -2.213355 1.311618
C -2.437151 -3.162711 2.358537
H -2.706989 -4.086139 1.839673
H -1.562710 -3.336354 3.001423
H -1.276250 -1.117381 -6.266931
H -2.441790 0.170078 -5.781219
H -0.830770 0.090406 -5.012608
C 0.566377 -4.561529 -3.104677
C -0.074115 -3.556916 -3.937005
H -0.051789 -5.445743 -2.935488
H 1.581632 -4.838527 -3.399576
H -1.043035 -3.798073 -4.378501
H 0.560813 -2.939732 -4.584050
C 1.104437 -4.193659 -1.307936
C 0.378637 -3.274592 -0.419907
H 2.154782 -3.930023 -1.459812
H 1.010656 -5.248297 -1.041818
H 0.958847 -2.482413 0.067033
H -0.401945 -3.688497 0.221306
H 2.628052 -2.034386 -2.932384
H 3.018322 -0.296640 -2.729522
H 2.341637 -0.904200 -4.295419

Geometry:



Spin state: singlet

E = -10886.12 kcal mol-1
H = -10461.38 kcal mol-1
TS = -73.89 kcal mol-1
G (298.15 K) = -10535.27 kcal mol-1

Cr -0.526374 -2.192872 -2.448268
P -2.819877 -2.742016 -2.105265
N -3.202895 -1.161324 -1.569856
P -1.665326 -0.575120 -1.147415
C -4.481648 -0.436911 -1.601751
H -4.654187 0.046821 -0.631681
H -5.295193 -1.146245 -1.780304
H -4.472551 0.313369 -2.404061
C -3.528774 -2.915404 -3.759539
C -4.760480 -3.546559 -3.990909
C -5.296993 -3.591893 -5.277484
C -4.593219 -3.013737 -6.335154
C -3.355671 -2.391006 -6.129517
C -2.826254 -2.344479 -4.840780
H -5.289191 -4.006778 -3.155320
H -6.255151 -4.079425 -5.454406
H -5.001462 -3.050300 -7.345569
H -2.830205 -1.961441 -6.979259
C -3.551194 -4.051566 -1.091273
C -4.459236 -3.860680 -0.015997
C -4.904761 -4.979498 0.706835
C -4.469363 -6.260892 0.372774
C -3.593880 -6.462292 -0.698946
C -3.146946 -5.360950 -1.421188
H -5.286654 -2.703212 2.308626
H -5.602648 -4.853555 1.531831
H -4.830366 -7.112309 0.950467
H -3.271941 -7.466127 -0.973421
H -2.483397 -5.518806 -2.270012
C -1.243621 0.892067 -2.139098
C -0.080664 0.792696 -2.919069
C 0.361640 1.843401 -3.715689
C -0.391538 3.022457 -3.746145
C -1.568112 3.139574 -3.000169
C -1.992385 2.080647 -2.196620
H 1.268600 1.758738 -4.312430
H -0.053927 3.852413 -4.367171
H -2.149262 4.060615 -3.037679
H -2.895758 2.181727 -1.594765
C -1.559120 -0.118939 0.588312
C -1.705536 -1.145669 1.561989
C -1.576728 -0.835735 2.920385
C -1.295294 0.476288 3.308422
C -1.128938 1.491193 2.360512
C -1.251393 1.191018 1.006877
H -2.738159 -3.458747 2.714537
H -1.685463 -1.609301 3.677859
H -1.194967 0.703655 4.370287
H -0.899902 2.508543 2.675626
H -1.100832 1.975965 0.267194
O -4.859171 -2.589008 0.250394
C -5.747718 -2.368939 1.367948
H -5.904751 -1.286995 1.403168
H -6.711025 -2.876011 1.216167
O -1.591989 -1.755562 -4.532900
C -0.838616 -1.205103 -5.653149
O 0.604370 -0.457171 -2.905383
C 2.074187 -0.396243 -2.799696
O -1.954171 -2.395040 1.075843
C -1.910492 -3.511396 1.993875
H -2.030127 -4.401396 1.368957
H -0.946950 -3.543675 2.521348
H -0.622662 -1.991539 -6.387522
H -1.397273 -0.380250 -6.112514
H 0.092204 -0.826691 -5.225803
C 0.386636 -5.004622 -2.106702
C -0.382049 -4.113762 -3.053034
H -1.102765 -4.600121 -3.723528
H 0.334675 -3.516063 -3.708668
C 1.372288 -4.112875 -1.345193
C 0.593770 -2.880972 -0.888086
H 1.218021 -2.061915 -0.493038
H -0.151012 -3.145549 -0.123442
H 1.834065 -4.640586 -0.495042
H 2.204381 -3.834352 -2.015847
H 0.881592 -5.832860 -2.642133
H -0.321409 -5.474892 -1.403283
H 2.405152 -1.417404 -2.590697
H 2.346117 0.274012 -1.976792
H 2.497931 -0.052548 -3.749545

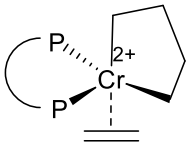
Spin state: triplet

E = -10899.09 kcal mol-1
H = -10474.30 kcal mol-1
TS = -73.94 kcal mol-1
G (298.15 K) = -10548.23 kcal mol-1

Cr -0.520755 -2.196751 -2.475236
P -2.827389 -2.743801 -2.105069
N -3.184557 -1.154413 -1.575841
P -1.646000 -0.580209 -1.136982
C -4.450646 -0.407894 -1.624827
H -4.648982 0.047865 -0.646299
H -5.267754 -1.097738 -1.855342
H -4.402369 0.366850 -2.401774
C -3.550591 -2.920910 -3.751089
C -4.781095 -3.559407 -3.969583
C -5.325451 -3.617647 -5.252110
C -4.629672 -3.046654 -6.319113
C -3.392874 -2.417861 -6.126838
C -2.855733 -2.357661 -4.842165
H -5.302832 -4.013944 -3.126401
H -6.283100 -4.109720 -5.419084
H -5.043574 -3.094358 -7.326794
H -2.873590 -1.995410 -6.984028
C -3.548664 -4.046313 -1.075999
C -4.504272 -3.848693 -0.045160
C -4.939049 -4.954837 0.703311
C -4.447047 -6.231231 0.434030
C -3.522896 -6.439881 -0.594487
C -3.083996 -5.349800 -1.339234
H -5.437012 -2.628224 2.201403
H -5.672165 -4.823714 1.496321
H -4.800917 -7.073665 1.029131

H -3.154258 -7.440491 -0.816624
H -2.377024 -5.512848 -2.150706
C -1.222799 0.892973 -2.120647
C -0.073589 0.797804 -2.921486
C 0.354554 1.855281 -3.717570
C -0.395158 3.036346 -3.724521
C -1.555807 3.150919 -2.953383
C -1.967986 2.085481 -2.152650
H 1.250342 1.772696 -4.331540
H -0.066929 3.870858 -4.344553
H -2.133844 4.074582 -2.969529
H -2.858180 2.185055 -1.531201
C -1.540141 -0.135963 0.600674
C -1.710678 -1.165857 1.566706
C -1.578583 -0.867708 2.927446
C -1.270441 0.435337 3.324734
C -1.080032 1.452927 2.383746
C -1.204842 1.164587 1.028092
H -2.765239 -3.484569 2.703871
H -1.707928 -1.643433 3.679513
H -1.169212 0.653957 4.388349
H -0.830685 2.463257 2.706127
H -1.035977 1.951107 0.293961
O -4.957005 -2.582302 0.152736
C -5.883136 -2.347114 1.236605
H -6.076865 -1.270546 1.223079
H -6.825278 -2.891129 1.079915
O -1.620590 -1.763717 -4.547571
C -0.883573 -1.201518 -5.672801
O 0.616714 -0.448160 -2.930439
C 2.084412 -0.375617 -2.796711
O -1.988126 -2.405545 1.071016
C -1.942391 -3.532438 1.977619
H -2.068674 -4.415385 1.344267
H -0.975196 -3.572351 2.497695
H -0.660152 -1.983965 -6.409182
H -1.458182 -0.385559 -6.128324
H 0.044041 -0.808373 -5.251110
C 0.466565 -4.983443 -2.113445
C -0.341789 -4.133649 -3.063149
H -1.074789 -4.646166 -3.698932
H 0.342267 -3.535176 -3.748302
C 1.425504 -4.052487 -1.363658
C 0.614599 -2.849755 -0.888187
H 1.219051 -2.016255 -0.495302
H -0.117200 -3.140976 -0.122225
H 1.917902 -4.566510 -0.521786
H 2.240174 -3.745553 -2.043686
H 0.991985 -5.795251 -2.645609
H -0.216050 -5.477121 -1.401526
H 2.421304 -1.397924 -2.603767
H 2.335593 0.279362 -1.955063
H 2.520495 -0.007368 -3.731599

Geometry:



Spin state: singlet

E = -11619.13 kcal mol-1
H = -11158.96 kcal mol-1
TS = -75.00 kcal mol-1
G (298.15 K) = -11233.96 kcal mol-1

Cr -0.439197 -2.409565 -2.392381
P -2.901162 -2.466339 -2.398479
N -3.099008 -0.909548 -1.754055
P -1.475497 -0.516905 -1.352204
C -4.335081 -0.246955 -1.296802
H -4.183290 0.161982 -0.289837
H -5.144443 -0.980333 -1.235683
H -4.619901 0.552729 -1.992074
C -3.740311 -2.540940 -4.035963
C -4.876762 -1.750013 -4.266302
C -5.538530 -1.788433 -5.493447
C -5.065964 -2.624290 -6.505361
C -3.938038 -3.422552 -6.301013
C -3.276491 -3.383947 -5.069707
H -5.260941 -1.096281 -3.487961
H -6.419722 -1.168100 -5.654093
H -5.577144 -2.662486 -7.467575
H -3.586643 -4.069027 -7.102455
C -3.862329 -3.699739 -1.444905
C -4.430352 -3.540850 -0.148689
C -5.187291 -4.584706 0.407388
C -5.344732 -5.791027 -0.270823
C -4.763387 -5.977738 -1.529009
C -4.045981 -4.936366 -2.105347
H -4.611925 -2.840092 2.523193
H -5.653802 -4.458303 1.382219
H -5.931399 -6.587917 0.187196
H -4.888371 -6.918370 -2.064147
H -3.621009 -5.079438 -3.098704
C -1.143132 1.189775 -1.927823
C 0.102222 1.598469 -2.466406
C 0.288488 2.925191 -2.877042
C -0.744717 3.852320 -2.747559
C -1.973487 3.472691 -2.205019
C -2.164161 2.153813 -1.801303
H 1.239956 3.242808 -3.297889
H -0.581618 4.880549 -3.071405
H -2.778792 4.197456 -2.090875
H -3.116563 1.885607 -1.354535
C -1.397983 -0.432438 0.465008
C -1.448778 -1.632224 1.220835
C -1.453980 -1.579785 2.617533
C -1.406437 -0.342655 3.267401
C -1.337025 0.845814 2.539225
C -1.321546 0.796106 1.145654
H -2.559471 -3.970513 1.866705
H -1.483780 -2.491472 3.210059
H -1.408819 -0.316487 4.357756
H -1.286591 1.806402 3.050868
H -1.253491 1.721972 0.576700
O -4.208350 -2.366615 0.505645
C -4.902350 -2.116782 1.747034
H -4.581000 -1.117063 2.054475

H -5.991821 -2.138581 1.602794
O -2.154745 -4.129231 -4.775127
C -1.610975 -4.968463 -5.820551
O 1.073845 0.637920 -2.572559
C 2.345875 1.013528 -3.152757
O -1.460801 -2.807052 0.505326
C -1.657535 -4.031733 1.245000
H -1.802807 -4.813542 0.495048
H -0.782674 -4.258799 1.870451
H -2.330530 -5.743697 -6.117927
H -1.315133 -4.368269 -6.692542
H -0.727494 -5.448486 -5.385233
C 0.665258 -4.494055 -1.311596
C -0.625896 -4.382443 -2.107280
H -1.500469 -4.915013 -1.729156
H -0.495017 -4.599660 -3.183099
C 1.610845 -3.272424 -1.552334
C 1.022676 -1.957621 -1.050312
H 1.568198 -1.044129 -1.293491
H 0.733481 -1.994246 0.002373
H 2.559743 -3.439396 -1.013273
H 1.918207 -3.222962 -2.612627
H 1.199190 -5.409285 -1.616495
H 0.460069 -4.570145 -0.238001
C -0.831625 -1.245417 -4.223305
C 0.354342 -1.997341 -4.265398
H -0.790012 -0.173974 -4.040528
H -1.708860 -1.575792 -4.772131
H 1.319622 -1.513199 -4.096205
H 0.389950 -2.942089 -4.815496
H 2.959086 0.106519 -3.123963
H 2.834769 1.796695 -2.557508
H 2.220107 1.342033 -4.193776

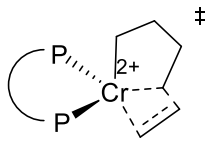
Spin state: triplet

E = -11634.09 kcal mol-1
H = -11174.22 kcal mol-1
TS = -79.43 kcal mol-1
G (298.15 K) = -11253.65 kcal mol-1

