Supporting Information for:

A Rare Terminal Dinitrogen Complex of Chromium

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Experimental Details

Physical Measurements and General Procedures.

NMR spectra were recorded in thin walled NMR tubes (25 °C, unless otherwise noted) on a Varian Inova 500 MHz (^{1}H) spectrometer or a 500 MHz Varian NMR S system. ^{1}H chemical shifts were referenced to residual proton resonances in deuterated solvent. ^{13}C chemical shifts were referenced to the solvent. ^{31}P chemical shifts were proton decoupled unless otherwise noted and referenced to 85 % H_3PO_4 (δ = 0) as an external reference. ^{15}N NMR chemical shifts were externally referenced to NH_4Cl (δ = -341) relative to CH_3NO_2 (δ = 0). Infrared spectra were recorded on a Nicolet Magna 860 FT-IR spectrometer at ambient temperature and under a purge stream of nitrogen gas. Solid-state FT-IR samples were prepared as KBr pellets. Solid-state magnetic moments were collected on a Johnson Matthey magnetic susceptibility balance. The magnetic susceptibility of the samples was adjusted for diamagnetic contributions using Pascal's constants.[1] Cyclic voltammetry was performed in a Vacuum Atmospheres Nexus II glovebox under an N_2 atmosphere using a CH Instruments model 660C potentiostat. A typical three-electrode single compartment electrochemical cell was used; that included a glassy carbon working electrode, a Ag^{+}/Ag pseudoreference electrode and a glassy carbon rod as auxiliary electrode in THF or fluorobenzene with 0.20 M tetrabutylammonium tetrakis(pentafluorophenyl)borate as the supporting electrolyte. Ferrocene or decamethylferrocene was used as an internal reference with all potentials reported versus the ferrocene/ferrocenium couple. Elemental analyses were performed by Atlantic Microlabs, Norcross, GA, combustion aid was used for all samples.

Synthesis and Materials.

All synthetic procedures were performed under an atmosphere of N_2 using standard Schlenk or glovebox techniques. Reactions performed with $^{15}N_2$ gas were handled in the glovebox under an atmosphere of argon. Unless described otherwise, all reagents were purchased from commercial sources and were used as received. Solvents were dried by passage through activated alumina in an Innovative Technology, Inc., PureSolv solvent purification system. $^{15}N_2$ (98%+) gas and Deuterated THF were purchased from Cambridge Isotope Laboratories. Deuterated THF was dried over NaK and vacuum transferred before use. $CrCl_3(THF)_3$ and magnesium powder were purchased from Strem Chemicals, Inc. CO (99%) and ^{13}CO gas (99 atom %) gas were purchased from Sigma-Aldrich. $P^{Ph}{}_2N^{Bn}{}_2$ ligand was prepared as previously described (ref 15 in main text).

Theoretical methods: All structures were fully optimized without symmetry constraints using B3P86[2] functional as impletemented in Gaussian 09.[3] Stugart basis set with effective core potential (ECP)[4] was used for Cr atom and 6-31G* basis set[5] was used for other non-metal atoms. Each stationary point was confirmed by frequency calculation at the same level of theory to be real minimium without imaginary frequency. The gas-phase free energy was corrected with ZPE, thermal corrections and entropy terms at the state of 1 atm and 298 K. The solvation free energy contribution to total free energy in THF was calculated by using the C-PCM model[6] in Gaussian 09 at the same level of theory as that for optimization. Bondi radii was used with a scale factor (α) of 1.0. All reported free energies are for THF solution as modelled by a polarized continuum model with standard correction for (harmonic) vibrational, rotational and translational thermal free energy contributions. NBO decomposition of the electronic structure; see E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, C. M. Bohmann, C. M. Morales and F. Weinhold, *NBO Version 5.0*, Theoretical Chemical Institute, University of Wisconsin, Madison, WI, 2001.

Note: Population analysis and fragment interaction energies as obtained with NBO have been strongly basis set dependent owing to the diffuse nature of the electron density build-up about the Cr/phosphine core. However, the relative strengths of metal ligand interactions reported here are preserved from minimal STO-6G to more complete cc-pvtz.

(κ^3-$P^{Ph}_2N^{Bn}_2$)$CrCl_3$, (1): $CrCl_3(THF)_3$ (0.40 g, 1.1 mmol) was added to a stirring solution of $P^{Ph}_2N^{Bn}_2$ (0.52 g, 1.1 mmol) in 50 mL THF resulting in a dark blue solution. After stirring for 2 hr, a purple precipitate formed. The reaction was stirred for an additional 12 h, and the purple solid was collected on a medium porosity glass frit, washed with Et_2O and dried under vacuum. **1** is sparingly soluble in THF and acetonitrile. Crystals for X-ray diffraction were grown by vapor diffusion of Et_2O into an acetonitrile solution. Yield: 0.56 g, 82%. ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ =18.5, 13.1, 11.8, 10.7, 7.4, 3.0, -0.43. No $^{31}P\{^1H\}$ NMR signal was observed. μ_{eff} (solid, 294 K) = 3.8(1) μB. Anal. Calcd. for $C_{30}H_{32}Cl_3CrN_2P_2$: C, 56.22; H, 5.03; N, 4.37. Found: C, 56.05; H, 5.29; N, 3.97.

***cis*-[$Cr(N_2)_2(P^{Ph}_2N^{Bn}_2)_2$], (*cis*-2)**: **1** (0.20 g, 0.32 mmol), $P^{Ph}_2N^{Bn}_2$ (0.14 g, 0.30 mmol), and Mg powder (1.0 g, 120 mmol) was stirred in 75 mL THF for 18 h. The brown reaction mixture was filtered through Celite and the solvent removed under vacuum. The dark solids were washed with ether and collected on a glass frit. ^{31}P NMR analysis indicated the composition of the solid to be a mixture of *cis*-**2** and $P^{Ph}_2N^{Bn}_2$ ligand. To remove the free ligand, the solids were dissolved in a minimal amount of THF and stored at -35 °C until the $P^{Ph}_2N^{Bn}_2$ ligand precipitated. The solution was decanted from the colorless ligand. This purification step was repeated as necessary. *cis*-**2** was isolated as a crystalline solid by diffusion of pentane into a THF solution. Dark yellow crystals were collected and dried under vacuum. Yield: 0.051 g, 15 %. Due to overlap of ^{1}H NMR resonances, ^{1}H-^{13}C HSQC NMR experiment was performed to corroborate assignments. ^{1}H NMR (500 MHz, THF-d_8, 298 K): δ =7.51 - 6.62 (40H, PC_6H_5 and $NCH_2C_6H_5$), 3.72 (d, $^2J_{H,H}$ = 13 Hz, 2H, $NCH_2C_6H_5$), 3.23 – 3.13 (8 H) {3.20 (m, 2H, NCH_2P), 3.19 (d, $^2J_{H,H}$ = 13 Hz, 2H, $NCH_2C_6H_5$), 3.19 (m, 2H, NCH_2P), 3.14 (d, $^2J_{H,H}$ = 13 Hz, 2H, $NCH_2C_6H_5$)], 3.05 (m, 2H, NCH_2P), 2.96 (dd, $^2J_{H,H}$ = 11 Hz, $^2J_{P,H}$ = 4 Hz, 2H, NCH_2P), 2.92 (d, $^2J_{H,H}$ = 13 Hz, 2H, $NCH_2C_6H_5$), 2.82 (dd, $^2J_{H,H}$ = 12 Hz, $^2J_{P,H}$ = 4 Hz, 2H, NCH_2P), 2.30 (m, 2H, NCH_2P), 2.28 (m, 2H, NCH_2P), 1.93 (dd, $^2J_{H,H}$ = 11 Hz, $^2J_{P,H}$ = 4 Hz, 2H, NCH_2P). $^{13}C\{^1H\}$ NMR (125 MHz, THF-d_8): δ =144.4 – 127.0 (PC_6H_5 and $NCH_2C_6H_5$), 66.2, 66.1 ($NCH_2C_6H_5$), 56.0, 53.5, 50.1, 49.3 (NCH_2P). $^{31}P\{^1H\}$ NMR (202 MHz, THF-d_8): δ =50.2 (t), 46.8 (t): AA'BB', splitting 50 Hz. $^{15}N\{^1H\}$ NMR (50 MHz, THF-d_8): δ =14.6 (d, $^2J_{N,N}$ = 6 Hz, N_β), 3.8 (br, N_α). UV-vis (THF): λ_{max} (ε, M^{-1} cm^{-1}) 329 (22,500), 429 (sh). IR (THF): ν_{NN} ($^{15}N_2$) cm^{-1} = 2009, 1937 (1942, 1873); (KBr) 2003, 1928; (hexanes) 2020, 1953. Anal. Calcd. for $C_{65}H_{76}CrN_8P_4$: C, 68.17; H, 6.68; N, 9.78. Found: C, 65.62; H, 6.64; N, 9.45.

***trans*-[$Cr(N_2)_2(P^{Ph}_2N^{Bn}_2)_2$], (*trans*-2)**: **1** (0.121 g, 0.19 mmol), $P^{Ph}_2N^{Bn}_2$ (0.088 g, 0.18 mmol), and potassium graphite (0.10 g, 0.78 mmol) was stirred in 30 mL Et_2O. 7 mL of THF was added in 2 mL portions over 60 min. The reaction was stirred for 4 h, filtered through Celite and the solvent removed under vacuum. The dark solids were extracted with pentane and filtered through Celite affording a yellow solution. Pentane was removed under vacuum and the solids were extracted two more time with pentane. An analytically pure sample of *trans*-**2** was not obtained. *cis*-**2**, $P^{Ph}_2N^{Bn}_2$, and an unidentified phosphorus

containing product (δ = 45.6 and 80.0 in ^{31}P NMR spectrum) were noted impurities. *Trans*-**2** decomposes in THF at room temperature over several days liberating $P^{Ph}{}_2N^{Bn}{}_2$ and unidentified decomposition products. ^{1}H and ^{13}C resonance assignments were obtained from 1D ^{1}H and 2D ^{1}H-^{13}C HSQC, ^{1}H-^{31}P HMBC NMR spectra. Yield, 0.009 g, 4 %. ^{1}H NMR (500 MHz, THF-d_8, 298 K): δ =7.80 (*o*-PC_6H_5), 7.40-7.00 (*m*-PC_6H_5, *p*-PC_6H_5 and $NCH_2C_6H_5$), 4.40 (m, 4H, $NCH_2C_6H_5$), 3.60 (d, 4H, NCH_2P), 3.46 (m, $NCH_2C_6H_5$), 2.95 (m, NCH_2P), 2.69 (d, $^{2}J_{H,H}$ = 13 Hz, 4H, NCH_2P), 2.52 (m, $^{2}J_{H,H}$ = 12 Hz, $^{2}J_{P,H}$ = 5 Hz, 4H, NCH_2P). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8): δ= 132.3 – 126.8 (PC_6H_5 and $NCH_2C_6H_5$), 76.5, 66.1 ($NCH_2C_6H_5$), 52.7, 49.5 (NCH_2P). ^{31}P{^{1}H} NMR (202 MHz, THF-d_8): δ = 52.8 (s). IR (hexanes): ν_{NN} ($^{15}N_2$) cm^{-1} = 2007 (1942); IR (KBr): ν_{NN} cm^{-1} = 1981.

***cis*-[Cr(CO)$_2$($P^{Ph}{}_2N^{Bn}{}_2$)$_2$], (3)** Exposure of *cis*-**2** to an atmosphere of CO shows full conversion to **3**. Due to overlap of ^{1}H NMR resonances, a ^{1}H-^{13}C HSQC NMR experiment was performed to corroborate assignments. ^{1}H NMR (500 MHz, THF-d_8, 298 K): δ =7.70 - 6.62 (PC_6H_5 and $NCH_2C_6H_5$, 40 H), 3.78 (d, $^{2}J_{H,H}$ = 13 Hz, 2H, $NCH_2C_6H_5$), 3.29 (m, 2H, NCH_2P), 3.14 (m, 4H, $NCH_2C_6H_5$), 3.01 (m, 2H, NCH_2P), 3.01 (d, $^{2}J_{H,H}$ = 13 Hz, 2H, $NCH_2C_6H_5$), 2.84 (m, 2H, NCH_2P), 2.77 (m, $^{2}J_{P,H}$ = 4 Hz, 2H, NCH_2P), 2.64 (m, $^{2}J_{P,H}$ = 4 Hz, 2H, NCH_2P), 2.41 (m, 2H, NCH_2P), 2.21 (m, $^{2}J_{P,H}$ = 4 Hz, 2H, NCH_2P), 2.05 (m, $^{2}J_{P,H}$ = 4 Hz, 2H, NCH_2P). ^{13}C{^{1}H} NMR (125 MHz, THF-d_8): δ = 238.6 (m, Cr*C*O), 130.9 – 126.6 (PC_6H_5 and $NCH_2C_6H_5$), 66.1 ($NCH_2C_6H_5$), 61.5, 60.3, 49.9, 49.5 (NCH_2P). ^{31}P{^{1}H} NMR (202 MHz, THF-d_8): δ =56.5 (m), 42.2 (m). IR (KBr): ν_{CO} (^{13}CO) cm^{-1} = 1837, 1777 (1794, 1736). Anal. Calcd. for $C_{62}H_{64}CrN_4O_2P_4$: C, 69.39; H, 6.01; N, 5.22. Found: C, 65.37; H, 6.20; N, 4.83.

Alternative Preparation of *cis*-[Cr(CO)$_2$($P^{Ph}{}_2N^{Bn}{}_2$)$_2$], (3): **1** (0.11 g, 0.17 mmol), $P^{Ph}{}_2N^{Bn}{}_2$ (0.078 g, 0.16 mmol), and Mg powder (0.27 g, 11 mmol) were combined in 25 mL THF. The solution was degassed by four freeze-pump-thaw cycles and was stirred under 1 atm CO for 18 hours. The yellow-brown reaction mixture was filtered through Celite, reduced in volume to 5 mL and stored in -35 °C freezer for 3 days to precipitate free ligand. The yellow solution was decanted from the colorless solid and this purification step was repeated as necessary. Recrystallization of **3** by diffusion of Et_2O into a THF solution yields a yellow microcrystalline solid. Yield: 0.065 g, 37 %.

Note: Repeated analysis on independently prepared samples of *cis*-**2** and **3** that were pure by spectroscopic studies failed to yield acceptable values for elemental analyses. We believe the low carbon analysis is due to the formation of metal carbides during combustion. Metal carbide formation during combustion analysis has been reported in the literature for low-valent Mo and W carbonyl complexes. See reference page 4985 in: J. Chatt and H. R. Watson *J. Chem. Soc.* 1961, 4980-4988, and for acetylide complexes: a) T. P. Vaid, A. S. Veige, E. B. Lobkovsky, W. V. Glassey, P. T. Wolczanski, L. M. Liable-Sands, A. L. Rheingold and T. Cundari, *J. Am. Chem. Soc.* 1998, **120**, 10067. b) L. A. Berben and J. R. Long, *Inorg. Chem.* 2005, **44**, 8459.

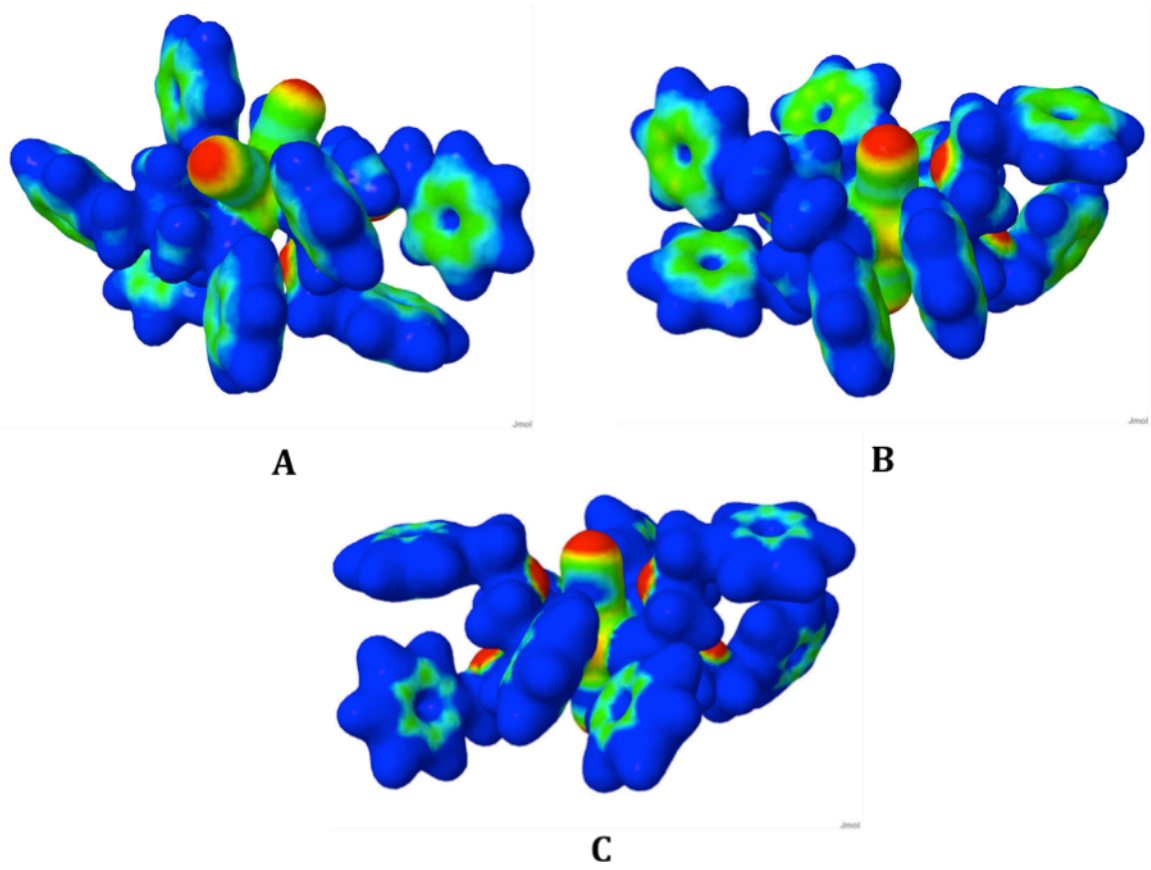


Figure S1. Plot of electrostatic potential projected onto electron density isosurface. A) *cis*-**2** (Structure A from Figure 2). B) *trans*-**2** (Conformer B from Figure 2). C) *trans*-**2** (Conformer C from Figure 2). Red indicates areas of negative charge density, green is neutral, blue is positive charge density. These diagrams highlight the repulsive interaction between the distal nitrogen atom of the N_2 ligand and the amine nitrogen of the $P^{Ph}{}_2N^{Bn}{}_2$ ligand. Density contour is chosen as 0.02 e-/Bohr^3.

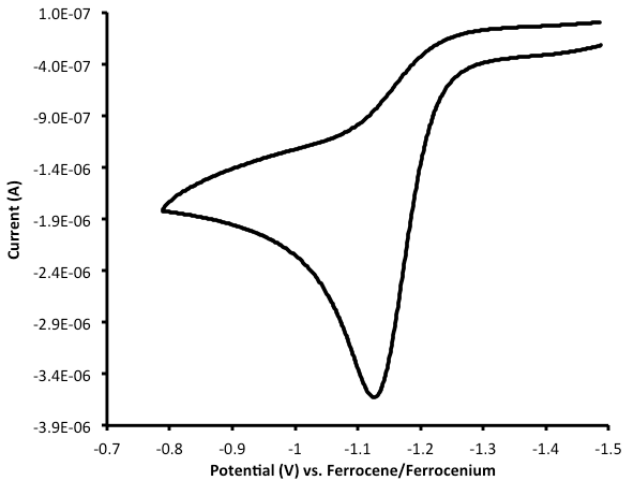


Figure S2. Cyclic voltammogram of *cis*-$[Cr(N_2)_2(P^{Ph}{}_2N^{Bn}{}_2)_2]$ (*cis*-**2**) in THF. E_{pa} = -1.11 V ($Cr^{I/0}$).

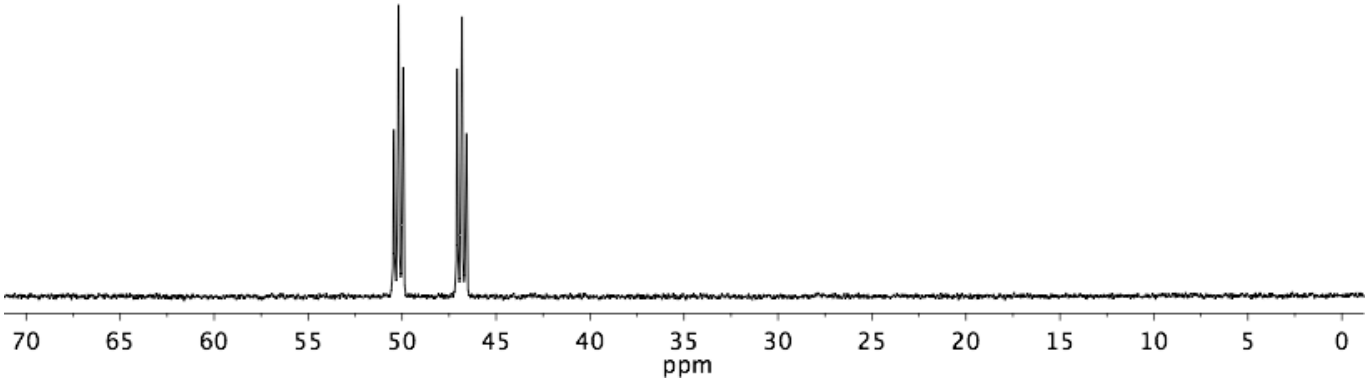


Figure S3. ^{31}P NMR spectrum of *cis*-[Cr(N$_2$)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$] (*cis*-**2**) in THF-d_8.

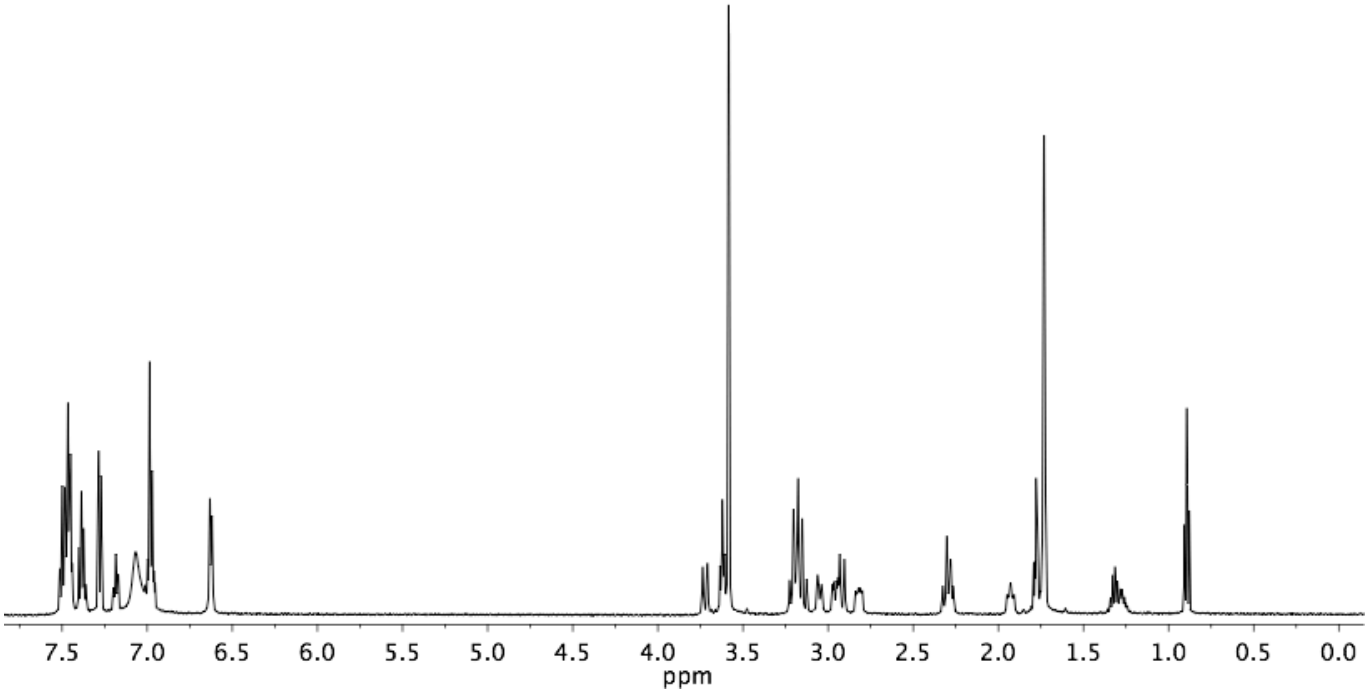


Figure S4. ^{1}H NMR spectrum of *cis*-[Cr(N$_2$)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$] (*cis*-**2**) in THF-d_8.