Cr -0.334834 -1.834940 -2.504366
P -2.708318 -2.421436 -2.227074
N -3.047242 -0.980334 -1.332904
P -1.485414 -0.428764 -0.975984
C -4.298368 -0.613335 -0.638206
H -4.219495 -0.851814 0.430279
H -5.119773 -1.189422 -1.074625
H -4.502049 0.456592 -0.769290
C -3.704263 -2.281673 -3.736183
C -4.415725 -1.109622 -4.034794
C -5.236366 -1.046538 -5.159242
C -5.343842 -2.162406 -5.995781
C -4.628982 -3.332955 -5.729766
C -3.793015 -3.392421 -4.608862
H -4.337719 -0.249667 -3.369234
H -5.792932 -0.136307 -5.380429
H -5.984857 -2.122166 -6.876941
H -4.716448 -4.183711 -6.402915
C -3.286272 -3.896169 -1.341747
C -4.663472 -4.235077 -1.260516
C -5.039158 -5.432963 -0.634372
C -4.068236 -6.281631 -0.099196
C -2.711762 -5.951037 -0.165999
C -2.335793 -4.760406 -0.782537
H -7.397368 -3.827946 -0.910890
H -6.089954 -5.707030 -0.560787
H -4.382080 -7.209543 0.380173
H -1.958461 -6.612556 0.260687
H -1.287243 -4.483439 -0.831526
C -1.091849 1.169345 -1.752926
C 0.112645 1.225987 -2.479448
C 0.547792 2.411487 -3.064936
C -0.250257 3.555261 -2.936648
C -1.458803 3.518333 -2.236494
C -1.873041 2.329131 -1.635564
H 1.481082 2.465637 -3.621830
H 0.084180 4.485222 -3.396952
H -2.068120 4.417257 -2.147399
H -2.794278 2.303908 -1.053227
C -1.212649 -0.199579 0.786016
C -1.610404 -1.193783 1.722475
C -1.302053 -1.028232 3.078243
C -0.585235 0.093188 3.498822
C -0.171614 1.069104 2.585873
C -0.483013 0.919812 1.238915
H -3.532855 -2.668558 2.858240
H -1.605581 -1.775526 3.808573
H -0.345748 0.202048 4.557184
H 0.384343 1.942454 2.924302
H -0.167757 1.682016 0.527286
O -5.546973 -3.351595 -1.802757
C -6.938362 -3.737326 -1.905606
H -7.418506 -2.927964 -2.462752
H -7.040107 -4.680600 -2.459983
O -3.009445 -4.462267 -4.276031
C -3.198483 -5.701583 -5.000292
O 0.824272 0.011183 -2.587105
C 2.178964 0.054614 -3.135282
O -2.283332 -2.265638 1.213835
C -2.881089 -3.197317 2.149075
H -3.471843 -3.881284 1.534545
H -2.107252 -3.760734 2.688464
H -4.243751 -6.033002 -4.932253
H -2.901202 -5.591073 -6.052672
H -2.547768 -6.428313 -4.505823
C 0.978494 -4.519301 -2.147607
C 0.035434 -3.765592 -3.054367
H -0.694388 -4.352265 -3.621933
H 0.630269 -3.120011 -3.773838
C 1.724949 -3.484405 -1.298887
C 0.712929 -2.450871 -0.811995
H 1.172579 -1.564114 -0.349200
H -0.005883 -2.882424 -0.098712
H 2.256052 -3.950482 -0.451640
H 2.512340 -3.008391 -1.909946
H 1.668473 -5.149842 -2.735899
H 0.414777 -5.220649 -1.513882
C -1.126495 -0.343728 -4.919185
C -0.757985 -1.571675 -5.314148

H -0.451701 0.508994 -4.998667
H -2.136497 -0.135871 -4.565382
H 0.227019 -1.756456 -5.748566
H -1.458411 -2.408101 -5.304998
H 2.592392 -0.945795 -2.977632
H 2.775087 0.790278 -2.582718
H 2.146782 0.291840 -4.206503

Geometry:

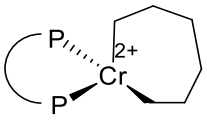


Spin state: triplet

E = -11625.77 kcal mol-1
H = -11167.81 kcal mol-1
TS = -75.46 kcal mol-1
G (298.15 K) = -11243.28 kcal mol-1

Cr -0.565465 -2.369445 -2.551915
P -2.897513 -2.562061 -1.976076
N -3.039475 -1.094268 -1.137206
P -1.417894 -0.513543 -1.184022
C -4.097962 -0.663729 -0.201086
H -4.357276 -1.485338 0.479071
H -4.995184 -0.348098 -0.744081
H -3.710350 0.171967 0.393169
C -3.552407 -2.367206 -3.653043
C -4.151538 -1.178471 -4.094453
C -4.606094 -1.068413 -5.405824
C -4.458417 -2.152265 -6.281019
C -3.854137 -3.342684 -5.865372
C -3.382523 -3.447013 -4.552398
H -4.263309 -0.349165 -3.397537
H -5.082846 -0.149653 -5.745915
H -4.815280 -2.071130 -7.308224
H -3.749096 -4.169472 -6.565773
C -3.797027 -3.904235 -1.174344
C -5.214326 -3.840443 -1.121060
C -5.932924 -4.917134 -0.582906
C -5.252883 -6.044736 -0.120787
C -3.857702 -6.125965 -0.188341
C -3.141203 -5.056411 -0.717708
H -7.647964 -2.626215 -0.659288
H -7.019234 -4.881849 -0.525426
H -5.826031 -6.875104 0.292952
H -3.339125 -7.017585 0.162164
H -2.057121 -5.123737 -0.796426
C -1.454048 1.142567 -1.920696
C -0.213188 1.764877 -2.189299
C -0.176111 3.028564 -2.786810
C -1.376636 3.660865 -3.124047
C -2.609217 3.052961 -2.870196
C -2.644735 1.793688 -2.270105
H 0.772130 3.521165 -2.993992
H -1.342893 4.645194 -3.592014
H -3.537101 3.561737 -3.129310
H -3.603368 1.323825 -2.054147
C -0.911674 -0.288806 0.543301
C -0.813302 -1.409621 1.404805
C -0.458702 -1.224033 2.746281
C -0.205787 0.062591 3.228804
C -0.302763 1.175008 2.390645
C -0.653887 0.995199 1.054922
H -1.717370 -3.711153 2.545121
H -0.381341 -2.069638 3.425855
H 0.067158 0.190166 4.276829
H -0.112844 2.176379 2.775266
H -0.742384 1.860595 0.399193
O -5.772500 -2.702333 -1.616243
C -7.216812 -2.608547 -1.670174
H -7.425159 -1.645581 -2.144733
H -7.636360 -3.420192 -2.280417
O -2.718258 -4.530307 -4.035366
C -2.717820 -5.759567 -4.800091
O 0.885323 1.028608 -1.825598
C 2.184194 1.664464 -1.895220
O -1.084542 -2.638572 0.847213
C -0.988221 -3.783197 1.726250
H -1.229670 -4.651982 1.110645
H 0.028718 -3.884585 2.131786
H -3.745612 -6.075890 -5.024155
H -2.145690 -5.645567 -5.732444
H -2.235729 -6.502196 -4.157742
C 0.332452 -4.430869 -2.300473
C 0.508130 -3.964136 -3.728181
H -0.039452 -4.562782 -4.456487
H 1.560622 -3.843008 -3.990822
C 1.294449 -3.743649 -1.297629
C 1.101429 -2.235596 -1.396239
H 1.714622 -1.732806 -2.165398
H 1.140557 -1.680991 -0.457339
H 1.075210 -4.094381 -0.282457
H 2.328615 -4.037164 -1.544265
H 0.376894 -5.531283 -2.255463
H -0.738706 -4.278264 -1.947571
C -0.419545 -0.970811 -4.157104
C 0.003573 -2.104843 -4.877395
H 0.316320 -0.218757 -3.866777
H -1.441738 -0.609829 -4.287530
H 1.031819 -2.165365 -5.227651
H -0.727242 -2.637845 -5.486383
H 2.886349 0.937492 -1.476742
H 2.199009 2.582550 -1.291966
H 2.456471 1.889624 -2.936459

Geometry:



Spin state: singlet

E = -11643.64 kcal mol-1
H = -11182.35 kcal mol-1

TS = -77.88 kcal mol-1
G (298.15 K) = -11260.24 kcal mol-1

Cr -0.518647 -1.811505 -2.374329
P -2.875415 -2.320956 -2.115748
N -3.232215 -0.979459 -1.093050
P -1.678208 -0.379258 -0.861243
C -4.473183 -0.635661 -0.382843
H -5.281767 -0.454901 -1.100168
H -4.299478 0.269564 0.211617
H -4.755442 -1.453237 0.291948
C -3.819680 -1.994369 -3.630290
C -4.133991 -0.661894 -3.949536
C -4.841054 -0.355497 -5.110294
C -5.236350 -1.389965 -5.963575
C -4.922307 -2.720224 -5.675926
C -4.200097 -3.033993 -4.516971
H -3.828896 0.138239 -3.273863
H -5.087203 0.679491 -5.345209
H -5.794034 -1.162157 -6.872676
H -5.236609 -3.506308 -6.359822
C -3.407706 -3.859590 -1.325804
C -4.785108 -4.138040 -1.138611
C -5.169308 -5.353949 -0.556047
C -4.197662 -6.284453 -0.179840
C -2.837225 -6.020919 -0.367274
C -2.453019 -4.808554 -0.937142
H -7.367521 -3.544336 -0.400715
H -6.221954 -5.584518 -0.402667
H -4.513557 -7.228315 0.265833
H -2.085776 -6.752972 -0.073180
H -1.396323 -4.592727 -1.083913
C -1.405398 1.188433 -1.746753
C -0.273678 1.224253 -2.575471
C 0.042217 2.341349 -3.340798
C -0.808438 3.450702 -3.277835
C -1.951787 3.436064 -2.471807
C -2.251334 2.308455 -1.706156
H 0.922257 2.357384 -3.982188
H -0.573544 4.332658 -3.874160
H -2.605130 4.307570 -2.436945
H -3.134036 2.299919 -1.065914
C -1.342370 -0.087050 0.875305
C -1.602890 -1.121401 1.816167
C -1.312996 -0.907587 3.168842
C -0.747839 0.303511 3.575247
C -0.468597 1.319885 2.654897
C -0.764051 1.122099 1.309668
H -3.267374 -2.918967 2.954162
H -1.514243 -1.680780 3.907380
H -0.520178 0.451211 4.631591
H -0.031141 2.260631 2.986859
H -0.560700 1.911990 0.586520
O -5.648148 -3.173457 -1.558770
C -7.068141 -3.424852 -1.451798
H -7.550310 -2.539654 -1.876067
H -7.351973 -4.314476 -2.031214
O -3.815831 -4.292662 -4.162536
C -4.244069 -5.400414 -4.986155
O 0.522238 0.044706 -2.617081
C 1.981880 0.250209 -2.637082
O -2.129309 -2.272564 1.307392
C -2.531848 -3.308136 2.236336
H -2.986442 -4.085444 1.616497
H -1.661158 -3.717288 2.767834
H -5.340913 -5.445415 -5.042937
H -3.814941 -5.328310 -5.995946
H -3.864355 -6.295123 -4.484852
C 1.457825 -4.665521 -2.052152
C 1.558304 -4.311101 -3.542715
C 1.737831 -3.472777 -1.119706
C 0.559297 -2.549042 -0.805536
H 0.895934 -1.660067 -0.245234
H -0.210477 -3.051700 -0.196806
H 2.091729 -3.862153 -0.148278
H 2.588889 -2.893340 -1.517725
H 2.183410 -5.464789 -1.848523
H 0.470553 -5.096568 -1.822242
C -0.815313 -3.317680 -3.751206
C 0.657574 -3.147674 -3.979681
H -1.454820 -2.951449 -4.563251
H -1.136681 -4.307428 -3.416388
H 1.299468 -5.185484 -4.157580
H 2.601901 -4.055765 -3.781300
H 1.057713 -2.228239 -3.417399
H 0.861467 -2.826951 -5.012981
H 2.424289 -0.663820 -2.230944
H 2.230538 1.104777 -1.998298
H 2.314262 0.415820 -3.667977

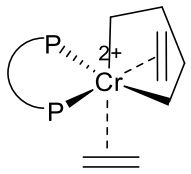
Spin state: triplet

E = -11655.92 kcal mol-1
H = -11194.68 kcal mol-1
TS = -78.14 kcal mol-1
G (298.15 K) = -11272.81 kcal mol-1

Cr -0.512771 -1.818804 -2.376462
P -2.884583 -2.329417 -2.113325
N -3.229978 -0.991785 -1.081207
P -1.679007 -0.380634 -0.851391
C -4.469776 -0.653384 -0.365504
H -5.275333 -0.444630 -1.078893
H -4.287800 0.232483 0.255038
H -4.762556 -1.486221 0.285569
C -3.821586 -1.986154 -3.627884
C -4.139274 -0.651445 -3.934924
C -4.841693 -0.335684 -5.095864
C -5.227836 -1.362560 -5.962672
C -4.909586 -2.694529 -5.687667
C -4.192966 -3.017508 -4.527904
H -3.840486 0.142658 -3.249440
H -5.091300 0.700700 -5.320803
H -5.781839 -1.127311 -6.872088
H -5.216131 -3.474449 -6.382112
C -3.429523 -3.866865 -1.331424
C -4.809317 -4.144372 -1.159418
C -5.200297 -5.361463 -0.583774
C -4.233261 -6.293078 -0.198675
C -2.870667 -6.030369 -0.370932

C -2.479224 -4.817512 -0.934971
H -7.400399 -3.555669 -0.449234
H -6.254619 -5.591488 -0.441567
H -4.554574 -7.237578 0.241757
H -2.123041 -6.763856 -0.070649
H -1.420859 -4.602525 -1.071252
C -1.410335 1.181055 -1.748872
C -0.271017 1.223122 -2.567797
C 0.042408 2.341827 -3.332162
C -0.817342 3.444630 -3.279463
C -1.968106 3.422949 -2.484278
C -2.265363 2.294755 -1.718822
H 0.927757 2.363904 -3.965960
H -0.583777 4.326825 -3.875980
H -2.628845 4.289149 -2.457771
H -3.153811 2.280182 -1.086626
C -1.347837 -0.075292 0.882569
C -1.596424 -1.109421 1.827486
C -1.308912 -0.887025 3.179243
C -0.756742 0.331670 3.580507
C -0.488387 1.347563 2.656125
C -0.781683 1.141640 1.311830
H -3.225205 -2.940229 2.974069
H -1.501547 -1.659399 3.920894
H -0.530804 0.486181 4.636254
H -0.060739 2.294062 2.984491
H -0.586656 1.930605 0.585481
O -5.667516 -3.177974 -1.585090
C -7.088488 -3.430962 -1.496032
H -7.566301 -2.544182 -1.921943
H -7.364671 -4.318127 -2.082970
O -3.805214 -4.277976 -4.184268
C -4.228088 -5.378905 -5.019865
O 0.533424 0.050404 -2.599591
C 1.990990 0.261540 -2.623210
O -2.108492 -2.268037 1.322685
C -2.482782 -3.311926 2.254087
H -2.920559 -4.100448 1.636202
H -1.600344 -3.698818 2.782844
H -5.324615 -5.425051 -5.081414
H -3.795064 -5.296488 -6.027176
H -3.848680 -6.277525 -4.525437
C 1.487472 -4.673114 -2.042691
C 1.591116 -4.317108 -3.532696
C 1.752608 -3.477468 -1.109503
C 0.562564 -2.573218 -0.794930
H 0.881529 -1.679912 -0.232050
H -0.207883 -3.086676 -0.197623
H 2.114746 -3.863265 -0.139297
H 2.595646 -2.886490 -1.507989
H 2.218697 -5.466516 -1.836632
H 0.502602 -5.111830 -1.816224
C -0.791439 -3.353921 -3.742144
C 0.678120 -3.164128 -3.974125
H -1.439077 -3.007955 -4.555954
H -1.096370 -4.342201 -3.389535
H 1.343954 -5.193978 -4.148872
H 2.632859 -4.050475 -3.767038
H 1.071667 -2.238594 -3.415641
H 0.877385 -2.846179 -5.009185
H 2.436956 -0.650936 -2.217102
H 2.238828 1.117379 -1.985739
H 2.321708 0.426783 -3.654790