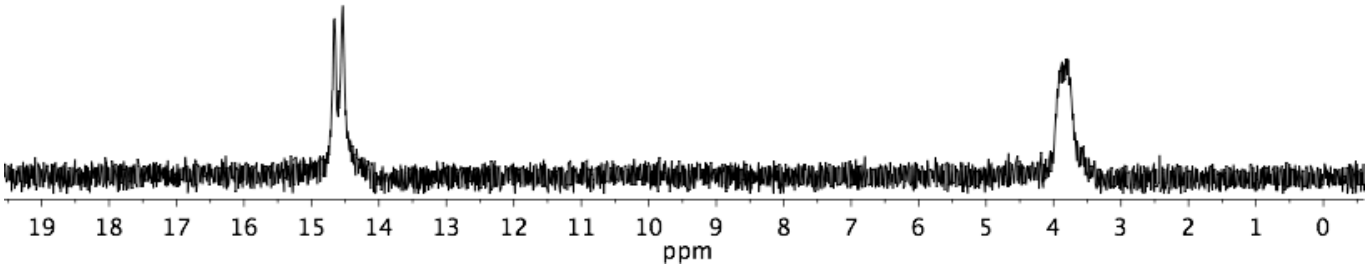


Figure S5. ^{15}N NMR spectrum of *cis*-[Cr(^{15}N$_2$)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$] (*cis*-**2**) in THF-d_8.

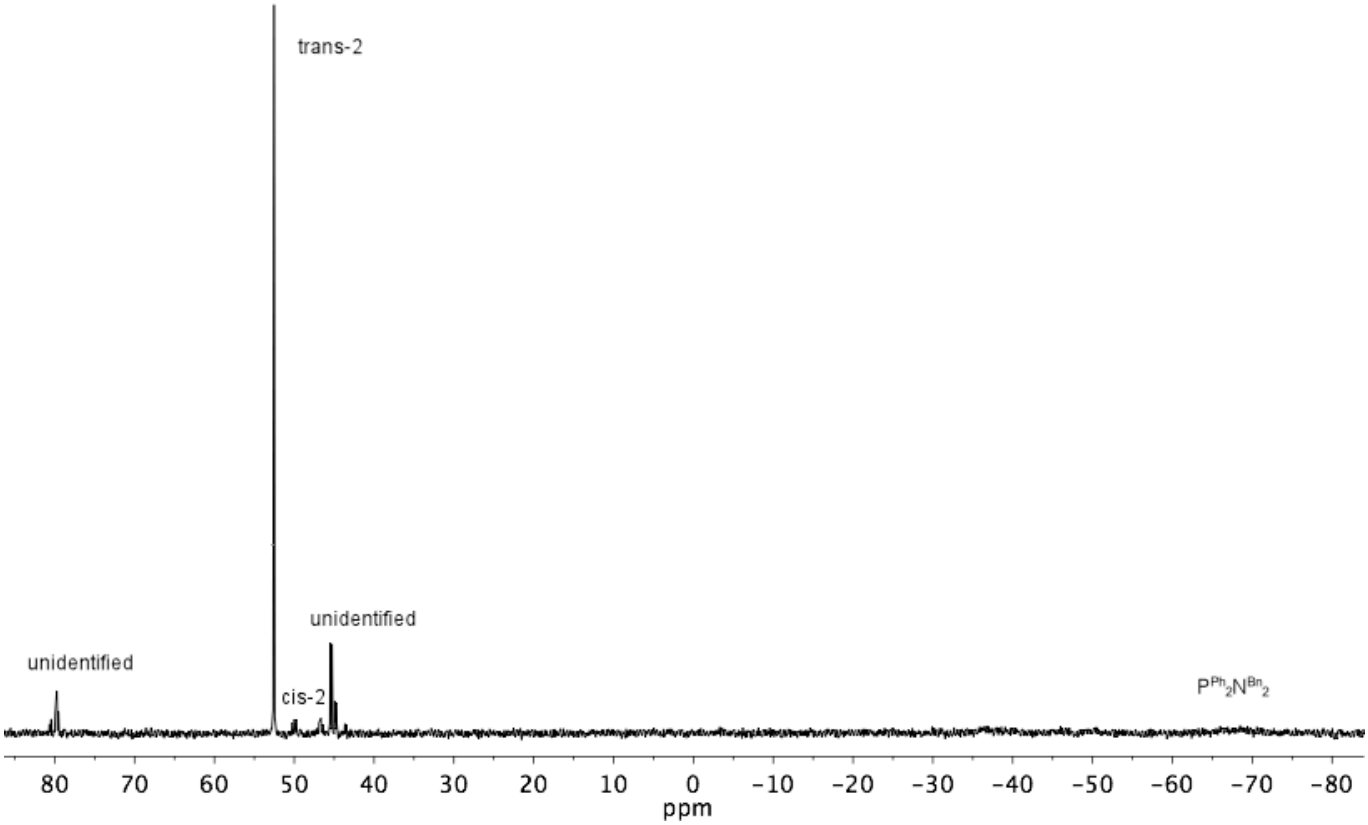


Figure S6. ^{31}P NMR spectrum of *trans*-[$Cr(N_2)_2(P^{Ph}{}_2N^{Bn}{}_2)_2$] (*trans*-**2**) in THF-d_8.

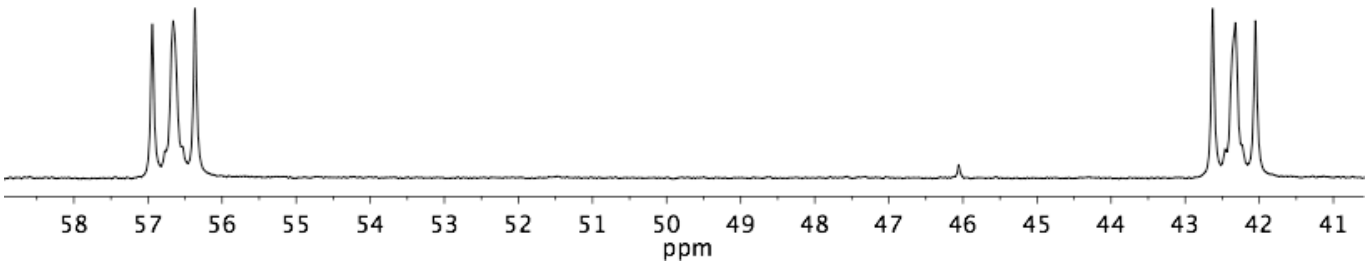


Figure S7. ^{31}P NMR spectrum of *cis*-[$Cr(CO)_2(P^{Ph}{}_2N^{Bn}{}_2)_2$] (**3**) in THF-$d_8$.

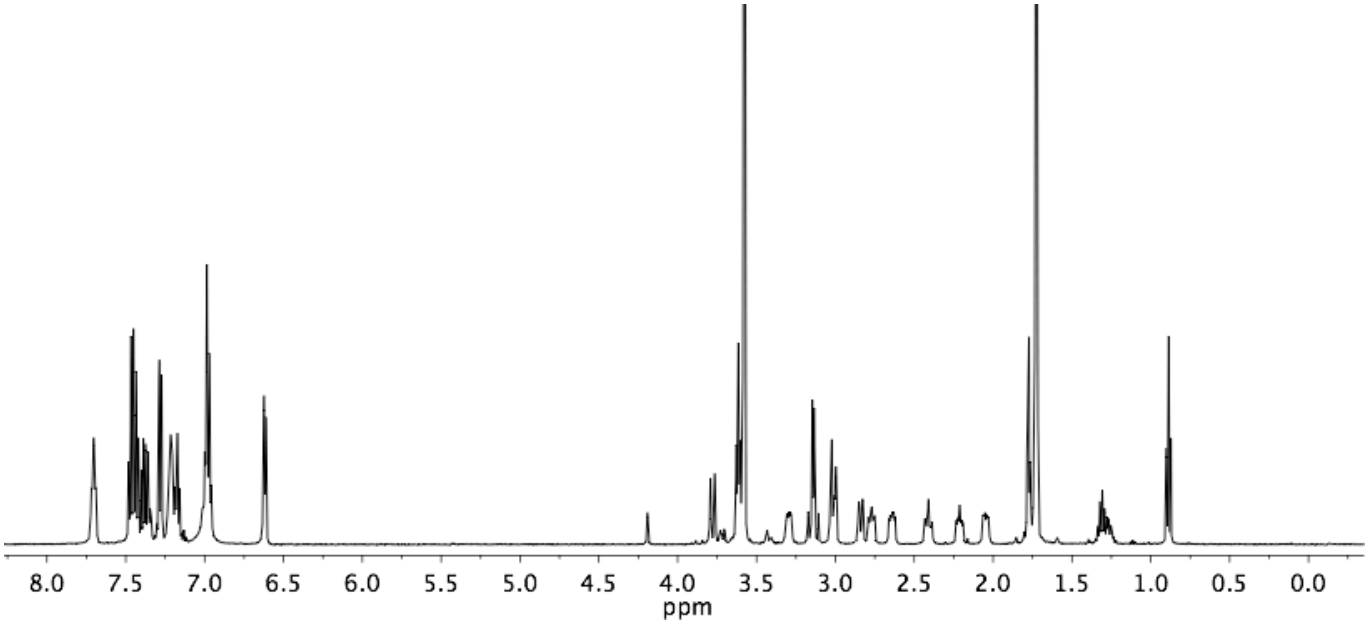


Figure S8. ^{1}H NMR spectrum of *cis*-[Cr(CO)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$] (**3**) in THF-d_8.

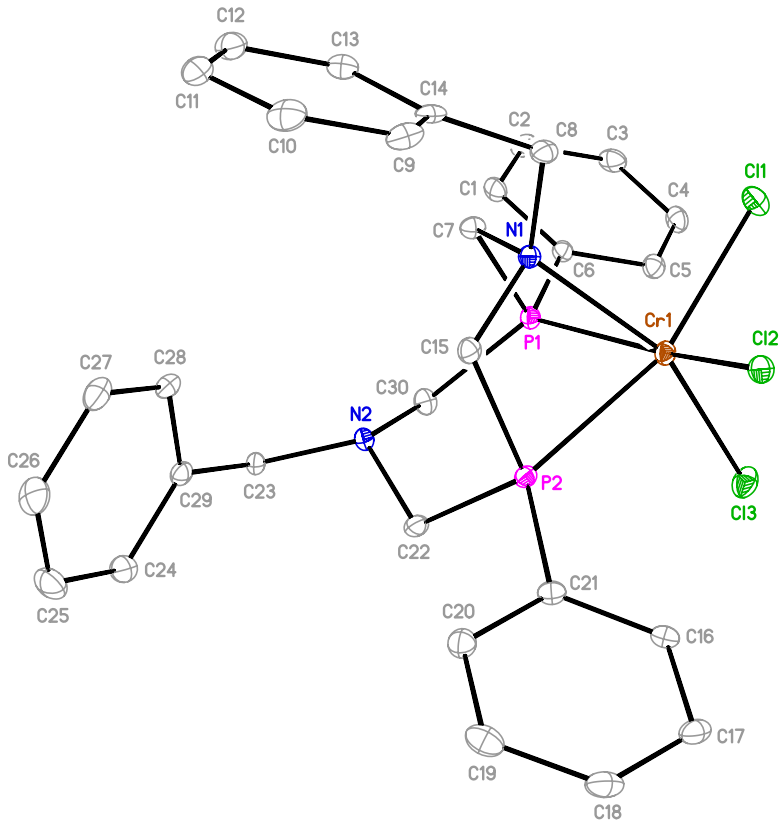


Figure S9. Molecular structure of **1**. Thermal ellipsoids drawn at 30 % probability. Hydrogen atoms omitted.