Geometry:



Spin state: singlet

E = -12356.32 kcal mol-1
H = -11860.85 kcal mol-1
TS = -82.58 kcal mol-1
G (298.15 K) = -11943.43 kcal mol-1

Cr -0.135390 -2.230685 -2.495034
P -2.575558 -2.588286 -2.220874
N -2.825094 -1.176501 -1.277277
P -1.284574 -0.462904 -1.180243
C -3.983314 -0.900196 -0.404979
H -4.211063 -1.788120 0.196963
H -4.862601 -0.630740 -1.001365
H -3.723400 -0.079792 0.274319
C -3.477513 -2.354147 -3.788652
C -4.010531 -1.101203 -4.120397
C -4.728481 -0.918254 -5.301059
C -4.919813 -2.002565 -6.162322
C -4.404541 -3.263377 -5.851232
C -3.680761 -3.445886 -4.666205
H -3.875407 -0.267671 -3.431998
H -5.141943 0.059929 -5.544442
H -5.478356 -1.872171 -7.089817
H -4.569656 -4.095056 -6.533587
C -3.433081 -3.956926 -1.365849
C -4.854686 -4.037447 -1.402745
C -5.504644 -5.134111 -0.817213
C -4.766884 -6.134714 -0.185310
C -3.374164 -6.053096 -0.114409
C -2.725783 -4.968387 -0.701149
H -7.463360 -3.093602 -1.222150
H -6.590273 -5.204774 -0.845976
H -5.290945 -6.979816 0.262607
H -2.797316 -6.826445 0.392056
H -1.646146 -4.905510 -0.630802
C -1.454269 1.214936 -1.906440
C -0.336180 1.970746 -2.326835
C -0.512506 3.230880 -2.909507
C -1.800013 3.742076 -3.084442
C -2.915884 3.008523 -2.678063
C -2.738159 1.754491 -2.095724
H 0.344766 3.818022 -3.232078
H -1.925774 4.724142 -3.541080
H -3.919612 3.412871 -2.804355
H -3.614691 1.198587 -1.772381
C -0.821291 -0.213629 0.558422
C -1.104455 -1.174688 1.571011

C -0.646543 -0.956728 2.877914
C 0.088898 0.187410 3.185995
C 0.366390 1.143447 2.204751
C -0.089731 0.940422 0.906629
H -2.828442 -2.677631 3.020807
H -0.862546 -1.678057 3.662817
H 0.438511 0.335116 4.208236
H 0.921610 2.046904 2.454182
H 0.113177 1.695325 0.150921
O -5.508032 -3.005764 -2.001704
C -6.938458 -3.098088 -2.188030
H -7.208927 -2.206688 -2.761067
H -7.201305 -3.998754 -2.760184
O -3.138493 -4.637691 -4.267083
C -3.449527 -5.824684 -5.034401
O 0.893855 1.387648 -2.134784
C 2.069716 2.202392 -2.370816
O -1.845534 -2.261996 1.207458
C -2.245084 -3.189405 2.242931
H -2.868525 -3.930311 1.734841
H -1.369645 -3.684651 2.687203
H -4.536088 -5.978607 -5.087677
H -3.024147 -5.763355 -6.046430
H -2.986767 -6.650941 -4.487260
C 0.320646 -5.189004 -2.318546
C -0.213526 -4.104526 -3.211952
H -0.920747 -4.412524 -3.988849
H 0.647920 -3.526084 -3.694391
C 1.112937 -4.527888 -1.178642
C 0.392341 -3.246818 -0.758797
H 0.962214 -2.625381 -0.054120
H -0.566055 -3.451542 -0.265754
H 1.242045 -5.214435 -0.325809
H 2.131689 -4.303381 -1.535296
H 0.945228 -5.886489 -2.906086
H -0.516997 -5.799309 -1.953380
C -0.744172 -0.434287 -4.622185
C -0.464109 -1.622170 -5.185438
H 0.009324 0.342423 -4.496951
H -1.764493 -0.161584 -4.358520
H 0.533000 -1.857782 -5.562075
H -1.258211 -2.342898 -5.387396
H 2.919610 1.583187 -2.069144
H 2.040557 3.113470 -1.758063
H 2.162064 2.463315 -3.434737
C 2.120694 -1.247714 -3.162545
C 2.215672 -1.333922 -1.817213
H 2.730310 -2.167740 -1.341990
H 1.884182 -0.519318 -1.172045
H 1.744538 -0.341948 -3.632864
H 2.565362 -2.006832 -3.810046

Spin state: triplet

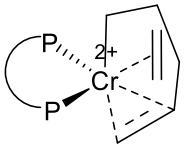
E = -12369.26 kcal mol-1
H = -11873.86 kcal mol-1
TS = -82.97 kcal mol-1
G (298.15 K) = -11956.83 kcal mol-1

Cr -0.128558 -2.234313 -2.495846
P -2.588093 -2.593030 -2.223354
N -2.828598 -1.181905 -1.272558
P -1.292381 -0.462019 -1.170127
C -3.988627 -0.905136 -0.401576
H -4.214710 -1.791526 0.203207
H -4.867733 -0.640264 -1.000230
H -3.731988 -0.081567 0.275133
C -3.491037 -2.344447 -3.787441
C -4.021816 -1.089120 -4.113165
C -4.735589 -0.898901 -5.295403
C -4.924541 -1.978088 -6.163383
C -4.409307 -3.240760 -5.859072
C -3.688623 -3.430273 -4.673256
H -3.886902 -0.259398 -3.420297
H -5.147209 0.081013 -5.534924
H -5.480070 -1.841977 -7.091878
H -4.571690 -4.068016 -6.547418
C -3.442894 -3.961217 -1.369041
C -4.864421 -4.041637 -1.394174
C -5.508536 -5.137084 -0.799787
C -4.764209 -6.136478 -0.173399
C -3.370603 -6.056488 -0.118211
C -2.727972 -4.972681 -0.712878
H -7.470173 -3.097263 -1.193136
H -6.594392 -5.208054 -0.817508
H -5.284028 -6.980364 0.281781
H -2.789014 -6.830531 0.381716
H -1.647214 -4.910043 -0.658313
C -1.460226 1.210269 -1.907247
C -0.341607 1.960438 -2.336074
C -0.517289 3.218706 -2.923114
C -1.804135 3.732409 -3.095246
C -2.920571 3.003610 -2.681499
C -2.743788 1.751844 -2.094540
H 0.339878 3.802489 -3.251828
H -1.929047 4.712861 -3.555601
H -3.923683 3.410341 -2.805129
H -3.620231 1.199653 -1.764539
C -0.830876 -0.206361 0.565950
C -1.110942 -1.167535 1.579861
C -0.654040 -0.945736 2.886597
C 0.077489 0.201432 3.192078
C 0.352692 1.156914 2.208952
C -0.102356 0.950642 0.911228
H -2.820570 -2.692548 3.030166
H -0.867707 -1.666388 3.672772
H 0.426603 0.352398 4.214031
H 0.904820 2.062510 2.457493
H 0.098154 1.704543 0.153593
O -5.522335 -3.012012 -1.991643
C -6.954536 -3.104447 -2.164033
H -7.230374 -2.214542 -2.736820
H -7.223016 -4.006623 -2.731126
O -3.141595 -4.622233 -4.281542
C -3.444857 -5.804500 -5.058860
O 0.887706 1.374875 -2.147451
C 2.063454 2.188704 -2.387693
O -1.847236 -2.256706 1.216248
C -2.233227 -3.193601 2.248309
H -2.849239 -3.939225 1.737958

H -1.350496 -3.680246 2.687629
H -4.530399 -5.964981 -5.114221
H -3.019373 -5.731878 -6.070106
H -2.977242 -6.632664 -4.518691
C 0.358654 -5.195707 -2.309013
C -0.176066 -4.134011 -3.226796
H -0.893209 -4.448257 -3.990918
H 0.675224 -3.556457 -3.715321
C 1.140853 -4.515506 -1.172386
C 0.405692 -3.246029 -0.744939
H 0.969817 -2.617591 -0.042352
H -0.551813 -3.463103 -0.257174
H 1.283469 -5.201118 -0.320553
H 2.155731 -4.277483 -1.531923
H 0.994186 -5.900923 -2.875623
H -0.476576 -5.805406 -1.937034
C -0.733832 -0.441056 -4.637772
C -0.470040 -1.633423 -5.197390
H 0.029562 0.326925 -4.516698
H -1.749852 -0.158047 -4.366559
H 0.524140 -1.883218 -5.573377
H -1.271564 -2.348753 -5.389208
H 2.913799 1.570236 -2.085225
H 2.035321 3.102140 -1.778363
H 2.154726 2.445982 -3.452626
C 2.171205 -1.266315 -3.166849
C 2.251833 -1.331281 -1.820607
H 2.759098 -2.158821 -1.326626
H 1.902730 -0.512436 -1.190429
H 1.788352 -0.373432 -3.657205
H 2.619764 -2.036455 -3.798522

Geometry:

‡



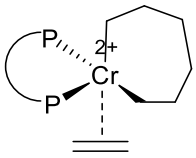
Spin state: triplet

E = -12356.10 kcal mol-1
H = -11861.71 kcal mol-1
TS = -79.14 kcal mol-1
G (298.15 K) = -11940.85 kcal mol-1

Cr -0.617268 -2.726577 -2.486559
P -3.296007 -2.549395 -2.365123
N -3.188115 -0.961427 -1.733451
P -1.548331 -0.815114 -1.262801
C -4.229985 -0.027080 -1.240099
H -5.218747 -0.477876 -1.350349
H -4.189726 0.918913 -1.794210
H -4.059003 0.178971 -0.177426
C -4.210451 -2.342872 -3.966802
C -4.795086 -1.092017 -4.240846
C -5.552518 -0.867097 -5.388909
C -5.734817 -1.902847 -6.304229
C -5.132067 -3.141511 -6.088219
C -4.356546 -3.360800 -4.944045
H -4.670064 -0.271116 -3.542989
H -6.003357 0.110124 -5.558391
H -6.334038 -1.748795 -7.201951
H -5.256188 -3.930345 -6.826821
C -4.331655 -3.676418 -1.340637
C -4.968966 -3.365006 -0.105544
C -5.711853 -4.352817 0.560214
C -5.815327 -5.642256 0.044229
C -5.178353 -5.970937 -1.153232
C -4.450842 -4.994526 -1.828382
H -5.042423 -2.419324 2.460027
H -6.216887 -4.112318 1.493289
H -6.399575 -6.389280 0.582437
H -5.256089 -6.976047 -1.566526
H -3.987083 -5.253729 -2.774270
C -0.931657 0.748280 -1.952312
C 0.374066 1.184516 -1.612489
C 0.882800 2.367625 -2.162974
C 0.113660 3.089037 -3.077911
C -1.158431 2.645179 -3.457017
C -1.671562 1.477976 -2.898303
H 1.876341 2.721792 -1.894375
H 0.519497 4.006208 -3.506140
H -1.747156 3.210786 -4.178446
H -2.655156 1.123940 -3.202362
C -1.571762 -0.673338 0.545797
C -1.889778 -1.818348 1.319853
C -1.941461 -1.721786 2.715473
C -1.713494 -0.489970 3.332905
C -1.429408 0.652217 2.577836
C -1.353188 0.555012 1.190030
H -3.117831 -4.177515 2.028769
H -2.158906 -2.597620 3.323908
H -1.760135 -0.425545 4.420617
H -1.266103 1.611496 3.067962
H -1.129209 1.440876 0.595709
O -4.819941 -2.108309 0.390535
C -5.433402 -1.781069 1.654336
H -5.148231 -0.743345 1.851453
H -6.528079 -1.862932 1.600932
O -3.662347 -4.531604 -4.741534
C -3.898255 -5.642338 -5.643346
O 1.053340 0.373856 -0.748692
C 2.258946 0.891225 -0.132640
O -2.126310 -2.967577 0.620455
C -2.253576 -4.203920 1.351370
H -2.429961 -4.970919 0.591127
H -1.332853 -4.420804 1.911274
H -4.960494 -5.921196 -5.645848
H -3.561772 -5.400700 -6.660915
H -3.299859 -6.468339 -5.246085
C 2.459931 -3.127951 -2.280734
C 1.339215 -2.781630 -3.214206
H 1.576471 -2.786029 -4.283230
H 0.927952 -1.737839 -2.950834
C 1.963403 -2.871070 -0.857135
C 0.487775 -3.233935 -0.732791
H 0.048240 -2.780290 0.155636
H 0.322024 -4.321493 -0.675298

H 2.565013 -3.416452 -0.112285
H 2.081829 -1.802432 -0.637302
H 3.356868 -2.532247 -2.528130
H 2.770925 -4.173163 -2.443173
C -1.004759 -2.426208 -5.281218
C -1.117011 -1.187956 -4.770486
H -1.868418 -3.083539 -5.376932
H -0.065539 -2.783948 -5.703266
H -2.086812 -0.796534 -4.465633
H -0.278173 -0.489765 -4.746095
C -1.163667 -4.894550 -2.889799
C 0.138729 -4.897527 -3.348485
H -1.984499 -4.858184 -3.602489
H -1.400139 -5.225160 -1.876200
H 0.342272 -4.872622 -4.419015
H 0.952901 -5.239066 -2.712795
H 2.533857 0.157127 0.630296
H 2.062518 1.861840 0.342804
H 3.068236 0.984050 -0.870262

Geometry:



Spin state: singlet

E = -12373.45 kcal mol-1
H = -11874.49 kcal mol-1
TS = -82.51 kcal mol-1
G (298.15 K) = -11957.00 kcal mol-1

Cr -0.977689 -2.903815 -1.966578
P -3.296398 -2.378178 -2.043010
N -3.193588 -0.855430 -1.272938
P -1.575015 -0.813762 -0.677293
C -4.328008 -0.126209 -0.661776
H -3.983338 0.864959 -0.345256
H -4.716242 -0.662761 0.214882
H -5.130057 -0.018266 -1.398904
C -4.031583 -2.137929 -3.669907
C -4.352339 -0.866317 -4.163763
C -4.904059 -0.727168 -5.436154
C -5.119839 -1.864215 -6.222374
C -4.768081 -3.137095 -5.764168
C -4.202717 -3.274981 -4.492160
H -4.175960 0.011964 -3.543674
H -5.167908 0.260118 -5.813716
H -5.556938 -1.761405 -7.216119
C -4.300637 -3.529491 -1.070795
C -5.711119 -3.414152 -0.991929
C -6.434044 -4.348113 -0.233851
C -5.763860 -5.371639 0.438324
C -4.371133 -5.492006 0.372895
C -3.653193 -4.571709 -0.385643
H -8.090958 -2.063640 -0.672390
H -7.517905 -4.279382 -0.161965
H -6.342841 -6.087123 1.023455
H -3.859431 -6.295518 0.901489
H -2.564770 -4.663947 -0.452113
C -0.811222 0.679497 -1.371491
C 0.580393 0.847025 -1.206734
C 1.216327 1.976218 -1.727999
C 0.464792 2.919224 -2.438998
C -0.906321 2.743373 -2.639886
C -1.540997 1.617681 -2.110664
H 2.285820 2.128150 -1.594338
H 0.966051 3.798017 -2.845760
H -1.480189 3.481047 -3.199869
H -2.609609 1.471978 -2.264921
C -1.766271 -0.677140 1.128669
C -1.244895 0.350145 1.961103
C -1.531586 0.325235 3.338313
C -2.316151 -0.686608 3.884169
C -2.842438 -1.699141 3.073558
C -2.561931 -1.685151 1.712911
H 0.645189 2.105547 2.960470
H -1.139104 1.104785 3.988085
H -2.521609 -0.681242 4.955244
H -3.466418 -2.484531 3.498306
H -2.988029 -2.466247 1.079645
O -6.263322 -2.374705 -1.672645
C -7.705135 -2.247882 -1.685079
H -7.912065 -1.384973 -2.324168
H -8.171508 -3.145915 -2.114202
O -3.747738 -4.452499 -3.954166
C -4.089476 -5.686383 -4.631141
O 1.212209 -0.163737 -0.523459
C 2.555191 0.084741 -0.047545
O -0.497675 1.318142 1.374423
C -0.047183 2.434988 2.172215
H 0.475855 3.089285 1.468350
H -0.897725 2.973132 2.614113
H -5.177695 -5.769466 -4.756724
H -3.588484 -5.750267 -5.607503
H -3.731027 -6.486758 -3.977319
C 0.836393 -4.022359 -4.791233
C 1.424703 -2.657218 -4.404558
C 0.625973 -5.028953 -3.648850
C -0.485723 -4.711182 -2.675402
H -0.828215 -5.588509 -2.110052
H -1.425472 -4.294186 -3.205878
H 0.407775 -6.016865 -4.093261
H 1.560288 -5.187589 -3.081437
H 1.514334 -4.479388 -5.525338
H -0.119501 -3.888607 -5.323559
C -0.867270 -1.695440 -3.613659
C 0.617080 -1.820940 -3.397624
H -1.271197 -0.680823 -3.577308
H -1.277617 -2.246313 -4.468280
H 1.528382 -2.054877 -5.319351
H 2.442409 -2.796480 -4.009233
H 0.836551 -2.253715 -2.353962
H 1.060146 -0.824892 -3.246091
C 0.131456 -3.124105 0.301444
C 0.691199 -4.134665 -0.423107
H -0.694694 -3.317950 0.987041

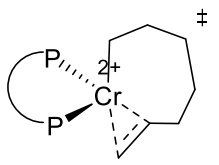
H 0.615908 -2.152191 0.384011
H -4.923639 -4.004142 -6.403705
H 0.357044 -5.163973 -0.299797
H 1.632985 -3.996576 -0.957142
H 2.818002 -0.781936 0.566909
H 2.581336 0.995491 0.566206
H 3.262402 0.168924 -0.884936

Spin state: triplet

E = -12384.36 kcal mol-1
H = -11888.14 kcal mol-1
TS = -83.19 kcal mol-1
G (298.15 K) = -11971.33 kcal mol-1

Cr -0.932072 -2.837099 -1.966871
P -3.291611 -2.402239 -1.999477
N -3.240569 -0.884434 -1.212392
P -1.624821 -0.763666 -0.642013
C -4.409858 -0.182580 -0.636145
H -4.074537 0.760748 -0.191117
H -4.885378 -0.790353 0.145661
H -5.141820 0.020766 -1.425200
C -3.965964 -2.148374 -3.651998
C -4.202917 -0.863396 -4.158685
C -4.685206 -0.698538 -5.455690
C -4.913748 -1.824330 -6.255476
C -4.643463 -3.111780 -5.784001
C -4.147924 -3.276423 -4.485804
H -4.010705 0.005044 -3.529429
H -4.885558 0.299923 -5.842689
H -5.296072 -1.700874 -7.269118
C -4.319341 -3.551361 -1.052643
C -5.733569 -3.451506 -1.032535
C -6.474918 -4.372777 -0.277019
C -5.819467 -5.367662 0.450669
C -4.424164 -5.470637 0.443872
C -3.686027 -4.563748 -0.311949
H -8.127304 -2.115683 -0.820996
H -7.561526 -4.316299 -0.249484
H -6.412736 -6.074050 1.032609
H -3.924541 -6.251261 1.016445
H -2.595898 -4.638460 -0.333692
C -0.922426 0.751808 -1.344953
C 0.478830 0.908473 -1.285748
C 1.079963 2.044843 -1.831624
C 0.280398 3.006107 -2.461238
C -1.103961 2.842692 -2.555566
C -1.703173 1.708555 -2.003976
H 2.157860 2.188010 -1.780810
H 0.753554 3.890589 -2.889017
H -1.714935 3.596682 -3.050746
H -2.781812 1.575045 -2.076210
C -1.784229 -0.647569 1.166423
C -1.166203 0.319123 2.006424
C -1.411251 0.279992 3.391198
C -2.238459 -0.696203 3.938734
C -2.850072 -1.656058 3.122770
C -2.615881 -1.625468 1.753911
H 0.877201 1.916009 2.975990
H -0.949797 1.016583 4.045689
H -2.409684 -0.705342 5.015747
H -3.504899 -2.413760 3.551387
H -3.104421 -2.367258 1.118737
O -6.270483 -2.437364 -1.762406
C -7.711801 -2.318753 -1.818350
H -7.904831 -1.470502 -2.480911
H -8.161761 -3.228204 -2.241014
O -3.774331 -4.472519 -3.930412
C -4.091934 -5.688538 -4.650204
O 1.151595 -0.122192 -0.675485
C 2.533742 0.097969 -0.314888
O -0.369891 1.244322 1.416745
C 0.180167 2.310213 2.222457
H 0.718670 2.947764 1.514816
H -0.617061 2.890638 2.707709
H -5.171157 -5.750571 -4.845854
H -3.530928 -5.743815 -5.593805
H -3.788733 -6.505131 -3.988800
C 0.772383 -4.120333 -4.788989
C 1.472754 -2.801890 -4.425582
C 0.499540 -5.098430 -3.633966
C -0.601477 -4.714094 -2.673672
H -1.018144 -5.559268 -2.113255
H -1.490784 -4.212404 -3.202599
H 0.230840 -6.078553 -4.068271
H 1.422806 -5.301710 -3.062215
H 1.401943 -4.634887 -5.528061
H -0.178352 -3.916197 -5.308339
C -0.718546 -1.642529 -3.618929
C 0.749880 -1.901386 -3.409371
H -1.035554 -0.600429 -3.536070
H -1.177557 -2.124799 -4.489504
H 1.604572 -2.215596 -5.347132
H 2.484261 -3.016839 -4.048309
H 0.925329 -2.378391 -2.376031
H 1.291436 -0.957217 -3.251769
C 0.121867 -3.115544 0.303308
C 0.574744 -4.203430 -0.378965
H -0.714271 -3.201552 0.998604
H 0.689367 -2.185781 0.338576
H -4.807033 -3.970571 -6.432510
H 0.134004 -5.187077 -0.220958
H 1.520927 -4.183755 -0.922180
H 2.835926 -0.783623 0.258827
H 2.629164 0.996203 0.310539
H 3.167230 0.188304 -1.208999

Geometry:



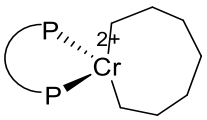
Spin state: triplet

E = -12381.23 kcal mol-1
H = -11885.89 kcal mol-1

TS = -81.74 kcal mol-1
G (298.15 K) = -11967.63 kcal mol-1

Cr -0.938702 -2.818996 -1.919437
P -3.296484 -2.405465 -1.963875
N -3.251457 -0.880645 -1.192716
P -1.619991 -0.753389 -0.669754
C -4.407296 -0.185976 -0.583495
H -4.061654 0.754327 -0.139775
H -4.861818 -0.800225 0.205913
H -5.158747 0.022764 -1.352474
C -3.934519 -2.168943 -3.634809
C -4.192022 -0.889703 -4.146178
C -4.636640 -0.734435 -5.457626
C -4.805666 -1.863350 -6.267471
C -4.516245 -3.144398 -5.789434
C -4.061075 -3.298957 -4.475510
H -4.045726 -0.018678 -3.508168
H -4.853326 0.259208 -5.848331
H -5.156809 -1.747514 -7.293226
C -4.349609 -3.544019 -1.034985
C -5.762477 -3.424399 -1.033503
C -6.527312 -4.342503 -0.297902
C -5.895980 -5.354094 0.428119
C -4.502186 -5.477167 0.439041
C -3.741143 -4.572563 -0.296378
H -8.136657 -2.052344 -0.838573
H -7.613239 -4.270538 -0.284022
H -6.507090 -6.057635 0.994798
H -4.021711 -6.270119 1.011029
H -2.652183 -4.659872 -0.304560
C -0.951331 0.782660 -1.359177
C 0.446098 0.963921 -1.297144
C 1.025905 2.120687 -1.821863
C 0.207574 3.078311 -2.433264
C -1.173326 2.890930 -2.530171
C -1.751352 1.735787 -1.998961
H 2.101050 2.282893 -1.768182
H 0.663529 3.979567 -2.844432
H -1.798241 3.642279 -3.011739
H -2.827512 1.583386 -2.072305
C -1.731310 -0.661364 1.145994
C -1.122603 0.313759 1.983924
C -1.331263 0.249477 3.373749
C -2.119337 -0.754118 3.929336
C -2.728016 -1.717548 3.116140
C -2.526974 -1.663951 1.742545
H 0.900918 1.949410 2.925245
H -0.873690 0.990393 4.026063
H -2.262775 -0.780950 5.010070
H -3.355198 -2.495493 3.549708
H -3.017498 -2.407493 1.110907
O -6.273914 -2.394957 -1.760309
C -7.712521 -2.252669 -1.832822
H -7.883882 -1.395144 -2.489408
H -8.171633 -3.150609 -2.269849
O -3.677089 -4.489062 -3.909763
C -3.946188 -5.709633 -4.641258
O 1.134975 -0.065318 -0.702129
C 2.498529 0.189661 -0.296739
O -0.373155 1.274280 1.389459
C 0.173362 2.339034 2.198440
H 0.676296 3.001519 1.487534
H -0.623203 2.891836 2.716097
H -5.016771 -5.793282 -4.872562
H -3.353317 -5.752509 -5.565879
H -3.650008 -6.521802 -3.971047
C 0.672693 -4.138979 -4.753953
C 1.425593 -2.842052 -4.423111
C 0.457268 -5.134378 -3.598753
C -0.619849 -4.779950 -2.583737
H -1.109893 -5.662176 -2.158901
H -1.491414 -4.209871 -3.075398
H 0.171114 -6.105932 -4.035592
H 1.410112 -5.336929 -3.081384
H 1.242601 -4.658968 -5.536809
H -0.304636 -3.910431 -5.210467
C -0.684946 -1.599163 -3.547411
C 0.773765 -1.929395 -3.371079
H -0.947396 -0.541141 -3.494366
H -1.188300 -2.085603 -4.392527
H 1.527898 -2.256273 -5.348799
H 2.447794 -3.086358 -4.095672
H 0.945781 -2.439203 -2.356594
H 1.360828 -1.014599 -3.207095
C 0.089180 -3.148600 0.029441
C 0.319027 -4.387348 -0.579454
H -0.652466 -3.079899 0.825936
H 0.871584 -2.389165 0.052505
H -4.635771 -4.005468 -6.444499
H -0.217717 -5.261998 -0.212740
H 1.286187 -4.596907 -1.036373
H 2.809393 -0.689160 0.276598
H 2.548510 1.082651 0.341185
H 3.156457 0.309554 -1.169576

Geometry:



Spin state: singlet

E = -12402.01 kcal mol-1
H = -11902.32 kcal mol-1
TS = -80.07 kcal mol-1
G (298.15 K) = -11982.39 kcal mol-1

Cr -1.202425 -2.362540 -1.484057
P -3.526806 -2.400684 -2.022891
N -3.812372 -0.763511 -1.569390
P -2.252844 -0.269657 -1.096346
C -5.103375 -0.202610 -1.127603
H -5.274232 -0.411491 -0.062284
H -5.910118 -0.657076 -1.714131
H -5.114482 0.881339 -1.297495
C -3.871868 -2.528234 -3.797955
C -4.411312 -1.467434 -4.535518