X-ray structural analysis for **(1)**: A single blue needle (0.01 X 0.02 X 0.20 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 100(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-Kα radiation. Unit cell parameters were obtained from 90 data frames, 0.3° Φ, from three different sections of the Ewald sphere yielding a = 11.801(3) Å, b = 19.066(5) Å, c = 15.474(4) Å, β = 112.14(1)°, V = 3225(2) Å^3. 49453 reflections (R_{int} = 0.1499) were collected (12404 unique) over θ = 1.78 to 33.43°. The systematic absences in the diffraction data were consistent with the centrosymmetric, monoclinic space group, $P2_1/c$. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data (Sheldrick, G,.Bruker-AXS, 2001) T_{max}/T_{min} = 1.14. The asymmetric unit contains one $Cl_3Cr(P^{Ph}{}_2N^{Bn}{}_2)$ molecule and one molecule of acetonitrile solvent, both located on general positions, yielding Z = 4, and Z' = 1. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.015 with $R1(wR2)$ 0.0675(0.0782) for [$I\theta$>2(I)] and with largest difference peak and hole of 0.621 and –0.820e/Å^3. The sample diffracted weakly at high angles due to the thin nature of the crystals leading to a large R_{int}. The space group was assigned from the systematic absences check in XPREP and was supported using PLATON's symmetry calculation. Sum Formula: C32 H35 Cl3 Cr N3 P2; Formula Weight: 681.92

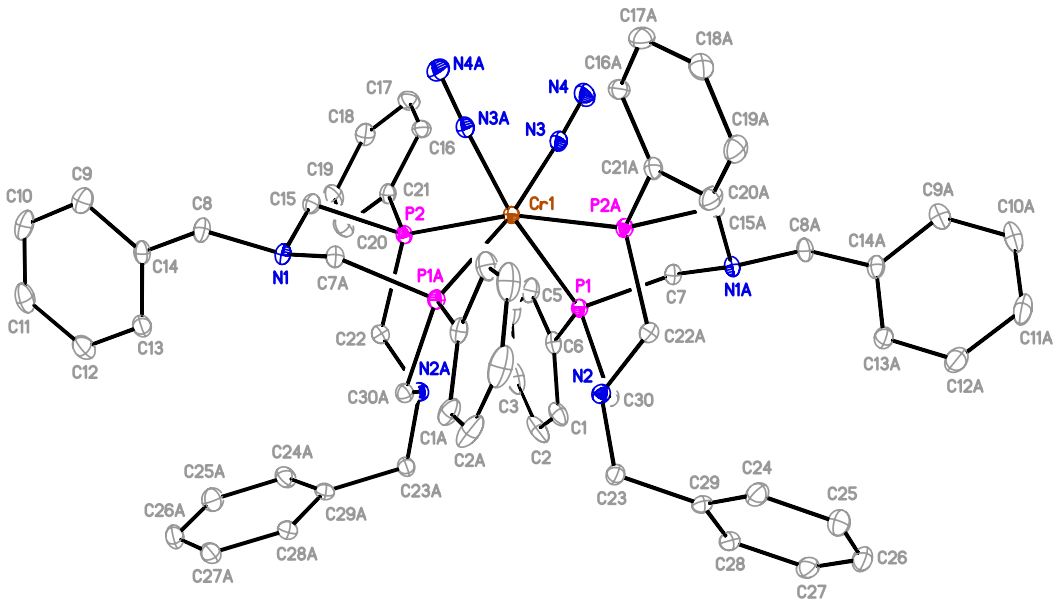


Figure S10. Molecular structure of *cis*-**2**. Thermal ellipsoids drawn at 30 % probability. Hydrogen atoms omitted.

X-ray structural analysis for **(*cis*-2)**: A single orange blade (0.06 X 0.08 X 0.14 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 100(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-Kα radiation. Unit cell parameters were obtained from 90 data frames, 0.3º Φ, from three different sections of the Ewald sphere yielding a = 27.27(1) Å, b = 41.84(2) Å, c = 9.362(2) Å, V = 10681(6) Å^3. 49496 reflections (R_{int} = 0.0958) were collected (10249 unique) over θ = 1.78 to 33.42°. The systematic absences in the diffraction data were consistent with the chiral, orthorhombic space group, *Fdd*2. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data (Sheldrick, G,.Bruker-AXS, 2001) T_{max}/T_{min} = 1.03. The molecule is located on a 2-fold rotation axis yielding Z = 8, and Z' = 1/2. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.009 with $R1(wR2)$ 0.0516(0.0967) for [$I\theta$>2(I)] and with largest difference peak and hole of 0.399 and –0.516e/Å^3. Sum Formula: C60 H64 Cr N8 P4; Formula Weight: 1073.07

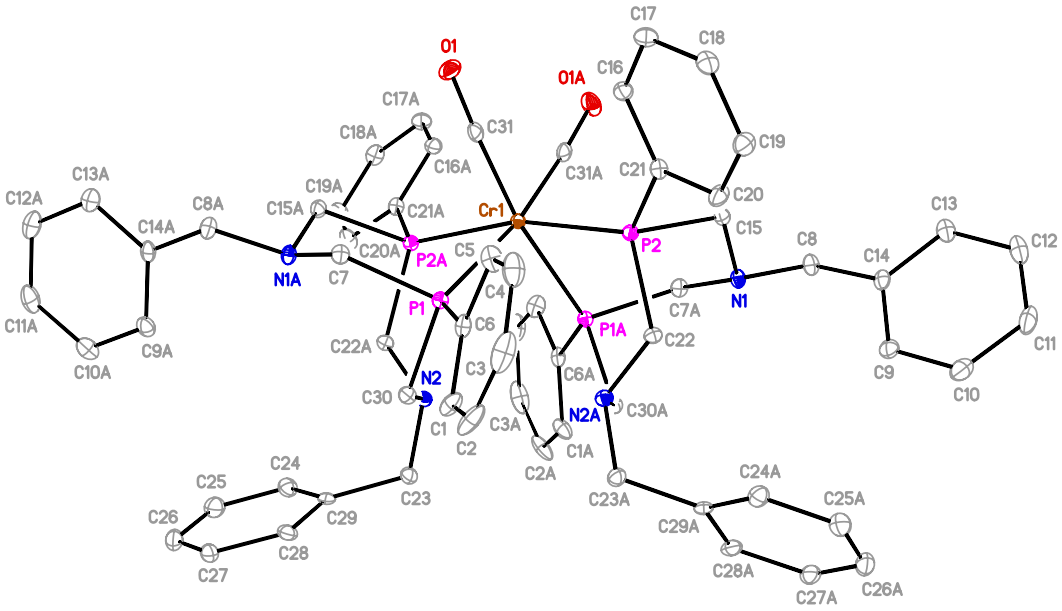


Figure S11. Molecular structure of **3**. Thermal ellipsoids drawn at 30 % probability. Hydrogen atoms omitted.

X-ray structural analysis for **(3)**: A single yellow needle (0.03 X 0.04 X 0.20 mm) was mounted using NVH immersion oil onto a nylon fiber and cooled to the data collection temperature of 100(2) K. Data were collected on a Brüker-AXS Kappa APEX II CCD diffractometer with 0.71073 Å Mo-Kα radiation. Unit cell parameters were obtained from 90 data frames, 0.3º Φ, from three different sections of the Ewald sphere yielding a = 27.386(2) Å, b = 41.872(2) Å, c = 9.257(1) Å, V = 10616(1) Å^3. 44110 reflections (R_{int} = 0.1084) were collected (10077 unique) over θ = 1.78 to 33.36°. The systematic absences in the diffraction data were consistent with the chiral, orthorhombic space group, *Fdd*2. The data-set was treated with SADABS absorption corrections based on redundant multi-scan data (Sheldrick, G,.Bruker-AXS, 2001) T_{max}/T_{min} = 1.07. The asymmetric unit contains one CrL2(CO)$_2$ molecule located on 2-fold rotation axis, yielding Z = 8, and Z' = 1/2. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were treated as idealized contributions. The goodness of fit on F^2 was 1.008 with $R1(wR2)$ 0.0540(0.0833) for [$I\theta$>2(I)] and with largest difference peak and hole of 0.460 and –0.488e/Å^3. Sum Formula: C62 H64 Cr N4 O2 P4; Formula Weight: 1073.05

Selected geometric parameters

Table S1 reports a comparison between selected theoretical and experimental geometric parameters and harmonic N_2/CO IR stretching frequencies. All data are compiled for optimized geometries with the methodology outlined in the main text.

Table S1. Selected calculated bond distance and vibrational frequencies of N_2/CO ligand. Experimental data is given in parenthesis.

	r(N-N/C-O) Å	r(Cr-N/C) Å	$\nu_{N2/CO}$(cm^{-1})
cis-[Cr(N$_2$)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$]	1.134(1.133)	1.854(1.861)	2133, 2177 (1953, 2020 in hexanes) (1937, 2009 in THF) (1928, 2003 in KBr)
trans-[Cr(N$_2$)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$]	1.133	1.870	2133 (1980 in KBr; 2007 in hexanes)
cis-[Cr(CO)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$]	1.178(1.179)	1.807	1908, 1951 (1784, 1843 in THF)
trans-[Cr(CO)$_2$(P$^{Ph}_2$N$^{Bn}_2$)$_2$]	1.174	1.853	1902
cis-[Cr(N$_2$)$_2$(dmpe)$_2$]	1.135	1.853	2130, 2176 (1895, 1920)[a]
trans-[Cr(N$_2$)$_2$(dmpe)$_2$]	1.135(1.122)	1.86(1.874)	2124 (1932 in hexanes) [a]
cis-[Cr(CO)$_2$(dmpe)$_2$]	1.177	1.807	1914, 1958 (1820, 1755 in hexanes) [a]
trans-[Cr(CO)$_2$(dmpe)$_2$]	1.174	1.844	1913
cis-[Cr(N$_2$)$_2$(PMe$_3$)$_4$]	1.136	1.845	2123, 2170 (1918, 1990)[b]
trans-[Cr(N$_2$)$_2$(PMe$_3$)$_4$]	1.137	1.86	2107, 2155
cis-[Cr(CO)$_2$(PMe$_3$)$_4$]	1.178	1.804	1911, 1957
trans-[Cr(CO)$_2$(PMe$_3$)$_4$]	1.175	1.846	1901
Free N$_2$ molecule	1.104(1.098)		2475 (2359)[c]
Free CO molecule	1.136(1.128)		2224 (2170) [c]

[a] experimental data from reference: J. E. Salt, G. S. Girolami, G. Wilkinson, M. Montevalli, M. Thornton-Pett and M. B. Hursthouse *J. Chem. Soc. Dalton Trans*. 1985, 685.
[b] experimental data from reference: H. H. Karsch, *Angew. Chem. Int. Ed. Engl*. 1977, **16**, 56.
[c] experimental data from: K. Huber, G. Herzberg, *Constants of Diatomic Molecules,* Van Nostrand Reinhold Co., New York, 1979.

Table S2. Reaction free energies (kcal mol^{-1}) for Cr(L$_2$)(N$_2$)$_2$ (L= P$^{Ph}_2$N$^{Bn}_2$ and dmpe) complexes.

	P$^{Ph}_2$N$^{Bn}_2$	dmpe
cis-Cr(L$_2$)(N$_2$)$_2$ → *trans*-Cr(L$_2$)(N$_2$)$_2$	6	-4
cis-Cr(L$_2$)(N$_2$)$_2$ → Cr(L$_2$)(N$_2$) + N$_2$	11	16
trans-Cr(L$_2$)(N$_2$)$_2$ → Cr(L$_2$)(N$_2$) + N$_2$	5	20
cis-Cr(L$_2$)(N$_2$)$_2$ + 2CO → *cis*-Cr(L$_2$)(CO)$_2$ + 2N$_2$	-56	-55

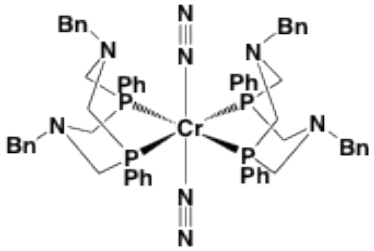
Ab Initio Molecular Dynamics (AIMD) Simulation of N_2 stretching frequencies.

The agreement between the observed N_2 IR stretching frequencies and those calculated within the harmonic approximation with the methodology reported here is of insufficient quality for accurate spectroscopic assignments: such as the identification of the *trans*-**2** IR active N_2 stretching frequency mode quoted in the text. The absolute values of these modes are significantly blue shifted with respect to experiment in part due to the basis set and in part due to the harmonic approximation. To overcome this we have resorted to finite temperature AIMD, using the PBE functional,[7] within the CP2K package.[8] All atoms are modeled by norm-conserving pseudopotentials.[9] Wavefunctions are expanded in a triple zeta polarized basis set[10] with an auxiliary planewave basis of 300Ry. All simulations are run at T = 300 K in a 30 periodic box for 4-6 ps (after equilibration). N_2 IR stretching frequencies are calculated by Fourier transform of the velocity-velocity time autocorrelation functional, see Table S3. Note the improved agreement (in terms of absolute frequencies) with respect to experimental data and the *trans*-**2** IR active band consistent with experiment for conformer B from Figure 2 in the text.

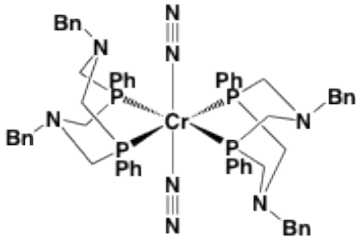
Table S3. Comparison between AIMD and experimental N_2 IR stretching frequencies.

	Calc. (cm^{-1})	Exp. (cm^{-1})
Free N_2	2333	2359(g)
cis-[Cr(N_2)$_2$($P^{Ph}_2N^{Bn}_2$)$_2$]	1979(s), 2025(a)	1928, 2003 (KBr) 1937, 2009 (THF) 1953, 2020 (hexanes)
trans-[Cr(N_2)$_2$($P^{Ph}_2N^{Bn}_2$)$_2$][a]	1963(a), 2034(s)	1980 (KBr) 2007 (hexanes)
trans-[Cr(N_2)$_2$($P^{Ph}_2N^{Bn}_2$)$_2$][b]	1966(a), 2011(s)	
Cr (N_2) (κ^1-$P^{Ph}_2N^{Bn}_2$) (κ^2-$P^{Ph}_2N^{Bn}_2$)	1946	N/A
cis-[Cr(N_2)$_2$(dmpe)$_2$]	1979, 2024	1895, 1920
trans-[Cr(N_2)$_2$(dmpe)$_2$]	1963(a), 2034(s)	1930

[a] conformer used:

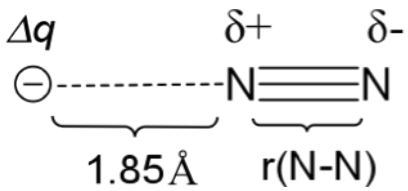


[b] conformer used (lower in energy):



Charge Model for N_2 bond polarization induced by charge on Cr

In this simple test calculation we employ the following scheme:



The value of Δq obtained from NBO population analysis is on the order of -2 electrons and δq = 0.2e- as obtained from our SSD/6-31G* and cc-PVTZ calculations. We note that this large negative charge on Cr is more a reflection of the excess charge build up (into very diffuse orbitals) from both the Cr and phosphine ligands as can be seen in the electrostatic potential plot of Figure S1 above. The Cr in both simulations shows a d-orbital population of about 6.5e- consistent with a d^6 Cr(0) oxidation state next to electron donating ligands. The remaining Cr electron population resides in very diffuse Cr s and p Rydberg states which overlap substantially with the P atoms. In this context we ascribe the large negative charge on Cr to be a reflection of the build-up of electron density at the metal center and not a reflection of the oxidation state of Cr. Finally, it is noted that a charge scheme based off of fitting of the electrostatic potential to point charges[11] also results in a large -1.5 charge to Cr in these species. Table S4 reports as a function of Δq, the electrostatic stabilization energy (relative to free N_2) for the model, the red shift in the vibrational frequency of the N_2 stretch Δ*v*, the charge build-up on the proximal nitrogen δ+, and the optimized N-N bond length, r(N-N).

Table S4. Calculated relative energies, N-N bond distance, N_2 vibrational frequencies and net charge on N(δ+) atom based on the above charge model.

Δq	ΔE(kcal/mol)	Δ*v*(cm^{-1})	N(δ+)	r(N-N) Å
0.0	0.0	0	0.000	1.104
-0.5	0.8	-31	0.112	1.107
-1.0	-5.3	-77	0.224	1.111
-1.5	-17.8	-139	0.333	1.116
-2.0	-36.1	-220	0.442	1.126
-2.5	-60.0	-321	0.550	1.131

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Cartesian coordinates of optimized structures.

cis-[$Cr(N_2)_2(P^{Ph}{}_2N^{Bn}{}_2)_2$]
E=-4225.45581

Cr	0.000005	-1.500165	0.000247
N	3.442515	-0.691001	1.920358
N	1.867978	1.503731	-0.482145
P	0.747972	0.042651	1.593419
P	2.236974	-1.274874	-0.517617
C	-0.029379	1.945024	3.620541
H	0.618579	2.675218	3.144174
C	-0.702084	2.306579	4.786353
H	-0.578580	3.308448	5.189591
C	-1.524345	1.388287	5.436506
H	-2.046962	1.671265	6.346087
C	-1.661805	0.103657	4.917323
H	-2.293463	-0.626473	5.415520
C	-0.991697	-0.254027	3.748571
H	-1.107515	-1.260319	3.354912
C	-0.178389	0.664049	3.073819
C	2.185587	-0.597208	2.638606
H	2.321564	0.117408	3.457965
H	1.872620	-1.556923	3.088893
C	4.560370	-0.900287	2.840795
H	4.531448	-1.911991	3.289248
H	4.431525	-0.189729	3.667795
C	6.906367	-1.645462	2.265558
H	6.694512	-2.593790	2.754557
C	8.164103	-1.417042	1.709334
H	8.928257	-2.187452	1.766887
C	8.435688	-0.207654	1.076329
H	9.414560	-0.027207	0.640329
C	7.443870	0.770259	1.003199
H	7.643252	1.718351	0.511561
C	6.191294	0.540979	1.562924
H	5.420082	1.304308	1.502567
C	5.909211	-0.670936	2.202815
C	3.439419	-1.685492	0.863575
H	3.196040	-2.698716	1.234417
H	4.443294	-1.722758	0.429021
C	2.739686	-3.609962	-1.952948
H	1.934423	-4.008780	-1.344966
C	3.386376	-4.438612	-2.867557
H	3.080511	-5.476981	-2.959870
C	4.411656	-3.936144	-3.663725
H	4.912591	-4.579673	-4.381757
C	4.795748	-2.603247	-3.531109
H	5.603838	-2.205496	-4.139577
C	4.155204	-1.776850	-2.611137
H	4.488996	-0.748320	-2.511246
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C	2.817692	0.475894	-0.885237
H	3.817651	0.613758	-0.442902
H	2.909072	0.552894	-1.974048
C	2.196842	2.810195	-1.063173
H	1.361261	3.484620	-0.831237
H	2.213534	2.683539	-2.151768
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H	4.652479	2.654977	-2.235266
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H	6.781528	3.664207	-1.485147
C	5.911534	4.600806	0.249327

H	6.844733	5.049523	0.578053
C	4.739222	4.814026	0.971817
H	4.755342	5.431691	1.865678
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H	0.833611	2.404680	1.050728
H	2.443378	1.830834	1.556697
N	-3.442580	-0.691867	-1.919980
N	-1.867945	1.503905	0.481625
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C	0.029247	1.943542	-3.621322
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C	0.702015	2.304650	-4.787233
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H	2.293705	-0.628538	-5.415004
C	0.991745	-0.255494	-3.748339
H	1.107611	-1.261603	-3.354230
C	0.178314	0.662807	-3.074045
C	-2.185659	-0.598285	-2.638288
H	-2.321690	0.116036	-3.457897
H	-1.872671	-1.558153	-3.088239
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C	-6.906745	-1.646191	-2.265586
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H	-8.928977	-2.187450	-1.767519
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C	-7.443829	0.769816	-1.003614
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C	-2.739548	-3.609202	1.954591
H	-1.934213	-4.008216	1.346843
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C	-4.795851	-2.601910	3.532109
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C	-1.562655	1.594125	-0.936523
H	-0.833569	2.404190	-1.051634
H	-2.443385	1.830256	-1.557330
N	-0.374573	-2.837219	-1.228624
N	-0.612053	-3.681499	-1.947912
N	0.374642	-2.836672	1.229692
N	0.612181	-3.680634	1.949339

trans-$[Cr(N_2)_2(P^{Ph}{}_2N^{Bn}{}_2)_2]$
E=-4225.44103

Cr	0.000016	0.341372	-0.00003200
N	-3.628447	0.601258	-1.65714000
N	-3.020849	-0.052129	1.82580000
P	-1.809730	1.771313	0.03564400
P	-1.775307	-1.103240	-0.38692200
C	-1.384008	3.888670	1.81273100
H	-1.161726	3.094926	2.52289100
C	-1.323502	5.213850	2.23013000
H	-1.070108	5.442212	3.26217500
C	-1.586061	6.244159	1.32874300
H	-1.542511	7.280154	1.65335300
C	-1.893107	5.936468	0.00735200
H	-2.082011	6.732331	-0.70800600
C	-1.963805	4.607540	-0.40837100
H	-2.200280	4.395567	-1.44690700
C	-1.728894	3.563987	0.49182000
C	-2.847418	1.820622	-1.52020300
H	-3.551192	2.657201	-1.44326200
H	-2.189138	2.007682	-2.38810700
C	-4.648631	0.741110	-2.69582900
H	-4.199945	0.751069	-3.70796900
H	-5.118781	1.723184	-2.55388600
C	-6.044384	-1.081285	-3.75569400
H	-5.499924	-0.920023	-4.68358900
C	-7.056764	-2.038268	-3.70223200
H	-7.298679	-2.618702	-4.58845900
C	-7.748766	-2.253710	-2.51396800
H	-8.536531	-3.000877	-2.46875900
C	-7.424086	-1.507246	-1.38132200
H	-7.954746	-1.666753	-0.44683200
C	-6.417056	-0.549338	-1.43962400
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C	-5.716083	-0.324987	-2.62963900
C	-2.843585	-0.607009	-1.85869300
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C	-2.591636	-3.850453	-0.62066000
H	-3.472250	-3.600140	-0.03550100
C	-2.446434	-5.151783	-1.09582100
H	-3.200088	-5.898536	-0.85981400
C	-1.345613	-5.492903	-1.87787100
H	-1.234277	-6.507643	-2.25011100

C	-0.390904	-4.526148	-2.18305700
H	0.468871	-4.783458	-2.79569300
C	-0.530230	-3.229644	-1.69545300
H	0.221702	-2.477930	-1.92391900
C	-1.627817	-2.875611	-0.90421300
C	-3.109109	-1.179446	0.92438600
H	-4.097744	-1.294289	0.44412400
H	-2.920754	-2.084273	1.51642000
C	-3.759811	-0.242371	3.07084200
H	-3.477186	0.575487	3.74517200
H	-3.395448	-1.171975	3.52693000
C	-5.923548	-1.531155	2.79004900
H	-5.341905	-2.450497	2.81189300
C	-7.306004	-1.593597	2.62915600
H	-7.795471	-2.558408	2.52480300
C	-8.060027	-0.421912	2.61533400
H	-9.139027	-0.466888	2.49592100
C	-7.422957	0.808004	2.77058700
H	-8.004818	1.725788	2.77329800
C	-6.041348	0.862835	2.93605300
H	-5.554196	1.825315	3.07527400
C	-5.269527	-0.304652	2.94217400
C	-3.175397	1.268024	1.25440900
H	-3.127941	1.983329	2.08086900
H	-4.138627	1.420162	0.73862600
N	3.628355	0.601291	1.65720600
N	3.020977	-0.051987	-1.82573800
P	1.809716	1.771380	-0.03563600
P	1.775357	-1.103217	0.38691100
C	1.384050	3.888698	-1.81273600
H	1.161841	3.094932	-2.52289500
C	1.323553	5.213870	-2.23016200
H	1.070224	5.442213	-3.26222800
C	1.586037	6.244196	-1.32877400
H	1.542490	7.280186	-1.65340100
C	1.893012	5.936533	-0.00735900
H	2.081864	6.732413	0.70799400
C	1.963710	4.607614	0.40839100
H	2.200136	4.395657	1.44694100
C	1.728857	3.564045	-0.49179700
C	2.847308	1.820649	1.52028900
H	3.551072	2.657243	1.44341100
H	2.188991	2.007664	2.38817000
C	4.648609	0.741172	2.69583300
H	4.199988	0.751284	3.70800000
H	5.118831	1.723187	2.55373300
C	6.043918	-1.081617	3.75563600
H	5.499315	-0.920454	4.68346400
C	7.056157	-2.038752	3.70216200
H	7.297817	-2.619407	4.58831400
C	7.748348	-2.254052	2.51398300
H	8.536003	-3.001334	2.46876700
C	7.424001	-1.507299	1.38143100
H	7.954809	-1.666700	0.44700700
C	6.417113	-0.549245	1.43974700
H	6.165040	0.029041	0.55501400
C	5.715951	-0.325030	2.62967900
C	2.843526	-0.606998	1.85875400
H	2.192383	-0.544010	2.74839200
H	3.544522	-1.430760	2.02476800
C	0.530319	-3.229716	1.69530000
H	-0.221592	-2.478008	1.92385600

C	0.390987	-4.526259	2.18279700
H	-0.468771	-4.783609	2.79544000
C	1.345669	-5.493003	1.87749300
H	1.234326	-6.507775	2.24964500
C	2.446471	-5.151832	1.09544000
H	3.200106	-5.898576	0.85934300
C	2.591681	-3.850462	0.62038900
H	3.472286	-3.600112	0.03523100
C	1.627885	-2.875629	0.90405200
C	3.109224	-1.179318	-0.92434200
H	4.097842	-1.294141	-0.44403900
H	2.920917	-2.084136	-1.51640400
C	3.759972	-0.242198	-3.07076400
H	3.477384	0.575687	-3.74507600
H	3.395609	-1.171780	-3.52689700
C	5.923688	-1.531018	-2.78992500
H	5.342040	-2.450355	-2.81183000
C	7.306135	-1.593476	-2.62896200
H	7.795588	-2.558294	-2.52460900
C	8.060167	-0.421798	-2.61506500
H	9.139161	-0.466786	-2.49559900
C	7.423116	0.808129	-2.77031800
H	8.004986	1.725907	-2.77297800
C	6.041515	0.862975	-2.93585300
H	5.554377	1.825462	-3.07507000
C	5.269685	-0.304506	-2.94204400
C	3.175504	1.268144	-1.25429700
H	3.128138	1.983490	-2.08072700
H	4.138679	1.420234	-0.73840100
N	-0.120439	0.423125	1.86438100
N	-0.138682	0.535113	2.99182400
N	0.120515	0.423021	-1.86445300
N	0.138751	0.534854	-2.99190900

cis-[$Cr(N_2)_2(dmpe)_2$]
E=-2151.93479

Cr	-0.009203	-0.018697	-0.476013
P	-2.225190	-0.664547	-0.448838
P	-0.759768	1.582908	1.059853
C	-2.868552	-2.199739	0.369163
C	-3.063597	-0.824710	-2.085368
C	-3.274321	0.638140	0.382676
H	-3.442354	1.430307	-0.358453
H	-4.257622	0.241305	0.664014
C	-2.514715	1.195352	1.581871
H	-2.455939	0.441495	2.378272
H	-3.005026	2.080999	2.006045
C	-0.041488	2.008506	2.716985
C	-0.985635	3.307427	0.418183
P	2.180459	0.694865	-0.513386
P	0.827119	-1.585416	1.052159
C	3.151219	0.288215	-2.034511
C	2.684182	2.463045	-0.311718
C	3.195576	-0.132423	0.815083
H	3.033856	0.429433	1.744706
H	4.268191	-0.088829	0.587930
C	2.699652	-1.566180	0.968282
H	2.977430	-2.155322	0.084515
H	3.136565	-2.066174	1.842119
C	0.538868	-3.391719	0.762385
C	0.597913	-1.558857	2.895286
H	-3.959624	-2.273849	0.292715