C -4.605240 -1.594757 -5.911845
C -4.246152 -2.784728 -6.550329
C -3.693648 -3.851588 -5.833513
C -3.499551 -3.721269 -4.455123
H -4.687764 -0.544127 -4.027815
H -5.037973 -0.773433 -6.481922
H -4.394920 -2.890606 -7.625256
C -4.753662 -3.423723 -1.183276
C -4.748513 -3.491555 0.231480
C -5.692463 -4.286078 0.892243
C -6.633512 -5.004074 0.149449
C -6.651326 -4.941008 -1.246513
C -5.711923 -4.154282 -1.907915
H -3.564834 -3.780109 2.676171
H -5.706610 -4.351321 1.978048
H -7.364615 -5.618660 0.675800
H -7.395820 -5.496927 -1.815413
H -5.724260 -4.092221 -2.995705
C -1.852102 1.244602 -1.987325
C -0.607864 1.863744 -1.712707
C -0.258143 3.045658 -2.373628
C -1.131496 3.585408 -3.322407
C -2.345263 2.961359 -3.628227
C -2.699438 1.786972 -2.966031
H 0.688094 3.542026 -2.166284
H -0.849847 4.504853 -3.836450
H -3.011574 3.391013 -4.375268
H -3.639404 1.288575 -3.199156
C -2.149723 0.111950 0.666359
C -1.241448 -0.623827 1.447119
C -1.039593 -0.284838 2.787625
C -1.776851 0.765824 3.347537
C -2.695983 1.489947 2.586998
C -2.864498 1.172843 1.239231
H 1.158834 -1.766790 2.010928
H -0.328723 -0.819251 3.412907
H -1.618374 1.017286 4.396634
H -3.261097 2.307462 3.033522
H -3.540097 1.764319 0.619927
O -3.791137 -2.738298 0.861355
C -3.776201 -2.766543 2.306139
H -2.977226 -2.082942 2.602972
H -4.731225 -2.407425 2.714952
O -2.952285 -4.680154 -3.638127
C -2.750246 -6.000511 -4.191506
O 0.182005 1.202354 -0.811375
C 1.390234 1.855357 -0.356957
O -0.572048 -1.682037 0.816276
C 0.355434 -2.425735 1.657941
H -0.176590 -2.878197 2.505119
H 0.778623 -3.211525 1.031057
H -3.683615 -6.390899 -4.620263
H -1.958105 -5.990511 -4.954328
H -2.448617 -6.630283 -3.348943
C 1.730059 -3.602778 -3.739043
C 1.763110 -2.083495 -3.496319
C 2.031927 -4.521531 -2.540522
C 1.070823 -4.411614 -1.347873
H 2.030073 -5.563370 -2.898792
H 3.054837 -4.327295 -2.184463
H 2.488258 -3.820378 -4.505155
H 0.776648 -3.887655 -4.215022
C -0.840773 -1.742222 -3.420948
C 0.523026 -1.385109 -2.883563
H -1.442951 -0.891672 -3.755633
H -0.872592 -2.535455 -4.175188
H 1.912012 -1.590900 -4.469010
H 2.644600 -1.826658 -2.888600
H 0.571466 -1.539401 -1.740661
H 0.661487 -0.294538 -2.899931
C -1.474256 -4.246249 -0.747862
C -0.400049 -4.567354 -1.750769
H -2.419766 -4.772257 -0.895033
H -1.188639 -4.198682 0.308865
H -3.418165 -4.766912 -6.354060
H -0.583612 -3.909369 -2.658936
H -0.584969 -5.540598 -2.233912
H 1.227131 -3.432840 -0.859396
H 1.320546 -5.165765 -0.585502
H 1.804338 1.197707 0.412850
H 1.162301 2.837606 0.079224
H 2.111103 1.962759 -1.180089

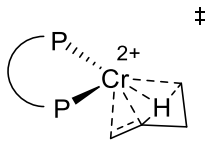
Spin state: triplet

E = -12414.30 kcal mol-1
H = -11915.01 kcal mol-1
TS = -80.30 kcal mol-1
G (298.15 K) = -11995.31 kcal mol-1

Cr -1.197565 -2.343442 -1.470530
P -3.541167 -2.391095 -2.019190
N -3.833933 -0.755410 -1.564645
P -2.282379 -0.247221 -1.085948
C -5.132651 -0.199313 -1.137911
H -5.323867 -0.426180 -0.079795
H -5.929115 -0.641000 -1.747797
H -5.138327 0.887392 -1.288535
C -3.863808 -2.518935 -3.796960
C -4.369154 -1.452301 -4.549963
C -4.529026 -1.581012 -5.930543
C -4.171141 -2.777950 -6.556809
C -3.651999 -3.850772 -5.823919
C -3.490131 -3.718407 -4.441708
H -4.642291 -0.522949 -4.051644
H -4.933967 -0.754805 -6.513818
H -4.293683 -2.884433 -7.634978
C -4.762678 -3.420128 -1.182110
C -4.750760 -3.492229 0.232195
C -5.690193 -4.290798 0.894529
C -6.632656 -5.008220 0.152926
C -6.656477 -4.940943 -1.242944
C -5.721507 -4.150356 -1.905934
H -3.555805 -3.787092 2.669030
H -5.699838 -4.359459 1.980188
H -7.360750 -5.625555 0.680220
H -7.402502 -5.496521 -1.810167
H -5.737611 -4.084462 -2.993562
C -1.883191 1.265209 -1.978847
C -0.626071 1.864210 -1.721318

C -0.265340 3.040011 -2.386539
C -1.143605 3.594273 -3.322631
C -2.372109 2.990710 -3.610527
C -2.736036 1.821293 -2.944724
H 0.691828 3.520643 -2.192636
H -0.854559 4.509124 -3.840696
H -3.042050 3.432058 -4.347428
H -3.686949 1.338581 -3.165943
C -2.177869 0.121651 0.679177
C -1.245809 -0.604027 1.441864
C -1.044622 -0.284505 2.786895
C -1.804452 0.737638 3.369361
C -2.746170 1.451433 2.626965
C -2.916318 1.153021 1.275016
H 1.202617 -1.640644 1.950530
H -0.317831 -0.812840 3.398951
H -1.645848 0.975056 4.421681
H -3.328169 2.246918 3.091212
H -3.611891 1.737099 0.671153
O -3.791576 -2.738639 0.859177
C -3.768296 -2.772033 2.303953
H -2.966616 -2.090747 2.598573
H -4.720734 -2.413351 2.719021
O -2.972641 -4.679243 -3.608101
C -2.776992 -6.005563 -4.149166
O 0.162781 1.187663 -0.829679
C 1.389747 1.816217 -0.392181
O -0.551014 -1.632871 0.787508
C 0.432843 -2.338362 1.597061
H -0.055267 -2.839323 2.443655
H 0.888622 -3.084860 0.945014
H -3.705675 -6.384670 -4.597678
H -1.967142 -6.011478 -4.893188
H -2.504879 -6.635026 -3.296244
C 1.711935 -3.659832 -3.778459
C 1.792818 -2.144964 -3.518228
C 2.011401 -4.605950 -2.600463
C 1.086687 -4.485680 -1.378927
H 1.965201 -5.640693 -2.975672
H 3.049201 -4.452748 -2.268142
H 2.446950 -3.889027 -4.563704
H 0.740991 -3.911288 -4.237956
C -0.797462 -1.740064 -3.415898
C 0.578497 -1.425775 -2.877216
H -1.382766 -0.868841 -3.726812
H -0.849159 -2.513941 -4.188592
H 1.941307 -1.643900 -4.486578
H 2.689452 -1.920607 -2.919718
H 0.635486 -1.621154 -1.743610
H 0.744982 -0.339244 -2.871193
C -1.438055 -4.244159 -0.714058
C -0.398535 -4.554392 -1.748657
H -2.393737 -4.758785 -0.829925
H -1.119336 -4.182185 0.331915
H -3.376221 -4.771456 -6.334872
H -0.563659 -3.842097 -2.624786
H -0.639248 -5.485797 -2.286231
H 1.302319 -3.532420 -0.866554
H 1.317037 -5.276456 -0.648995
H 1.801872 1.150057 0.371440
H 1.187428 2.802545 0.047414
H 2.101090 1.909884 -1.225298

Geometry:



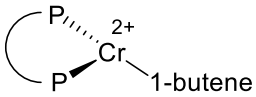
Spin state: triplet

E = -10861.87 kcal mol-1
H = -10441.32 kcal mol-1
TS = -72.30 kcal mol-1
G (298.15 K) = -10513.61 kcal mol-1

Cr -0.725954 -4.580857 -3.134318
H 1.880112 -4.640889 -1.734632
H -2.685424 -5.640707 -1.432732
H -2.521465 -3.831378 -1.196543
C 0.239636 -3.774438 -0.562408
H 1.460369 -3.017776 -2.339981
C -0.699706 -4.984360 -0.804807
C -2.015277 -4.778349 -1.389328
H 0.166238 -5.212587 -1.756822
C 1.051922 -3.929226 -1.877861
H -0.319048 -2.830725 -0.511611
H -0.535157 -5.900473 -0.221654
H 0.840942 -3.860150 0.352155
H -3.242208 -9.611038 -2.407062
P 0.502222 -4.071593 -5.130429
N 0.710388 -5.713655 -5.568474
P -0.163972 -6.545525 -4.369403
C 1.437198 -6.238950 -6.734909
H 1.445928 -7.334358 -6.688051
H 2.473990 -5.880046 -6.706487
H 0.959372 -5.924631 -7.673255
C -0.712937 -3.350934 -6.257434
C -0.431216 -2.894464 -7.556428
C -1.461287 -2.471840 -8.395234
C -2.778979 -2.507324 -7.934283
C -3.084712 -2.970542 -6.649405
C -2.051051 -3.394904 -5.817040
H 0.602995 -2.871716 -7.902230
H -1.238622 -2.114815 -9.400309
H -3.591883 -2.168193 -8.576906
H -4.122419 -2.981720 -6.325847
C 2.050092 -3.165678 -5.220916
C 3.236628 -3.749841 -4.695708
C 4.418805 -3.000559 -4.667175
C 4.415488 -1.677470 -5.114909
C 3.245124 -1.079409 -5.592502
C 2.067665 -1.820152 -5.640919
H 4.685169 -5.182749 -2.840574
H 5.341415 -3.437096 -4.289482
H 5.342960 -1.105112 -5.080561
H 3.251233 -0.042554 -5.926537
H 1.152360 -1.352832 -6.003116
C -1.760362 -7.038571 -5.069639

C -2.693715 -7.663986 -4.206347
C -3.948344 -8.044837 -4.695611
C -4.275692 -7.770430 -6.027316
C -3.376647 -7.113822 -6.875916
C -2.121459 -6.743307 -6.393208
H -4.670772 -8.545812 -4.053829
H -5.254268 -8.071289 -6.403223
H -3.648123 -6.906288 -7.910439
H -1.413764 -6.230002 -7.043640
C 0.693815 -8.070248 -3.922939
C 1.570815 -8.174820 -2.816199
C 2.226168 -9.389398 -2.574102
C 2.014290 -10.481858 -3.418315
C 1.139562 -10.393348 -4.503852
C 0.475584 -9.193424 -4.745023
H 3.544355 -7.410845 -1.036514
H 2.899359 -9.496560 -1.726000
H 2.533080 -11.418538 -3.211220
H 0.969589 -11.252196 -5.152248
H -0.228991 -9.122385 -5.574815
O 3.121173 -5.031617 -4.240119
C 4.301669 -5.691604 -3.737207
H 3.970899 -6.702542 -3.481837
H 5.085470 -5.742695 -4.506161
O -2.300336 -3.895888 -4.508883
C -3.694697 -4.301121 -4.260492
O -2.267814 -7.816843 -2.916617
C -3.089763 -8.596980 -2.013531
O 1.714360 -7.063396 -2.028623
C 2.488256 -7.200516 -0.815159
H 2.413616 -6.234186 -0.305842
H 2.073774 -7.987832 -0.170051
H -4.329430 -3.410801 -4.189563
H -4.019445 -4.971880 -5.064967
H -3.683932 -4.831559 -3.309674
H -4.058903 -8.106512 -1.841888
H -2.528001 -8.644044 -1.076667

Geometry:



Spin state: singlet

E = -10891.70 kcal mol-1
H = -10467.15 kcal mol-1
TS = -74.28 kcal mol-1
G (298.15 K) = -10541.43 kcal mol-1

Cr -0.499673 -2.008561 -2.283564
P -2.823879 -2.342573 -2.036897
N -3.004399 -1.100352 -0.868850
P -1.404191 -0.502705 -0.771315
C -4.183981 -0.658762 -0.110621
H -5.066664 -1.176708 -0.499965
H -4.330560 0.424797 -0.224074
H -4.057609 -0.901297 0.953238
C -3.631406 -1.775202 -3.560497
C -4.049810 -0.442460 -3.692960
C -4.590663 0.015814 -4.894571
C -4.711159 -0.865692 -5.974229
C -4.293257 -2.195481 -5.867924
C -3.742300 -2.656176 -4.664956
H -3.954162 0.236252 -2.845551
H -4.926554 1.048272 -4.985512
H -5.138495 -0.518918 -6.915798
H -4.398903 -2.862542 -6.721644
C -3.614060 -3.856388 -1.436839
C -5.023149 -4.021140 -1.468932
C -5.586056 -5.228413 -1.030600
C -4.764725 -6.252278 -0.555986
C -3.376074 -6.095691 -0.505140
C -2.813993 -4.900117 -0.947608
H -7.651004 -3.265157 -1.079679
H -6.664428 -5.373815 -1.052671
H -5.220554 -7.184125 -0.219680
H -2.742537 -6.899777 -0.131969
H -1.732147 -4.774062 -0.910385
C -1.384606 1.048540 -1.720212
C -1.037364 0.912551 -3.075653
C -1.109884 1.981487 -3.961310
C -1.564504 3.216548 -3.484175
C -1.950813 3.372862 -2.151457
C -1.863852 2.291589 -1.273601
H -0.823968 1.882060 -5.005975
H -1.617857 4.060552 -4.172126
H -2.319153 4.335190 -1.796464
H -2.174736 2.407400 -0.235079
C -0.944830 -0.214871 0.943658
C -1.130122 -1.281867 1.863946
C -0.772721 -1.108769 3.205683
C -0.192385 0.093175 3.618587
C 0.049480 1.127788 2.709771
C -0.322517 0.971425 1.376778
H -2.722422 -3.129489 3.011028
H -0.928167 -1.906842 3.928840
H 0.086551 0.213503 4.665927
H 0.522390 2.052305 3.038745
H -0.123468 1.772548 0.666291
O -5.744657 -2.958521 -1.924563
C -7.179185 -3.105319 -2.059547
H -7.524548 -2.160208 -2.487699
H -7.424023 -3.932666 -2.740194
O -3.273023 -3.921080 -4.456774
C -3.492470 -4.911967 -5.488806
O -0.615285 -0.384257 -3.517358
C -0.787831 -0.662260 -4.958370
O -1.641625 -2.441211 1.341355
C -2.008325 -3.498131 2.261491
H -2.485293 -4.263241 1.642226
H -1.119542 -3.913602 2.757679
H -4.564093 -5.015619 -5.708541
H -2.942291 -4.655559 -6.405923
H -3.108432 -5.849131 -5.075934
C 0.950014 -3.415115 -0.751920
C 1.572850 -2.731707 -1.972722
H 2.669245 -2.660991 -1.931892
H 1.463199 -2.726718 -4.177106

H -0.702794 -1.745881 -5.063386
H 0.007587 -0.157962 -5.517174
H 1.313886 -1.584057 -1.825019
H -1.788179 -0.336040 -5.265382
H 1.374822 -3.026548 0.179972
H 1.051822 -4.506263 -0.804050
C -0.147710 -3.928343 -3.386554
C 1.012719 -3.168164 -3.283803
H -0.588123 -4.117143 -4.364772
H -0.456920 -4.639559 -2.618986
H -0.159765 -3.228206 -0.629667

Spin state: triplet

E = -10903.48 kcal mol-1
H = -10477.22 kcal mol-1
TS = -74.28 kcal mol-1
G (298.15 K) = -10551.49 kcal mol-1