H	-2.425071	-3.078616	-0.108873
H	-2.587376	-2.209963	1.427386
H	-2.884077	0.081801	-2.671133
H	-2.623876	-1.665169	-2.631836
H	-4.142926	-0.987145	-1.989197
H	0.996422	2.339270	2.606817
H	-0.611020	2.809401	3.202553
H	-0.051467	1.131454	3.368833
H	-0.009959	3.747529	0.191133
H	-1.557636	3.291477	-0.513239
H	-1.499898	3.943387	1.147327
H	2.322382	2.850224	0.645944
H	2.230720	3.057683	-1.111397
H	3.772163	2.588356	-0.354498
H	4.206201	0.569858	-1.942951
H	2.713092	0.819079	-2.885927
H	3.078066	-0.781992	-2.248031
H	-0.472079	-3.665163	1.077343
H	1.255025	-4.004435	1.321977
H	0.636399	-3.612222	-0.304582
H	-0.466894	-1.509227	3.144566
H	1.088146	-0.677291	3.318075
H	1.027348	-2.451892	3.363827
N	-0.395683	1.188348	-1.828665
N	0.329001	-1.298064	-1.772741
N	-0.617319	1.907150	-2.678713
N	0.523688	-2.076939	-2.575363

trans-[Cr(N$_2$)$_2$(dmpe)$_2$]
E=-2151.94048

Cr	0.000000	0.000000	0.000000
P	-0.623023	-2.198206	-0.301918
P	-2.239628	0.312148	0.447933
C	-0.222207	-3.448064	1.001652
C	-0.213427	-3.166048	-1.823961
C	-2.491960	-2.332362	-0.358635
H	-2.793829	-2.072990	-1.382364
H	-2.821410	-3.362559	-0.173047
C	-3.094399	-1.346314	0.632652
H	-2.908800	-1.682004	1.661867
H	-4.180825	-1.247882	0.513204
C	-2.859213	1.134325	1.984596
C	-3.318550	1.122016	-0.817982
P	0.623023	2.198206	0.301918
P	2.239628	-0.312148	-0.447933
C	0.222207	3.448064	-1.001652
C	0.213427	3.166048	1.823961
C	2.491960	2.332362	0.358635
H	2.793829	2.072990	1.382364
H	2.821410	3.362559	0.173047
C	3.094399	1.346314	-0.632652
H	2.908800	1.682004	-1.661867
H	4.180825	1.247882	-0.513204
C	2.859213	-1.134325	-1.984596
C	3.318550	-1.122016	0.817982
H	-0.705350	-4.412021	0.806812
H	0.861341	-3.597880	1.043494
H	-0.538018	-3.078238	1.981518
H	-0.378447	-2.541259	-2.707191
H	0.839365	-3.462421	-1.810553
H	-0.827902	-4.070030	-1.905000
H	-2.719495	2.216965	1.915958

H	-3.923510	0.931155	2.149852
H	-2.288342	0.772937	2.845518
H	-3.031422	2.172955	-0.924612
H	-3.173510	0.644221	-1.791329
H	-4.378554	1.070896	-0.545270
H	0.378447	2.541259	2.707191
H	-0.839365	3.462421	1.810553
H	0.827902	4.070030	1.905000
H	0.705350	4.412021	-0.806812
H	-0.861341	3.597880	-1.043494
H	0.538018	3.078238	-1.981518
H	2.719495	-2.216965	-1.915958
H	3.923510	-0.931155	-2.149852
H	2.288342	-0.772937	-2.845518
H	3.031422	-2.172955	0.924612
H	3.173510	-0.644221	1.791329
H	4.378554	-1.070896	0.545270
N	0.290862	-0.295952	1.813476
N	-0.290862	0.295952	-1.813476
N	0.460432	-0.463530	2.923650
N	-0.460432	0.463530	-2.923650

cis-[$Cr(CO)_2(P^{Ph}{}_2N^{Bn}{}_2)_2$]
E=-4233.10847

Cr	-0.000015	-1.535048	-0.000031
N	-3.431818	-0.710877	-1.946205
N	-1.848423	1.492222	0.448519
P	-0.739972	0.009125	-1.614105
P	-2.239867	-1.287911	0.503394
C	0.078538	1.887133	-3.638357
H	-0.570554	2.623983	-3.174176
C	0.768653	2.238145	-4.797051
H	0.657042	3.238798	-5.206631
C	1.593056	1.311067	-5.431857
H	2.130141	1.586375	-6.335321
C	1.714256	0.027915	-4.905424
H	2.347422	-0.708737	-5.391753
C	1.026001	-0.319997	-3.744381
H	1.129542	-1.324190	-3.343605
C	0.211858	0.607395	-3.084302
C	-2.173636	-0.626697	-2.661012
H	-2.303494	0.082982	-3.485921
H	-1.858676	-1.591706	-3.098939
C	-4.550180	-0.918477	-2.866262
H	-4.527754	-1.932604	-3.309217
H	-4.416833	-0.212882	-3.696816
C	-6.899666	-1.646775	-2.282538
H	-6.693976	-2.599537	-2.765447
C	-8.154849	-1.407984	-1.724777
H	-8.923187	-2.174680	-1.775568
C	-8.418506	-0.193173	-1.098838
H	-9.395422	-0.004656	-0.661859
C	-7.421375	0.780042	-1.034517
H	-7.614662	1.732613	-0.549109
C	-6.171448	0.540447	-1.596041
H	-5.396468	1.300523	-1.543442
C	-5.897197	-0.677207	-2.228577
C	-3.433429	-1.700353	-0.884586
H	-3.183198	-2.713735	-1.248707
H	-4.441270	-1.736473	-0.459648
C	-2.678182	-3.448366	2.265654
H	-1.738895	-3.829874	1.882473

C	-3.383109	-4.188128	3.214803
H	-2.987086	-5.142722	3.550027
C	-4.582074	-3.706412	3.731187
H	-5.129077	-4.281320	4.473532
C	-5.081794	-2.484126	3.284619
H	-6.022839	-2.103891	3.673351
C	-4.382734	-1.749577	2.331380
H	-4.803060	-0.810755	1.980959
C	-3.163430	-2.215526	1.817961
C	-2.814569	0.476862	0.842751
H	-3.800356	0.622147	0.372231
H	-2.934805	0.559210	1.928368
C	-2.168466	2.804298	1.022881
H	-1.326778	3.471056	0.790476
H	-2.189959	2.681653	2.111790
C	-4.645219	3.265292	1.276057
H	-4.628977	2.670096	2.186371
C	-5.838886	3.842945	0.849409
H	-6.747508	3.694836	1.427039
C	-5.864524	4.620207	-0.306892
H	-6.793085	5.075448	-0.639746
C	-4.688225	4.822567	-1.025973
H	-4.696557	5.438175	-1.921352
C	-3.497154	4.247065	-0.590561
H	-2.578791	4.428367	-1.144903
C	-3.457929	3.453565	0.561356
C	-1.540619	1.574219	-0.969950
H	-0.803631	2.376046	-1.088632
H	-2.419552	1.814401	-1.591908
N	3.431791	-0.710939	1.946197
N	1.848422	1.492206	-0.448496
P	0.739953	0.009079	1.614099
P	2.239851	-1.287920	-0.503416
C	-0.078506	1.887049	3.638411
H	0.570589	2.623903	3.174241
C	-0.768594	2.238037	4.797128
H	-0.656962	3.238677	5.206734
C	-1.592997	1.310953	5.431925
H	-2.130060	1.586243	6.335407
C	-1.714219	0.027816	4.905461
H	-2.347383	-0.708842	5.391782
C	-1.025990	-0.320073	3.744395
H	-1.129547	-1.324255	3.343599
C	-0.211855	0.607329	3.084320
C	2.173606	-0.626781	2.660997
H	2.303460	0.082874	3.485928
H	1.858640	-1.591802	3.098895
C	4.550153	-0.918552	2.866251
H	4.527744	-1.932693	3.309175
H	4.416792	-0.212984	3.696826
C	6.899664	-1.646770	2.282524
H	6.694003	-2.599544	2.765420
C	8.154841	-1.407931	1.724769
H	8.923203	-2.174604	1.775552
C	8.418460	-0.193104	1.098845
H	9.395371	-0.004551	0.661870
C	7.421298	0.780080	1.034533
H	7.614555	1.732662	0.549134
C	6.171377	0.540438	1.596052
H	5.396372	1.300488	1.543458
C	5.897165	-0.677232	2.228574
C	3.433407	-1.700390	0.884557

H	3.183180	-2.713782	1.248652
H	4.441248	-1.736495	0.459618
C	2.678236	-3.448394	-2.265639
H	1.738984	-3.829950	-1.882421
C	3.383180	-4.188138	-3.214789
H	2.987204	-5.142764	-3.549978
C	4.582102	-3.706365	-3.731218
H	5.129119	-4.281259	-4.473563
C	5.081764	-2.484039	-3.284693
H	6.022775	-2.103757	-3.673461
C	4.382688	-1.749509	-2.331450
H	4.802967	-0.810653	-1.981065
C	3.163424	-2.215515	-1.817988
C	2.814564	0.476850	-0.842747
H	3.800354	0.622125	-0.372227
H	2.934800	0.559213	-1.928363
C	2.168474	2.804289	-1.022837
H	1.326795	3.471052	-0.790415
H	2.189958	2.681663	-2.111749
C	4.645235	3.265240	-1.276010
H	4.628981	2.670056	-2.186331
C	5.838916	3.842856	-0.849350
H	6.747535	3.694733	-1.426980
C	5.864570	4.620100	0.306963
H	6.793141	5.075313	0.639826
C	4.688275	4.822478	1.026045
H	4.696620	5.438071	1.921434
C	3.497190	4.247010	0.590622
H	2.578832	4.428323	1.144967
C	3.457949	3.453529	-0.561308
C	1.540620	1.574177	0.969975
H	0.803640	2.376008	1.088671
H	2.419556	1.814338	1.591938
C	-0.390948	-2.865407	-1.159147
O	-0.665017	-3.774648	-1.855368
C	0.390903	-2.865459	1.159033
O	0.665046	-3.774743	1.855167

trans-[$Cr(CO)_2(P^{Ph}{}_2N^{Bn}{}_2)_2$]
E=-4233.09109

Cr	0.000000	0.369708	-0.000002
N	-3.614185	0.622284	-1.678520
N	-2.969281	-0.086653	1.785846
P	-1.795752	1.771868	0.026265
P	-1.726892	-1.071336	-0.452096
C	-1.373010	3.872598	1.828011
H	-1.150157	3.073580	2.531396
C	-1.317830	5.194781	2.255960
H	-1.069993	5.415393	3.291050
C	-1.577942	6.231801	1.361619
H	-1.537727	7.265266	1.694727
C	-1.878290	5.934304	0.036349
H	-2.064791	6.735429	-0.673714
C	-1.944724	4.608552	-0.389984
H	-2.175710	4.403919	-1.431117
C	-1.710758	3.558611	0.503013
C	-2.852005	1.850089	-1.517405
H	-3.568883	2.672617	-1.411184
H	-2.203410	2.069234	-2.385212
C	-4.646375	0.765463	-2.704014
H	-4.209594	0.794913	-3.720959
H	-5.125988	1.739999	-2.542951