Cr -0.494221 -2.009311 -2.277919
P -2.829807 -2.340310 -2.055335
N -3.001775 -1.099214 -0.879302
P -1.408847 -0.484837 -0.764575
C -4.183426 -0.670955 -0.114560
H -5.067683 -1.171181 -0.523407
H -4.320892 0.416332 -0.198803
H -4.064922 -0.943842 0.942794
C -3.657878 -1.765750 -3.563556
C -4.084552 -0.435546 -3.685226
C -4.629125 0.027548 -4.883867
C -4.746247 -0.847849 -5.968428
C -4.320168 -2.176112 -5.871385
C -3.764549 -2.640274 -4.672326
H -3.987879 0.239086 -2.834619
H -4.969766 1.058964 -4.968479
H -5.176891 -0.497694 -6.907226
H -4.422389 -2.838245 -6.729380
C -3.610779 -3.855921 -1.446457
C -5.019027 -4.029443 -1.470810
C -5.571665 -5.240139 -1.028400
C -4.741725 -6.258426 -0.557142
C -3.353827 -6.092950 -0.513510
C -2.801837 -4.894486 -0.960331
H -7.653285 -3.295315 -1.076259
H -6.649202 -5.392326 -1.045023
H -5.189954 -7.192990 -0.218127
H -2.713160 -6.892872 -0.143510
H -1.720570 -4.762149 -0.930658
C -1.385830 1.059222 -1.724795
C -1.038165 0.916856 -3.080076
C -1.093786 1.985481 -3.966546
C -1.532281 3.227532 -3.492324
C -1.919934 3.390568 -2.160913
C -1.848763 2.309828 -1.281247
H -0.804972 1.879390 -5.009890
H -1.572135 4.071257 -4.181520
H -2.277471 4.357742 -1.808125
H -2.161978 2.431491 -0.244206
C -0.959802 -0.196795 0.951448
C -1.135464 -1.272258 1.864109
C -0.780712 -1.105064 3.207103
C -0.210732 0.099027 3.628083
C 0.023437 1.141578 2.726123
C -0.346237 0.991459 1.391986
H -2.698143 -3.153593 2.998851
H -0.929068 -1.909521 3.924666
H 0.066757 0.214824 4.676308
H 0.489148 2.067462 3.061450
H -0.150966 1.797850 0.686644
O -5.750356 -2.972491 -1.922921
C -7.183650 -3.131687 -2.056544
H -7.537401 -2.189641 -2.484612
H -7.421783 -3.961278 -2.736836
O -3.280750 -3.901680 -4.472501
C -3.484065 -4.885882 -5.513826
O -0.634951 -0.384577 -3.526208
C -0.851198 -0.672772 -4.960289
O -1.634045 -2.432633 1.332039
C -1.981767 -3.504086 2.242867
H -2.450206 -4.269649 1.617798
H -1.084672 -3.911064 2.731007
H -4.553703 -5.003873 -5.736090
H -2.936829 -4.612749 -6.427884
H -3.086446 -5.821178 -5.109535
C 1.011097 -3.491119 -0.714917
C 1.629445 -2.800753 -1.937039
H 2.729168 -2.828162 -1.932187
H 1.465720 -2.726401 -4.140142
H -0.811340 -1.760879 -5.052514
H -0.046658 -0.207568 -5.539307
H 1.459422 -1.660481 -1.778919
H -1.842718 -0.310221 -5.253345
H 1.462878 -3.125204 0.213684
H 1.100796 -4.582538 -0.783289
C -0.127315 -3.960932 -3.378317
C 1.021191 -3.187561 -3.253148
H -0.557043 -4.138700 -4.363005
H -0.443170 -4.676408 -2.617735
H -0.088969 -3.291930 -0.573438

Spin state: quintet

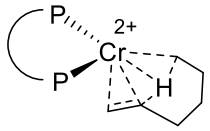
E = -10913.82 kcal mol-1
H = -10488.05 kcal mol-1
TS = -78.44 kcal mol-1
G (298.15 K) = -10566.49 kcal mol-1

Cr -0.578084 -1.766224 -2.563706
P -2.940251 -2.271346 -2.192640
N -3.166696 -0.893669 -1.187247
P -1.577891 -0.364762 -0.877115
C -4.393519 -0.474532 -0.484711
H -5.241766 -1.013344 -0.917961
H -4.556325 0.603575 -0.608417
H -4.317391 -0.720942 0.582727
C -3.958663 -1.973330 -3.658403
C -4.462715 -0.688015 -3.918831
C -5.269534 -0.457039 -5.030935
C -5.568648 -1.515672 -5.894829
C -5.050843 -2.794579 -5.673903

C -4.225731 -3.027039 -4.567299
H -4.229640 0.128303 -3.234796
H -5.669893 0.538411 -5.219412
H -6.207348 -1.346023 -6.762338
H -5.284105 -3.597678 -6.370489
C -3.435903 -3.802461 -1.365773
C -4.793244 -4.157525 -1.165544
C -5.099790 -5.390142 -0.570183
C -4.072874 -6.254496 -0.182527
C -2.730539 -5.908978 -0.367602
C -2.424292 -4.684061 -0.956431
H -7.398582 -3.724819 -0.397124
H -6.135400 -5.683191 -0.408363
H -4.331247 -7.209635 0.276067
H -1.935932 -6.584823 -0.053405
H -1.380262 -4.398779 -1.094210
C -1.277832 1.238932 -1.682632
C -0.260932 1.304529 -2.654668
C -0.010997 2.479548 -3.358372
C -0.794345 3.608001 -3.089124
C -1.809882 3.568486 -2.130597
C -2.045985 2.388186 -1.427231
H 0.770803 2.538761 -4.112895
H -0.600124 4.528187 -3.640904
H -2.407786 4.456436 -1.926421
H -2.816002 2.356882 -0.655538
C -1.295349 -0.137365 0.885264
C -1.675239 -1.156842 1.801618
C -1.418492 -0.985193 3.167381
C -0.764749 0.165196 3.613508
C -0.363556 1.162583 2.718341
C -0.626900 1.009090 1.360877
H -3.568066 -2.750509 2.848033
H -1.712226 -1.748575 3.885145
H -0.563124 0.279077 4.679208
H 0.145562 2.055909 3.077797
H -0.322079 1.786385 0.660763
O -5.720029 -3.248915 -1.577436
C -7.121074 -3.591002 -1.452363
H -7.663985 -2.740205 -1.873271
H -7.353939 -4.499188 -2.025663
O -3.624271 -4.220089 -4.280676
C -4.002426 -5.379977 -5.057869
O 0.485826 0.115873 -2.886527
C 1.796107 0.276501 -3.523190
O -2.280378 -2.253620 1.260588
C -2.852954 -3.229436 2.164710
H -3.370678 -3.946647 1.522476
H -2.067327 -3.743719 2.735619
H -5.086612 -5.550328 -5.000515
H -3.691533 -5.270268 -6.106601
H -3.472039 -6.220262 -4.600622
C 1.522496 -4.544448 -1.886687
C 1.962671 -3.700340 -3.084164
H 2.661065 -4.277188 -3.718816
H 1.187047 -2.514490 -4.788047
H 2.313301 -0.677637 -3.389224
H 2.353327 1.073798 -3.017408
H 2.568617 -2.842601 -2.743678
H 1.674369 0.494139 -4.591176
H 2.394855 -4.865355 -1.305330
H 0.980040 -5.446797 -2.198143
C -0.408916 -3.675345 -4.048806
C 0.871408 -3.215819 -4.004701
H -1.093523 -3.373471 -4.845076
H -0.762182 -4.476529 -3.396411
H 0.872453 -3.972685 -1.202111

Geometry:

‡



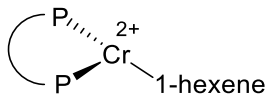
Spin state: triplet

E = -11643.53 kcal mol-1
H = -11184.14 kcal mol-1
TS = -79.61 kcal mol-1
G (298.15 K) = -11263.74 kcal mol-1

H -1.936203 7.448281 14.317935
C -0.808970 4.025442 9.681126
C -0.856185 7.311033 14.355893
C 1.354995 8.166565 14.918335
C 1.106857 5.948634 13.946039
C -0.283519 6.132714 13.879390
H -0.478335 9.232718 15.265216
H -0.101471 4.854964 9.692293
O -1.150287 0.748602 11.262303
H -3.029265 -0.117308 11.659255
H 5.317198 2.009154 17.096996
C -0.186775 2.633327 13.985004
O 3.277563 6.756368 14.322857
C 1.747147 1.182006 11.433700
C -0.535440 2.875789 10.440040
C -1.463430 1.801942 10.456664
C 3.078480 -1.276064 11.478643
H 3.587951 -2.240294 11.492532
C -2.625030 1.894096 9.679438
Cr 2.902310 4.232982 11.112817
H -3.348967 1.081420 9.669863
C 1.934563 6.992717 14.424218
C -0.034603 8.311920 14.885071
C 2.669374 3.779537 15.913198
H 5.691004 3.200475 8.410867
P 0.986094 2.821221 11.393862
H 3.398718 -0.895671 13.587566
C 3.497329 3.140433 16.835380
H 5.937266 2.032897 14.728852
C 5.017212 2.525211 15.032602
H 1.759993 4.285544 16.241428
H 0.798596 -0.714765 8.032633
H -3.780126 3.096433 8.325446
C -2.867959 3.041684 8.920552
C 1.351961 0.224473 7.894673
H 1.973666 8.971886 15.309888
H 2.375767 0.014164 7.553200

H 0.837866 0.853528 7.162927
N 0.677441 3.312085 12.995122
P 1.906247 4.475784 13.291724
C 3.001808 3.788890 14.550662
C 4.661342 2.513696 16.386981
H -0.912763 5.354466 13.447378
H 3.238836 3.132480 17.893970
H -2.181910 5.010699 8.336611
C -1.972976 4.116167 8.922127
H 2.632963 -1.415626 9.375681
C 2.536869 -0.812939 10.276772
C 4.189922 3.174854 14.114550
O 4.485708 3.258485 12.737749
C 2.978090 -0.522502 12.654175
O 1.363489 0.996249 9.119436
C 1.883379 0.424628 10.240325
H 2.231332 1.287771 13.541345
C 2.315042 0.701654 12.627207
H 5.705218 4.288971 9.789412
H 5.527058 5.508267 7.585045
H 3.989845 4.711014 7.256958
C 3.920038 6.184650 8.864393
C 4.638229 5.081417 8.067819
C 2.320371 6.201467 10.889711
C 2.614400 5.748029 9.545135
H 3.045646 6.854673 11.389159
H 1.291507 6.411917 11.187914
H 3.669850 7.029158 8.202464
H 4.607191 6.587666 9.626472
H 1.760502 5.645444 8.862811
H 2.914385 4.354790 9.465112
C 5.062401 3.907986 8.975779
C 3.856374 3.153381 9.537140
H 4.102858 2.430897 10.348759
H 3.302591 2.604059 8.763836
C -2.038094 -0.395745 11.274347
H -2.128712 -0.830000 10.268947
H -1.567055 -1.116679 11.948087
H -0.874990 3.350668 14.446785
C 4.183464 7.698987 14.945566
H 5.181834 7.271563 14.816451
H 3.958859 7.802919 16.016183
H 4.131648 8.678055 14.448561
C 5.718285 2.586262 12.336198
H 5.853070 2.788534 11.272897
H 5.625041 1.505011 12.501917
H 6.568554 3.001757 12.890028
H -0.763361 1.857493 13.468772
H 0.422116 2.164412 14.770566

Geometry:



Spin state: singlet

E = -11651.42 kcal mol-1
H = -11189.55 kcal mol-1
TS = -77.78 kcal mol-1
G (298.15 K) = -11267.33 kcal mol-1

Cr -0.446550 -1.882676 -2.225291
P -2.753592 -2.286725 -2.074749
N -3.059336 -0.994550 -0.988953
P -1.488560 -0.375144 -0.745563
C -4.297612 -0.612448 -0.295675
H -5.125884 -0.557172 -1.010204
H -4.154441 0.371520 0.167908
H -4.534417 -1.345955 0.486601
C -3.575991 -1.834743 -3.627704
C -3.932450 -0.494046 -3.849828
C -4.495494 -0.097691 -5.061890
C -4.698952 -1.049340 -6.067392
C -4.348272 -2.387335 -5.872182
C -3.782745 -2.790664 -4.654183
H -3.767279 0.240003 -3.061148
H -4.783233 0.941620 -5.218141
H -5.141360 -0.751461 -7.018636
H -4.521400 -3.109509 -6.667706
C -3.430524 -3.822132 -1.392420
C -4.831433 -4.018714 -1.299138
C -5.326173 -5.212068 -0.752814
C -4.440969 -6.199445 -0.315804
C -3.057640 -6.019672 -0.411270
C -2.564651 -4.832428 -0.949588
H -7.412604 -3.280409 -0.709747
H -6.398555 -5.378771 -0.670562
H -4.842400 -7.123300 0.102432
H -2.374378 -6.798807 -0.074832
H -1.486978 -4.694682 -1.032566
C -1.410018 1.199156 -1.645460
C -1.016251 1.101806 -2.993019
C -1.046802 2.209306 -3.835097
C -1.483228 3.436492 -3.321559
C -1.896915 3.554780 -1.993741
C -1.864461 2.437056 -1.160695
H -0.738954 2.150888 -4.875799
H -1.498545 4.305991 -3.978966
H -2.246850 4.512718 -1.609670
H -2.198359 2.518542 -0.126061
C -1.161157 -0.113561 1.005811
C -1.505387 -1.144196 1.923983
C -1.198946 -0.990961 3.281534
C -0.517758 0.148196 3.716625
C -0.125033 1.141851 2.814760
C -0.443415 1.007929 1.465815
H -3.323045 -2.852152 2.989587
H -1.474740 -1.759388 4.001101
H -0.280484 0.250848 4.776011
H 0.422955 2.017201 3.161097
H -0.127056 1.776991 0.761811
O -5.607940 -3.000208 -1.760100
C -7.044774 -3.168483 -1.739692
H -7.448423 -2.251995 -2.179415
H -7.344887 -4.033846 -2.347002
O -3.397734 -4.064958 -4.363364
C -3.644270 -5.100728 -5.343268
O -0.595243 -0.183816 -3.467069