C	-6.034969	-1.059355	-3.771155
H	-5.505349	-0.878997	-4.704114
C	-7.034681	-2.029623	-3.716784
H	-7.281563	-2.601195	-4.607395
C	-7.707597	-2.269719	-2.522292
H	-8.485293	-3.027321	-2.476568
C	-7.376799	-1.534324	-1.384127
H	-7.892664	-1.713025	-0.444766
C	-6.382603	-0.563215	-1.443475
H	-6.125347	0.006408	-0.554647
C	-5.700544	-0.314150	-2.639601
C	-2.809443	-0.567157	-1.909087
H	-2.157446	-0.470121	-2.795615
H	-3.496739	-1.398610	-2.094522
C	-2.500882	-3.817617	-0.763194
H	-3.396157	-3.586876	-0.192350
C	-2.334199	-5.106888	-1.262967
H	-3.086383	-5.864690	-1.059910
C	-1.213430	-5.421871	-2.027623
H	-1.085372	-6.427165	-2.419601
C	-0.260904	-4.440780	-2.290405
H	0.613556	-4.677390	-2.890646
C	-0.422124	-3.156032	-1.778429
H	0.325378	-2.391354	-1.975901
C	-1.539718	-2.828697	-1.004453
C	-3.060587	-1.193777	0.861116
H	-4.049636	-1.294967	0.380730
H	-2.868436	-2.112347	1.429874
C	-3.664213	-0.312290	3.049653
H	-3.367768	0.494039	3.731588
H	-3.275358	-1.247447	3.472669
C	-5.821360	-1.617612	2.795427
H	-5.229717	-2.530526	2.773372
C	-7.207004	-1.690958	2.671024
H	-7.689040	-2.657780	2.551770
C	-7.973401	-0.527963	2.712638
H	-9.054748	-0.581659	2.621453
C	-7.345223	0.703944	2.886669
H	-7.936318	1.614665	2.932391
C	-5.960141	0.769597	3.014932
H	-5.479163	1.733184	3.167516
C	-5.176348	-0.388641	2.964914
C	-3.155508	1.240456	1.240956
H	-3.112219	1.942961	2.078589
H	-4.124604	1.381496	0.734887
N	3.614186	0.622281	1.678522
N	2.969279	-0.086649	-1.785851
P	1.795754	1.771867	-0.026264
P	1.726893	-1.071335	0.452092
C	1.372996	3.872600	-1.828002
H	1.150133	3.073584	-2.531386
C	1.317812	5.194784	-2.255948
H	1.069963	5.415398	-3.291035
C	1.577936	6.231802	-1.361609
H	1.537717	7.265268	-1.694714
C	1.878298	5.934303	-0.036343
H	2.064806	6.735426	0.673719
C	1.944735	4.608550	0.389987
H	2.175732	4.403915	1.431117
C	1.710759	3.558610	-0.503009
C	2.852007	1.850086	1.517406
H	3.568886	2.672614	1.411186

H	2.203412	2.069231	2.385213
C	4.646372	0.765459	2.704020
H	4.209587	0.794913	3.720963
H	5.125988	1.739994	2.542956
C	6.034950	-1.059365	3.771170
H	5.505319	-0.879010	4.704124
C	7.034660	-2.029636	3.716807
H	7.281530	-2.601211	4.607419
C	7.707589	-2.269729	2.522322
H	8.485284	-3.027332	2.476605
C	7.376807	-1.534328	1.384156
H	7.892683	-1.713027	0.444801
C	6.382613	-0.563218	1.443496
H	6.125369	0.006410	0.554667
C	5.700539	-0.314155	2.639615
C	2.809441	-0.567159	1.909086
H	2.157442	-0.470122	2.795612
H	3.496735	-1.398614	2.094523
C	0.422121	-3.156034	1.778417
H	-0.325381	-2.391355	1.975887
C	0.260898	-4.440782	2.290390
H	-0.613564	-4.677392	2.890627
C	1.213424	-5.421873	2.027609
H	1.085364	-6.427167	2.419585
C	2.334196	-5.106890	1.262957
H	3.086380	-5.864692	1.059902
C	2.500882	-3.817618	0.763187
H	3.396158	-3.586877	0.192346
C	1.539718	-2.828698	1.004445
C	3.060587	-1.193774	-0.861121
H	4.049636	-1.294964	-0.380736
H	2.868435	-2.112343	-1.429881
C	3.664210	-0.312284	-3.049660
H	3.367765	0.494047	-3.731592
H	3.275354	-1.247439	-3.472677
C	5.821358	-1.617608	-2.795444
H	5.229715	-2.530522	-2.773393
C	7.207002	-1.690954	-2.671047
H	7.689038	-2.657778	-2.551799
C	7.973399	-0.527960	-2.712658
H	9.054746	-0.581657	-2.621477
C	7.345220	0.703948	-2.886680
H	7.936316	1.614669	-2.932399
C	5.960138	0.769603	-3.014938
H	5.479160	1.733190	-3.167517
C	5.176345	-0.388635	-2.964923
C	3.155508	1.240458	-1.240958
H	3.112218	1.942966	-2.078589
H	4.124605	1.381497	-0.734891
C	-0.172425	0.485768	1.841484
C	0.172424	0.485769	-1.841487
O	-0.195056	0.646582	3.004059
O	0.195132	0.646612	-3.004057

cis-$[Cr(CO)_2(dmpe)_2]$
E=-2159.58913

Cr	0.000064	-0.000120	0.470449
P	-2.188279	0.660513	0.515961
P	-0.800117	-1.549666	-1.104540
C	-2.795209	2.265331	-0.190326
C	-3.002500	0.744571	2.167888
C	-3.288089	-0.557409	-0.380506

H	-3.494160	-1.375422	0.321586
H	-4.251402	-0.107125	-0.649962
C	-2.542713	-1.087984	-1.600133
H	-2.459602	-0.304117	-2.364762
H	-3.056328	-1.941866	-2.060495
C	-0.093733	-1.945384	-2.774762
C	-1.060911	-3.287018	-0.522885
P	2.188583	-0.660253	0.515848
P	0.799752	1.549371	-1.104816
C	3.001864	-0.747190	2.168056
C	2.796952	-2.263063	-0.193828
C	3.288068	0.559931	-0.377765
H	4.252430	0.111256	-0.646168
H	3.491878	1.377681	0.325288
C	2.543695	1.090260	-1.598130
H	3.056796	1.945071	-2.057326
H	2.462801	0.306684	-2.363301
C	1.057227	3.287483	-0.523921
C	0.094696	1.942788	-2.776151
H	-3.870146	2.403244	-0.025645
H	-2.260218	3.094444	0.283720
H	-2.598402	2.303215	-1.266124
H	-2.837804	-0.198078	2.697791
H	-2.535544	1.541290	2.755436
H	-4.078178	0.938972	2.091095
H	0.855347	-2.476922	-2.656631
H	-0.773820	-2.581855	-3.352918
H	0.100113	-1.032795	-3.344478
H	-0.091716	-3.750657	-0.314717
H	-1.627155	-3.286865	0.412066
H	-1.588482	-3.890416	-1.270338
H	2.601991	-2.297786	-1.270072
H	2.261398	-3.093738	0.276833
H	3.871657	-2.401156	-0.027777
H	4.077705	-0.940784	2.091555
H	2.535019	-1.545351	2.753732
H	2.836263	0.194314	2.699712
H	0.087202	3.749490	-0.316068
H	1.583908	3.891553	-1.271462
H	1.623331	3.288599	0.411127
H	-0.855699	2.472353	-2.659614
H	-0.096417	1.029512	-3.345689
H	0.774210	2.580418	-3.353701
C	0.331541	1.209980	1.771463
O	0.526592	1.980388	2.639675
C	-0.331169	-1.210682	1.771127
O	-0.526084	-1.981566	2.638946

trans-$[Cr(CO)_2(dmpe)_2]$
E=-2159.58786

Cr	0.000000	0.000000	0.000000
P	-0.607912	-2.185221	-0.298386
P	-2.222384	0.320933	0.442121
C	-0.205556	-3.451265	0.990480
C	-0.201537	-3.155639	-1.820322
C	-2.475073	-2.324309	-0.355404
H	-2.775913	-2.072625	-1.381148
H	-2.799997	-3.354467	-0.162328
C	-3.080446	-1.333980	0.628101
H	-2.900697	-1.665215	1.659597
H	-4.165641	-1.231960	0.501537
C	-2.845176	1.141720	1.978813

C	-3.314658	1.138594	-0.808652
P	0.607912	2.185221	0.298386
P	2.222384	-0.320933	-0.442121
C	0.205556	3.451265	-0.990480
C	0.201537	3.155639	1.820322
C	2.475073	2.324309	0.355404
H	2.775913	2.072625	1.381148
H	2.799997	3.354467	0.162328
C	3.080446	1.333980	-0.628101
H	2.900697	1.665215	-1.659597
H	4.165641	1.231960	-0.501537
C	2.845176	-1.141720	-1.978813
C	3.314658	-1.138594	0.808652
H	-0.664081	-4.422165	0.770791
H	0.880011	-3.579363	1.050288
H	-0.547228	-3.102793	1.969487
H	-0.380084	-2.537216	-2.705048
H	0.853039	-3.445682	-1.816009
H	-0.809281	-4.065379	-1.887953
H	-2.699046	2.223884	1.917763
H	-3.912827	0.945924	2.131551
H	-2.284270	0.771530	2.842164
H	-3.007394	2.181579	-0.935816
H	-3.200358	0.644358	-1.777885
H	-4.369384	1.114986	-0.511776
H	0.380084	2.537216	2.705048
H	-0.853039	3.445682	1.816009
H	0.809281	4.065379	1.887953
H	0.664081	4.422165	-0.770791
H	-0.880011	3.579363	-1.050288
H	0.547228	3.102793	-1.969487
H	2.699046	-2.223884	-1.917763
H	3.912827	-0.945924	-2.131551
H	2.284270	-0.771530	-2.842164
H	3.007394	-2.181579	0.935816
H	3.200358	-0.644358	1.777885
H	4.369384	-1.114986	0.511776
C	0.276049	-0.276792	1.801714
O	0.439124	-0.432744	2.953767
C	-0.276049	0.276792	-1.801714
O	-0.439124	0.432744	-2.953767

$Cr(N_2)(P^{Ph}{}_2N^{Bn}{}_2)_2$
E=-4115.64146

Cr	0.000284	0.000862	-0.886670
N	3.926618	-0.464342	-1.484883
N	2.031444	-0.901836	1.605779
P	1.486895	-1.714726	-0.939065
P	1.938363	1.104781	-0.367743
C	1.882959	-4.548416	-1.168273
H	2.677745	-4.452034	-0.431905
C	1.625143	-5.797541	-1.726506
H	2.205129	-6.661129	-1.411065
C	0.631734	-5.938167	-2.693775
H	0.435046	-6.911630	-3.134898
C	-0.104442	-4.826496	-3.094230
H	-0.876987	-4.928496	-3.851659
C	0.143285	-3.580381	-2.522379
H	-0.433358	-2.711770	-2.830427
C	1.138606	-3.426239	-1.552899

C	2.993499	-1.435295	-2.031731
H	3.518933	-2.392091	-2.123884
H	2.623609	-1.161235	-3.037446
C	5.227471	-0.540369	-2.148791
H	5.179121	-0.151789	-3.184662
H	5.485070	-1.604336	-2.228896
C	7.145776	1.103643	-2.031425
H	6.972841	1.337706	-3.079771
C	8.181782	1.731868	-1.341615
H	8.812426	2.453534	-1.853862
C	8.401695	1.439499	0.001322
H	9.206122	1.930254	0.542417
C	7.582315	0.515022	0.648888
H	7.742316	0.279463	1.697400
C	6.553531	-0.114318	-0.043955
H	5.914854	-0.832373	0.463039
C	6.323722	0.173137	-1.393876
C	3.431105	0.900913	-1.476704
H	3.161621	1.250732	-2.492471
H	4.238162	1.538433	-1.101274
C	2.910497	3.819689	-0.577279
H	3.530377	3.508781	-1.412566
C	2.937332	5.158491	-0.187306
H	3.576122	5.858912	-0.718794
C	2.155662	5.596851	0.876130
H	2.180560	6.639335	1.180943
C	1.333080	4.689559	1.542699
H	0.713512	5.023079	2.371271
C	1.299234	3.358205	1.143991
H	0.637182	2.659209	1.653956
C	2.097347	2.897265	0.087460
C	2.630526	0.374182	1.232720
H	3.729935	0.334848	1.149654
H	2.386638	1.089100	2.024731
C	2.278288	-1.234299	3.014104
H	1.681297	-2.126019	3.243785
H	1.873459	-0.411217	3.615951
C	4.533745	-0.432180	3.849175
H	4.109747	0.564256	3.950857
C	5.870662	-0.648101	4.175683
H	6.480526	0.179066	4.529104
C	6.420121	-1.923511	4.061336
H	7.461059	-2.095994	4.320375
C	5.622379	-2.979901	3.626105
H	6.039516	-3.980093	3.545804
C	4.285843	-2.757850	3.304388
H	3.664761	-3.590746	2.981877
C	3.722371	-1.480963	3.404352
C	2.322354	-2.014229	0.708763
H	1.866042	-2.913120	1.139862
H	3.402024	-2.201844	0.582633
N	-3.925918	0.463280	-1.484671
N	-2.032600	0.902918	1.606798
P	-1.487307	1.715771	-0.938088
P	-1.936984	-1.103914	-0.366409
C	-1.887417	4.548679	-1.168368
H	-2.684033	4.450795	-0.434168
C	-1.630091	5.798357	-1.725557
H	-2.212305	6.660946	-1.411489
C	-0.634244	5.940813	-2.690065
H	-0.437859	6.914719	-3.130346
C	0.104758	4.830423	-3.088843