C -0.621596 -0.342608 -4.933545
O -2.100697 -2.252913 1.385988
C -2.591628 -3.273936 2.286121
H -3.073508 -4.013566 1.640098
H -1.765438 -3.744847 2.838039
H -4.717376 -5.180376 -5.566364
H -3.077167 -4.911675 -6.266344
H -3.295122 -6.026328 -4.877265
C 1.532263 -4.910509 -1.611010
C 1.965811 -4.026741 -2.791411
C 1.497690 -4.163919 -0.271526
C 0.720677 -2.851524 -0.302033
H 0.591282 -2.394006 0.686723
H -0.341468 -3.050994 -0.638034
H 1.059131 -4.810256 0.503080
H 2.524506 -3.942028 0.058772
H 2.228878 -5.754258 -1.519430
H 0.548943 -5.363020 -1.816804
C -0.418560 -3.566738 -3.682907
C 0.893220 -3.172975 -3.443603
H -0.996796 -3.183730 -4.524795
H -0.806411 -4.507257 -3.288551
H 2.363370 -4.671289 -3.594110
H 2.811946 -3.390048 -2.487531
H 1.241319 -2.086691 -0.925495
H 1.302617 -2.367769 -4.073307
H -0.414002 -1.393686 -5.133109
H 0.163178 0.278053 -5.378242
H -1.620878 -0.080441 -5.300434

Spin state: triplet

E = -11662.72 kcal mol-1
H = -11200.82 kcal mol-1
TS = -77.73 kcal mol-1
G (298.15 K) = -11278.55 kcal mol-1

Cr -0.437965 -1.887709 -2.227135
P -2.755547 -2.292060 -2.069369
N -3.052497 -1.002522 -0.978703
P -1.484177 -0.372504 -0.739604
C -4.289629 -0.623085 -0.280653
H -5.118464 -0.558072 -0.993725
H -4.142709 0.355687 0.192575
H -4.527814 -1.363325 0.494735
C -3.572889 -1.832083 -3.621224
C -3.926580 -0.489926 -3.839722
C -4.484272 -0.088361 -5.052316
C -4.685522 -1.036162 -6.062181
C -4.338208 -2.375441 -5.870618
C -3.778126 -2.784480 -4.651935
H -3.763850 0.240921 -3.047646
H -4.770044 0.951892 -5.205761
H -5.123054 -0.733817 -7.014280
H -4.508893 -3.094318 -6.669657
C -3.435277 -3.827482 -1.391476
C -4.836967 -4.019165 -1.298303
C -5.335570 -5.212670 -0.755927
C -4.453638 -6.204979 -0.323671
C -3.069677 -6.030536 -0.420562
C -2.572449 -4.843204 -0.954719
H -7.416621 -3.274260 -0.708704
H -6.408502 -5.375501 -0.673010
H -4.858193 -7.128929 0.091334
H -2.389201 -6.814329 -0.089369
H -1.494362 -4.710961 -1.041360
C -1.414188 1.195617 -1.650146
C -1.018440 1.095843 -2.997065
C -1.057867 2.200372 -3.842631
C -1.505066 3.426022 -3.334600
C -1.921712 3.546020 -2.008101
C -1.880915 2.431463 -1.171358
H -0.748543 2.141185 -4.882758
H -1.526180 4.292658 -3.995640
H -2.280027 4.502385 -1.627858
H -2.217398 2.513797 -0.137633
C -1.162809 -0.101456 1.011064
C -1.497210 -1.133838 1.931287
C -1.194740 -0.974202 3.288875
C -0.527366 0.173658 3.722515
C -0.145340 1.170161 2.819164
C -0.459429 1.029550 1.469919
H -3.290601 -2.866915 3.001762
H -1.462883 -1.744162 4.009684
H -0.293368 0.281544 4.782107
H 0.391572 2.052721 3.164536
H -0.151206 1.800884 0.764829
O -5.609763 -2.996475 -1.755975
C -7.047262 -3.160260 -1.737852
H -7.447406 -2.241083 -2.175160
H -7.349306 -4.022701 -2.348341
O -3.396904 -4.059868 -4.364454
C -3.634070 -5.090511 -5.352207
O -0.585786 -0.187514 -3.469918
C -0.607049 -0.345224 -4.936570
O -2.080345 -2.250219 1.395460
C -2.553839 -3.277739 2.297345
H -3.025682 -4.025107 1.652720
H -1.719371 -3.735075 2.848304
H -4.705343 -5.170878 -5.583623
H -3.060225 -4.894841 -6.269665
H -3.286387 -6.017940 -4.888820
C 1.520388 -4.923351 -1.631708
C 1.966278 -4.024471 -2.796322
C 1.471851 -4.200101 -0.279596
C 0.709081 -2.878688 -0.297764
H 0.573521 -2.434842 0.696308
H -0.353258 -3.065826 -0.642283
H 1.017450 -4.856356 0.477211
H 2.495337 -3.991444 0.069036
H 2.215361 -5.769114 -1.545487
H 0.539430 -5.373080 -1.854217
C -0.415200 -3.554585 -3.692154
C 0.900659 -3.161991 -3.451195
H -0.987737 -3.176972 -4.540416
H -0.803775 -4.495562 -3.299772
H 2.371865 -4.661197 -3.601359
H 2.810544 -3.392846 -2.476507
H 1.243450 -2.113118 -0.905190
H 1.318741 -2.371330 -4.092493

H -0.385672 -1.393164 -5.136853
H 0.171252 0.285030 -5.378938
H -1.608504 -0.094226 -5.305380

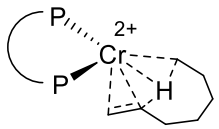
Spin state: quintet

E = -11674.83 kcal mol-1
H = -11213.25 kcal mol-1
TS = -78.03 kcal mol-1
G (298.15 K) = -11291.28 kcal mol-1

Cr -0.541123 -2.316678 -1.926359
P -2.969762 -2.381122 -1.912910
N -3.136945 -1.024288 -0.895568
P -1.528534 -0.535839 -0.597521
C -4.363471 -0.422764 -0.349356
H -5.227524 -0.839562 -0.878880
H -4.347715 0.666672 -0.494327
H -4.445988 -0.652597 0.721226
C -3.538515 -1.884291 -3.562332
C -3.935856 -0.569340 -3.837226
C -4.300673 -0.201224 -5.133289
C -4.256046 -1.151336 -6.158552
C -3.835038 -2.462248 -5.909537
C -3.462980 -2.827671 -4.611162
H -3.957207 0.166508 -3.033582
H -4.627101 0.817610 -5.340169
H -4.547921 -0.873193 -7.171967
H -3.800764 -3.182364 -6.725309
C -3.926134 -3.773570 -1.277121
C -5.325414 -3.886821 -1.477926
C -5.997784 -5.018378 -0.993135
C -5.293814 -6.005263 -0.300524
C -3.918376 -5.888559 -0.072272
C -3.244016 -4.773104 -0.563890
H -7.931814 -2.994026 -1.500594
H -7.069595 -5.130986 -1.144326
H -5.833924 -6.877738 0.068706
H -3.381256 -6.660168 0.478376
H -2.172736 -4.663257 -0.385079
C -1.340530 1.039258 -1.483052
C -0.964463 0.974212 -2.843818
C -0.995691 2.119562 -3.639967
C -1.405751 3.334683 -3.081588
C -1.792286 3.416402 -1.742395
C -1.763320 2.270076 -0.949439
H -0.704373 2.086560 -4.687422
H -1.421345 4.225834 -3.709531
H -2.118592 4.365788 -1.318790
H -2.075000 2.323704 0.094073
C -1.214609 -0.264987 1.156224
C -1.718312 -1.183263 2.118130
C -1.426681 -0.987946 3.474261
C -0.601741 0.068151 3.866048
C -0.051399 0.941296 2.922700
C -0.357392 0.772941 1.575328
H -3.763658 -2.564317 3.248874
H -1.828199 -1.662281 4.227872
H -0.379215 0.201206 4.925256
H 0.602470 1.754182 3.236394
H 0.069037 1.453890 0.839086
O -5.925597 -2.851207 -2.127806
C -7.339033 -2.952820 -2.425254
H -7.581852 -2.042538 -2.980379
H -7.544104 -3.833658 -3.049661
O -2.985890 -4.062437 -4.246501
C -3.075472 -5.138336 -5.210489
O -0.579246 -0.277308 -3.340640
C -0.542408 -0.419395 -4.790357
O -2.460195 -2.222350 1.631702
C -3.085937 -3.116391 2.582375
H -3.655627 -3.824580 1.973848
H -2.330809 -3.655684 3.171795
H -4.113504 -5.277093 -5.542204
H -2.424237 -4.948838 -6.076362
H -2.734625 -6.033206 -4.682026
C 2.831829 -3.770328 -2.760706
C 1.811820 -3.592228 -3.901390
C 3.118652 -2.501717 -1.941644
C 1.889085 -1.827721 -1.321772
H 2.151771 -1.016922 -0.630024
H 1.298652 -2.554806 -0.717514
H 3.821313 -2.754682 -1.135097
H 3.632652 -1.762912 -2.575367
H 3.782100 -4.104791 -3.197747
H 2.519895 -4.587457 -2.092384
C -0.159188 -4.590941 -2.572946
C 0.361476 -3.893979 -3.621932
H -1.201099 -4.914740 -2.603420
H 0.469045 -4.997686 -1.776647
H 2.073276 -4.270059 -4.735385
H 1.900592 -2.585491 -4.346290
H 1.293169 -1.324145 -2.119546
H -0.339040 -3.651425 -4.432789
H -0.368000 -1.482019 -4.978580
H 0.280590 0.168704 -5.215527
H -1.508989 -0.126570 -5.220364

Geometry:

‡



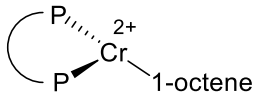
Spin state: triplet

E = -12414.29 kcal mol-1
H = -11914.52 kcal mol-1
TS = -80.10 kcal mol-1
G (298.15 K) = -11994.62 kcal mol-1

Cr -1.185938 -2.328440 -1.451298
P -3.531307 -2.393687 -2.011531
N -3.835701 -0.757363 -1.566125
P -2.289291 -0.238927 -1.082983
C -5.139270 -0.210157 -1.143359
H -5.358526 -0.489494 -0.103321
H -5.925896 -0.607211 -1.795531

H -5.127748 0.882852 -1.235250
C -3.836756 -2.526890 -3.792501
C -4.313974 -1.453675 -4.554600
C -4.454176 -1.581310 -5.937366
C -4.104010 -2.783716 -6.557340
C -3.610691 -3.862585 -5.815661
C -3.467947 -3.731140 -4.431183
H -4.579371 -0.519420 -4.061434
H -4.837696 -0.749593 -6.527236
H -4.211099 -2.889424 -7.637238
C -4.752874 -3.425204 -1.176595
C -4.773867 -3.461579 0.239275
C -5.716556 -4.258453 0.899319
C -6.630463 -5.008803 0.155033
C -6.623239 -4.975326 -1.242244
C -5.684687 -4.187478 -1.903107
H -3.691105 -3.586138 2.763961
H -5.749917 -4.300389 1.985859
H -7.360552 -5.625108 0.680779
H -7.348695 -5.554872 -1.812171
H -5.679371 -4.146518 -2.991938
C -1.905022 1.282529 -1.966373
C -0.644222 1.877263 -1.719351
C -0.292782 3.062606 -2.372115
C -1.185012 3.630633 -3.286601
C -2.417405 3.030914 -3.565682
C -2.772140 1.852076 -2.911493
H 0.667319 3.540284 -2.185609
H -0.903576 4.552999 -3.795506
H -3.098600 3.483430 -4.285289
H -3.727206 1.374270 -3.125265
C -2.182473 0.114760 0.686471
C -1.239330 -0.612209 1.434137
C -1.038249 -0.318339 2.784413
C -1.808695 0.683598 3.388072
C -2.761970 1.398549 2.661462
C -2.933068 1.123819 1.304364
H 0.076667 -2.839009 2.365972
H -0.306040 -0.852726 3.384770
H -1.651146 0.902422 4.444540
H -3.352540 2.177709 3.142287
H -3.639514 1.709193 0.714719
O -3.844500 -2.675678 0.871181
C -3.912833 -2.607795 2.314315
H -3.152960 -1.880510 2.608844
H -4.902027 -2.257429 2.641103
O -2.972206 -4.697306 -3.590508
C -2.796012 -6.029032 -4.125541
O 0.155894 1.187735 -0.847221
C 1.388736 1.810113 -0.417669
O -0.531332 -1.618053 0.757219
C 0.512714 -2.282226 1.526213
H 1.001336 -2.977707 0.841679
H 1.241860 -1.545035 1.885398
H -3.725819 -6.390529 -4.586045
H -1.976381 -6.053368 -4.858412
H -2.548661 -6.661852 -3.267428
C 1.656607 -3.705379 -3.847896
C 1.793122 -2.198022 -3.568088
C 1.969429 -4.679570 -2.696614
C 1.091345 -4.559915 -1.439859
H 1.883807 -5.705307 -3.088723
H 3.021735 -4.559287 -2.397830
H 2.353613 -3.944631 -4.664261
H 0.661413 -3.919762 -4.273344
C -0.775853 -1.722116 -3.397922
C 0.618493 -1.460396 -2.874932
H -1.334344 -0.827381 -3.691189
H -0.861659 -2.482098 -4.181022
H 1.924176 -1.684322 -4.532256
H 2.714174 -2.010126 -2.994575
H 0.696810 -1.707434 -1.754052
H 0.816951 -0.380119 -2.836102
C -1.396471 -4.235093 -0.682029
C -0.406886 -4.555913 -1.757702
H -2.364217 -4.735606 -0.752387
H -1.029318 -4.173424 0.347946
H -3.339257 -4.787431 -6.321429
H -0.568202 -3.809757 -2.610442
H -0.705543 -5.455466 -2.318479
H 1.363836 -3.635896 -0.903056
H 1.311659 -5.384423 -0.745289
H 1.812653 1.132413 0.329108
H 1.192316 2.789340 0.040217
H 2.088070 1.917500 -1.259243

Geometry:



Spin state: singlet

E = -12410.44 kcal mol-1
H = -11909.34 kcal mol-1
TS = -80.19 kcal mol-1
G (298.15 K) = -11989.53 kcal mol-1

Cr -0.427834 -1.876293 -2.231350
P -2.748743 -2.289816 -2.057695
N -3.052929 -1.027770 -0.937280
P -1.488168 -0.378845 -0.769114
C -4.276648 -0.694769 -0.197620
H -5.087780 -0.433943 -0.887660
H -4.068326 0.158121 0.460146
H -4.582599 -1.548888 0.420518
C -3.577818 -1.811374 -3.603999
C -3.920851 -0.465213 -3.808209
C -4.465933 -0.042654 -5.020295
C -4.668119 -0.974790 -6.043279
C -4.337842 -2.320510 -5.863356
C -3.792402 -2.748944 -4.645060
H -3.762308 0.254420 -3.005361
H -4.740675 1.002264 -5.161770
H -5.095072 -0.656782 -6.995071
H -4.513034 -3.029019 -6.670674
C -3.449152 -3.822958 -1.395357
C -4.852456 -4.017683 -1.341610
C -5.363533 -5.217213 -0.824521

C -4.491667 -6.208923 -0.371008
C -3.106020 -6.027006 -0.418902
C -2.597112 -4.835136 -0.932167
H -7.448654 -3.279641 -0.810950
H -6.437990 -5.383899 -0.775737
H -4.906074 -7.137242 0.024060
H -2.433811 -6.808816 -0.066529
H -1.517915 -4.689861 -0.977462
C -1.454915 1.185569 -1.694169
C -1.052929 1.093164 -3.039931
C -1.135242 2.191107 -3.892712
C -1.636425 3.399145 -3.395675
C -2.065519 3.509275 -2.071821
C -1.979468 2.403317 -1.227740
H -0.825018 2.136584 -4.932716
H -1.693629 4.259136 -4.063316
H -2.470217 4.450706 -1.700956
H -2.329405 2.477373 -0.197819
C -1.120765 -0.067700 0.967600
C -1.355863 -1.113922 1.901043
C -0.985724 -0.943722 3.240746
C -0.358335 0.237223 3.644091
C -0.085700 1.257344 2.727748
C -0.463032 1.101345 1.396106
H -2.965809 -2.961949 3.076297
H -1.174563 -1.727784 3.971198
H -0.072583 0.354801 4.689898
H 0.416418 2.169082 3.048923
H -0.230475 1.887027 0.678487
O -5.614457 -2.989696 -1.805615
C -7.051177 -3.154418 -1.828294
H -7.439638 -2.230835 -2.266742
H -7.336603 -4.010611 -2.455623
O -3.434899 -4.035147 -4.366920
C -3.674993 -5.048948 -5.369672
O -0.578979 -0.173157 -3.500529
C -0.558943 -0.337054 -4.963444
O -1.919189 -2.252877 1.393850
C -2.260976 -3.317101 2.311526
H -2.735489 -4.083472 1.691763
H -1.360574 -3.728569 2.791225
H -4.744839 -5.113045 -5.613098
H -3.090055 -4.849350 -6.279419
H -3.344364 -5.987178 -4.915460
C 1.391185 -5.097598 -1.723363
C 1.848772 -4.295299 -2.951466
C 1.486993 -4.357460 -0.379673
C 0.832007 -2.966552 -0.344037
H 0.511193 -2.707226 0.674375
H -0.201592 -3.117886 -0.819984
H 1.029466 -4.983235 0.399772
H 2.544115 -4.235278 -0.094783
H 2.001591 -6.008142 -1.652201
H 0.358979 -5.451667 -1.875881
C -0.482740 -3.552945 -3.722695
C 0.866542 -3.294616 -3.535328
H -1.053190 -3.088485 -4.528536
H -0.939925 -4.466963 -3.341186
H 2.060243 -5.004238 -3.770850
H 2.813855 -3.809804 -2.746427
C 1.733192 -1.827787 -0.874869
H 1.335335 -2.520689 -4.157913
H -0.254028 -1.366026 -5.153549
H 0.180993 0.343748 -5.396833
H -1.568249 -0.159176 -5.354379
C 2.384617 -1.041189 0.271472
H 1.192766 -1.034078 -1.480298
H 2.506380 -2.232167 -1.534094
H 2.985089 -1.726261 0.886144
H 1.629546 -0.573712 0.915563
H 3.051355 -0.260649 -0.114567

Spin state: triplet

E = -12417.55 kcal mol-1
H = -11919.78 kcal mol-1
TS = -79.92 kcal mol-1
G (298.15 K) = -11999.70 kcal mol-1

Cr -0.388388 -1.905717 -2.240518
P -2.722590 -2.279356 -2.115812
N -3.024335 -0.921910 -1.120395
P -1.453885 -0.381516 -0.711105
C -4.288141 -0.371881 -0.606845
H -5.073873 -0.497032 -1.357896
H -4.154576 0.699092 -0.405360
H -4.578786 -0.887069 0.317704
C -3.583072 -1.925149 -3.670812
C -3.882926 -0.591152 -3.997233
C -4.492652 -0.272831 -5.208756
C -4.798925 -1.297206 -6.112346
C -4.498410 -2.628327 -5.818285
C -3.883377 -2.953986 -4.600675
H -3.635165 0.200361 -3.288898
H -4.737452 0.762739 -5.444032
H -5.277764 -1.059723 -7.062936
H -4.741813 -3.406260 -6.539424
C -3.355703 -3.798114 -1.349582
C -4.746785 -3.979997 -1.148962
C -5.210021 -5.152458 -0.534905
C -4.302585 -6.137839 -0.138190
C -2.929819 -5.975219 -0.344366
C -2.468848 -4.806860 -0.949543
H -7.261091 -3.193944 -0.383827
H -6.274812 -5.306440 -0.370366
H -4.678899 -7.046378 0.333237
H -2.229492 -6.753475 -0.043014
H -1.400181 -4.690166 -1.129378
C -1.293556 1.214444 -1.570204
C -0.882891 1.142442 -2.912690
C -0.806972 2.282432 -3.708032
C -1.171033 3.517210 -3.157538
C -1.620106 3.609701 -1.839976
C -1.680827 2.461255 -1.050927
H -0.465944 2.242581 -4.739317
H -1.103471 4.410767 -3.778304
H -1.920663 4.572144 -1.426626
H -2.033846 2.526954 -0.021924
C -1.354188 -0.086021 1.068380
C -1.949870 -1.015448 1.965913

C -1.840655 -0.810718 3.346458
C -1.093773 0.263862 3.834022
C -0.441180 1.140974 2.962759
C -0.570977 0.962850 1.587745
H -3.981022 -2.625643 2.849428
H -2.314557 -1.497107 4.045135
H -1.010345 0.404941 4.912122
H 0.160178 1.961659 3.351825
H -0.055331 1.642178 0.909675
O -5.547759 -2.970277 -1.587777
C -6.979281 -3.117624 -1.443778
H -7.408564 -2.209256 -1.876264
H -7.339063 -3.996013 -1.997671
O -3.525231 -4.213642 -4.229279
C -3.887068 -5.317744 -5.090992
O -0.567763 -0.151737 -3.441765
C -0.638655 -0.234678 -4.913743
O -2.555006 -2.098582 1.393694
C -3.175038 -3.079539 2.255513
H -3.588538 -3.831796 1.576905
H -2.431797 -3.544461 2.918530
H -4.975322 -5.357381 -5.238755
H -3.373778 -5.244449 -6.060576
H -3.553382 -6.214822 -4.562342
C 1.714144 -4.896635 -2.160901
C 2.013588 -3.874193 -3.264221
C 1.779240 -4.308274 -0.750601
C 0.975351 -3.027981 -0.501351
C 1.037739 -2.554329 0.961261
H -0.111536 -3.237609 -0.771351
H 1.439279 -5.060832 -0.022682
H 2.826472 -4.085639 -0.489411
H 2.441393 -5.717392 -2.223544
H 0.731082 -5.364711 -2.329663
C -0.468581 -3.442150 -3.828884
C 0.853302 -3.007228 -3.713314
H -1.143949 -3.046723 -4.588927
H -0.771320 -4.424424 -3.461552
H 2.354210 -4.408872 -4.167851
H 2.863595 -3.239525 -2.966180
H 1.381850 -2.206534 -1.150165
H 1.166617 -2.164629 -4.344156
H -0.664799 -1.293076 -5.168078
H 0.250892 0.238051 -5.344043
H -1.565187 0.241088 -5.251368
C 2.205808 -1.595969 1.211418
H 1.124109 -3.442133 1.604405
H 0.103467 -2.061223 1.241950
H 3.170243 -2.039559 0.928510
H 2.261738 -1.324569 2.273009
H 2.073583 -0.665568 0.637763

Spin state: quintet

E = -12426.80 kcal mol-1
H = -11928.96 kcal mol-1
TS = -82.44 kcal mol-1
G (298.15 K) = -12011.40 kcal mol-1

Cr -0.454131 -2.062715 -2.101593
P -2.893486 -2.291748 -2.049667
N -3.116442 -1.003111 -0.950427
P -1.545945 -0.371903 -0.761448
C -4.359353 -0.500693 -0.344385
H -5.206591 -1.036247 -0.786402
H -4.476750 0.574412 -0.541506
H -4.341657 -0.677835 0.739353
C -3.658792 -1.774276 -3.613791
C -4.001965 -0.428766 -3.814276
C -4.516950 -0.000037 -5.037949
C -4.686547 -0.923604 -6.073408
C -4.339784 -2.267029 -5.900953
C -3.817503 -2.697614 -4.674983
H -3.865512 0.288145 -3.005384
H -4.793493 1.044587 -5.177775
H -5.095175 -0.600838 -7.031616
H -4.480258 -2.968143 -6.721556
C -3.651896 -3.803656 -1.413576
C -5.045881 -4.048338 -1.488034
C -5.554556 -5.270358 -1.024155
C -4.692507 -6.225352 -0.481335
C -3.317756 -5.985615 -0.384251
C -2.809107 -4.776567 -0.854280
H -7.708892 -3.420627 -1.190597
H -6.620976 -5.480985 -1.078333
H -5.106619 -7.169613 -0.125808
H -2.654968 -6.734542 0.048172
H -1.738788 -4.570991 -0.778551
C -1.511445 1.207976 -1.651393
C -1.104643 1.179861 -3.005432
C -1.245314 2.314087 -3.806242
C -1.794801 3.478476 -3.261291
C -2.214366 3.521381 -1.929540
C -2.076418 2.387275 -1.131106
H -0.931323 2.309428 -4.847830
H -1.893707 4.361734 -3.893089
H -2.649415 4.431324 -1.516968
H -2.412744 2.409271 -0.093756
C -1.116728 -0.098521 0.965817
C -1.334403 -1.149700 1.896983
C -0.916672 -0.996319 3.224336
C -0.249181 0.167734 3.612850
C 0.019013 1.186157 2.693275
C -0.410704 1.049685 1.375531
H -2.912122 -2.979632 3.126411
H -1.097215 -1.780765 3.956314
H 0.072384 0.272592 4.649620
H 0.553470 2.083529 3.002413
H -0.196602 1.839144 0.655987
O -5.804102 -3.044341 -2.008324
C -7.226037 -3.266268 -2.165981
H -7.608956 -2.352613 -2.628971
H -7.416097 -4.124591 -2.825564
O -3.422083 -3.978984 -4.403873
C -3.662900 -4.996123 -5.403590
O -0.580191 -0.021803 -3.491671
C -0.590793 -0.198235 -4.938394
O -1.935799 -2.272792 1.400555
C -2.250806 -3.339399 2.325971
H -2.769646 -4.092708 1.726752

H -1.333904 -3.767974 2.756575
H -4.733827 -5.064544 -5.640627
H -3.085935 -4.796091 -6.318467
H -3.325500 -5.932628 -4.950578
C 1.564394 -4.912021 -1.320130
C 1.994793 -4.361004 -2.701261
C 2.018623 -4.083406 -0.105491
C 1.369255 -2.703143 0.086787
H 1.571498 -2.353497 1.111757
H 0.262898 -2.821619 0.064764
H 1.799349 -4.674984 0.795787
H 3.114266 -3.979324 -0.125496
H 1.980998 -5.921471 -1.205132
H 0.470496 -5.049167 -1.283755
C -0.365344 -3.948998 -3.614318
C 0.961062 -3.658628 -3.544216
H -0.998756 -3.527299 -4.397217
H -0.819738 -4.746517 -3.022259
H 2.342737 -5.195735 -3.337008
H 2.877710 -3.714988 -2.594895
C 1.816049 -1.558326 -0.848604
H 1.362456 -2.945179 -4.276162
H -0.316956 -1.244026 -5.110744
H 0.151355 0.453601 -5.415565
H -1.599789 -0.012024 -5.329917
C 3.321757 -1.267612 -0.831388
H 1.286260 -0.637412 -0.558017
H 1.578695 -1.758145 -1.932812
H 3.911772 -2.115012 -1.201707
H 3.642214 -1.061533 0.199348
H 3.563288 -0.391277 -1.445253

7. References

1 S. C. Eady, T. Breault, L. Thompson and N. Lehnert, *Dalton Trans.*, 2016, **45**, 1138–1151.

2 E. J. M. De Boer, H. Van Der Heijden, A. O. Quoc, J. P. Smit, A. Van Zon. Catalytic Oligomerization of Olefin. US patent WO2007057455A1. May 24, 2007.

3 S. A. Bartlett, J. Moulin, M. Tromp, G. Reid, A. J. Dent, G. Cibin, D. S. McGuinness and J. Evans, *Catal. Sci. Technol.*, 2016, **6**, 6237–6246.

4 T. Agapie, J. A. Labinger and J. E. Bercaw, *J. Am. Chem. Soc.*, 2007, **129**, 14281–14295.

5 S. Stoll and A. Schweiger, *J. Magn. Reson.*, 2006, **178**, 42–55.

6 B. Ravel, M. Newville and IUCr, *J. Synchrotron Radiat.*, 2005, **12**, 537–541.

7 G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders and T. Ziegler, *J. Comput. Chem.*, 2001, **22**, 931–967.

8 C. Fonseca Guerra, J. G. Snijders, G. te Velde and E. J. Baerends, *Theor. Chem. Acc.*, 1998, **99**, 391–403.

9 D. S. McGuinness, B. Chan, G. J. P. Britovsek and B. F. Yates, *Aust. J. Chem.*, 2014, **67**, 1481.

10 B. Venderbosch, J. P. H. Oudsen, L. A. Wolzak, D. J. Martin, T. J. Korstanje and M. Tromp, *ACS Catal.*, 2019, **9**, 1197–1210.

11 S. Teo, Z. Weng and T. S. A. Hor, *Organometallics*, 2008, **27**, 4188–4192.

12 Z. Falls, N. Tymińska and E. Zurek, *Macromolecules*, 2014, **47**, 8556–8569.

13 V. Busico, R. Cipullo, F. Cutillo, N. Friederichs, S. Ronca and B. Wangt, *J. Am. Chem. Soc.*, 2003, **125**, 12402–12403.

14 W. J. Van Rensburg, J. A. Van Den Berg and P. J. Steynberg, *Organometallics*, 2007, **26**, 1000–1013.

15 T. Agapie, S. J. Schofr, J. A. Labinger and J. E. Bercaw, *J. Am. Chem. Soc.*, 2004, **126**, 1304–1305.