H	0.879234	4.933872	-3.844093
C	-0.142602	3.583751	-2.518044
H	0.436249	2.716086	-2.824617
C	-1.140233	3.427776	-1.551290
C	-2.993332	1.434983	-2.031221
H	-3.519549	2.391322	-2.123640
H	-2.622865	1.161137	-3.036763
C	-5.226475	0.538186	-2.149297
H	-5.177211	0.149628	-3.185132
H	-5.484948	1.601928	-2.229574
C	-7.143398	-1.107501	-2.033006
H	-6.969601	-1.341473	-3.081231
C	-8.179281	-1.736598	-1.343809
H	-8.808973	-2.458843	-1.856411
C	-8.400288	-1.444347	-0.001026
H	-9.204622	-1.935773	0.539597
C	-7.582121	-0.519115	0.646993
H	-7.742987	-0.283625	1.695388
C	-6.553452	0.111089	-0.045240
H	-5.915738	0.829743	0.462114
C	-6.322548	-0.176243	-1.394998
C	-3.429312	-0.901609	-1.476178
H	-3.158931	-1.251191	-2.491774
H	-4.236027	-1.539829	-1.101185
C	-1.297515	-3.355955	1.147404
H	-0.637145	-2.656010	1.658233
C	-1.330499	-4.687201	1.546552
H	-0.711973	-5.019701	2.376316
C	-2.150976	-5.595668	0.878985
H	-2.175229	-6.638057	1.184175
C	-2.931376	-5.158599	-0.185913
H	-3.568479	-5.859950	-0.718193
C	-2.905407	-3.819921	-0.576358
H	-3.524240	-3.509971	-1.412780
C	-2.094426	-2.896328	0.089383
C	-2.630604	-0.373502	1.233505
H	-3.729977	-0.334853	1.149629
H	-2.386892	-1.088141	2.025815
C	-2.280525	1.235475	3.014912
H	-1.684230	2.127608	3.244782
H	-1.875535	0.412760	3.617156
C	-4.535931	0.432090	3.848897
H	-4.111333	-0.564040	3.951079
C	-5.873173	0.647214	4.174606
H	-6.482685	-0.180262	4.527910
C	-6.423406	1.922232	4.059620
H	-7.464603	2.094103	4.318022
C	-5.626110	2.979035	3.624571
H	-6.043861	3.978932	3.543787
C	-4.289246	2.757785	3.303671
H	-3.668523	3.591010	2.981315
C	-3.724993	1.481291	3.404266
C	-2.323677	2.014896	0.709395
H	-1.868215	2.914211	1.140515
H	-3.403406	2.201800	0.582634
N	-0.000724	0.000862	-2.700424
N	-0.001474	0.000778	-3.843601

$Cr(N_2)_2(\kappa^2\text{-}P^{Ph}{}_2N^{Bn}{}_2)(\kappa^1\text{-}P^{Ph}{}_2N^{Bn}{}_2)$
E=-4225.40272

Cr	0.402774	0.025183	0.767022
N	-3.886763	-0.336671	-1.754250

N	-3.281135	1.090971	1.537154
P	-2.789544	2.047858	-1.034125
P	-1.730554	-0.747302	0.088474
C	-2.533656	4.799725	-0.880702
H	-1.848159	4.553344	-0.072216
C	-2.745131	6.129026	-1.230953
H	-2.241254	6.916985	-0.677488
C	-3.584558	6.449619	-2.297132
H	-3.742728	7.487612	-2.576737
C	-4.211434	5.429869	-3.006951
H	-4.863856	5.669080	-3.842876
C	-4.014300	4.097402	-2.646641
H	-4.521555	3.323067	-3.214254
C	-3.179746	3.762541	-1.573170
C	-3.842660	1.046149	-2.197803
H	-4.871433	1.428937	-2.219602
H	-3.418822	1.146803	-3.216963
C	-4.776090	-1.135930	-2.596562
H	-4.316444	-1.366668	-3.576283
H	-5.657511	-0.516533	-2.805411
C	-4.926070	-3.661592	-2.471808
H	-4.343345	-3.718180	-3.388742
C	-5.361317	-4.832970	-1.852221
H	-5.114769	-5.797852	-2.286637
C	-6.106902	-4.764222	-0.679190
H	-6.450372	-5.674852	-0.196026
C	-6.415582	-3.519207	-0.128514
H	-6.999411	-3.455170	0.785555
C	-5.979095	-2.353766	-0.749967
H	-6.216909	-1.384915	-0.318651
C	-5.228182	-2.412029	-1.929951
C	-2.567380	-0.940753	-1.614200
H	-1.866609	-0.576432	-2.379255
H	-2.673662	-2.020276	-1.753105
C	-2.563636	-3.443757	0.720890
H	-3.596719	-3.135263	0.583154
C	-2.289232	-4.758680	1.090852
H	-3.109787	-5.455292	1.240035
C	-0.972255	-5.180634	1.262930
H	-0.761949	-6.206590	1.553120
C	0.074213	-4.284297	1.057647
H	1.104349	-4.604850	1.186181
C	-0.201077	-2.969768	0.686737
H	0.650253	-2.304392	0.493274
C	-1.521400	-2.531304	0.518597
C	-3.175649	-0.316211	1.210353
H	-4.101813	-0.743297	0.794987
H	-2.938745	-0.852137	2.133911
C	-3.852961	1.328352	2.865860
H	-3.749622	2.400454	3.073779
H	-3.219584	0.798510	3.586714
C	-5.623848	-0.371629	3.499586
H	-4.824956	-1.055451	3.777747
C	-6.951122	-0.777093	3.618881
H	-7.180622	-1.774454	3.985148
C	-7.982008	0.098576	3.284309
H	-9.018283	-0.213620	3.381330
C	-7.675635	1.382493	2.838468
H	-8.473224	2.077149	2.588387
C	-6.346547	1.782514	2.723052
H	-6.115989	2.792187	2.390144
C	-5.299945	0.910928	3.044053

C	-3.858282	1.933498	0.510885
H	-3.916651	2.951442	0.911828
H	-4.882940	1.634826	0.219185
N	3.746157	1.633054	-0.679990
N	3.040645	-1.909994	-0.249967
P	1.482468	0.146505	-1.270975
P	2.573210	0.233898	1.433957
C	0.470244	-1.014660	-3.693671
H	0.837710	-1.973576	-3.338689
C	-0.220529	-0.973754	-4.903236
H	-0.355928	-1.888009	-5.475121
C	-0.736854	0.229820	-5.376228
H	-1.273546	0.262495	-6.320260
C	-0.562905	1.391048	-4.625407
H	-0.968702	2.335944	-4.976631
C	0.129271	1.348480	-3.417679
H	0.230819	2.261119	-2.837632
C	0.671068	0.146610	-2.937343
C	2.531503	1.695704	-1.474597
H	2.816013	1.774650	-2.529563
H	1.907447	2.571594	-1.222719
C	4.717646	2.640019	-1.108887
H	4.391125	3.661919	-0.836489
H	4.753059	2.605909	-2.205643
C	6.798791	3.397603	0.110426
H	6.319393	4.360481	0.272805
C	8.093413	3.179059	0.579265
H	8.618656	3.972199	1.104378
C	8.706318	1.945189	0.381716
H	9.714148	1.771224	0.748821
C	8.018905	0.932743	-0.287532
H	8.485195	-0.035663	-0.446254
C	6.729363	1.156061	-0.758711
H	6.195792	0.364528	-1.277879
C	6.104674	2.393074	-0.565493
C	3.514135	1.706302	0.753092
H	2.954918	2.615755	1.043297
H	4.487000	1.738996	1.253793
C	4.282794	-0.089626	3.720499
H	4.955714	-0.668610	3.093858
C	4.629679	0.136725	5.050081
H	5.552217	-0.280745	5.444902
C	3.802354	0.902623	5.868428
H	4.073580	1.078314	6.905842
C	2.628244	1.442916	5.350564
H	1.977405	2.041611	5.981654
C	2.275566	1.207992	4.023974
H	1.353280	1.622607	3.628257
C	3.096133	0.435438	3.193207
C	3.667768	-1.166159	0.836470
H	4.671258	-0.785784	0.580205
H	3.774106	-1.860561	1.678252
C	3.698130	-3.201076	-0.487177
H	3.081572	-3.749565	-1.210251
H	3.659739	-3.758980	0.456981
C	6.197104	-3.180214	-0.070716
H	5.989807	-3.285024	0.992098
C	7.516321	-3.097226	-0.510291
H	8.329369	-3.134976	0.209741
C	7.791898	-2.978518	-1.870954
H	8.819781	-2.919460	-2.217819
C	6.741331	-2.951506	-2.786231

H	6.947839	-2.871973	-3.850033
C	5.425076	-3.039307	-2.340365
H	4.612354	-3.036042	-3.063198
C	5.132017	-3.147473	-0.976321
C	2.822737	-1.157778	-1.479166
H	2.486400	-1.870425	-2.237163
H	3.733886	-0.669749	-1.860007
N	0.114417	1.814202	0.823352
N	-0.060281	2.937276	0.866247
N	-0.234257	-0.206179	2.492497
N	-0.626326	-0.381934	3.540875

$Cr(N_2)(dmpe)_2$
E=-2042.12105

Cr	-0.000001	-0.014482	-0.132011
P	-1.709782	1.528114	-0.177858
P	-1.716746	-1.525803	-0.181770
C	-3.381492	0.686065	-0.365721
H	-4.187565	1.310762	0.039402
H	-3.566185	0.579091	-1.443577
C	-3.323695	-0.684210	0.294159
H	-4.191307	-1.306316	0.038960
P	1.716955	-1.525605	-0.181059
P	1.709524	1.528345	-0.178671
C	3.323271	-0.683579	0.296131
H	4.191256	-1.305656	0.042129
C	3.381556	0.686404	-0.364300
H	3.567389	0.578940	-1.441910
H	4.187131	1.311398	0.041351
N	0.000255	-0.055143	1.673972
N	0.000518	-0.099441	2.817683
H	-3.303928	-0.578937	1.386968
H	3.302281	-0.577846	1.388872
C	-2.225722	-2.327069	-1.781237
H	-3.140158	-2.921585	-1.669860
H	-2.395358	-1.563028	-2.547252
H	-1.422263	-2.981098	-2.135415
C	2.227323	-2.326957	-1.780029
H	3.141780	-2.921298	-1.667892
H	1.424253	-2.981175	-2.134743
H	2.397395	-1.562978	-2.546009
C	-1.934476	2.870591	-1.442024
H	-1.848686	2.451354	-2.450162
H	-2.911580	3.358818	-1.346224
H	-1.154237	3.628939	-1.326113
C	1.934701	2.868862	-1.444837
H	2.911417	3.357820	-1.348817
H	1.850289	2.447827	-2.452345
H	1.153869	3.626922	-1.331125
C	1.807906	-2.988294	0.948084
H	1.505690	-2.680189	1.953781
H	1.122551	-3.770770	0.610346
H	2.821037	-3.405065	0.988984
C	1.987261	2.514638	1.362695
H	1.950286	1.852455	2.232394
H	2.947171	3.042983	1.342552
H	1.182942	3.247967	1.475670
C	-1.988907	2.511928	1.364842
H	-1.184437	3.244726	1.480090
H	-2.948603	3.040649	1.344416
H	-1.953223	1.848294	2.233483
C	-1.808257	-2.988680	0.947093

H	-1.506786	-2.680726	1.953059
H	-2.821351	-3.405620	0.987207
H	-1.122541	-3.770983	0.609692

$Cr(N_2)_2(\kappa^2\text{-dmpe})(\kappa^1\text{-dmpe})$
E=-2151.88884

Cr	-0.879437	0.450700	-0.227634
P	4.535652	-0.715970	-1.219182
P	1.014587	1.459339	0.674115
C	2.973737	-0.373282	-0.254851
C	2.620902	1.112456	-0.204384
P	-1.217317	-1.189133	1.403877
P	-2.679098	-0.568995	-1.226020
C	-2.601589	-2.345229	0.884834
H	-2.138149	-3.151603	0.300477
H	-3.072015	-2.811875	1.759321
C	-3.610312	-1.590647	0.023537
H	-4.183885	-0.885075	0.638138
H	-4.327456	-2.267407	-0.457573
N	-1.983531	1.609346	0.634424
N	-2.668396	2.339982	1.176023
N	-0.677218	1.544047	-1.699367
N	-0.523672	2.176334	-2.631057
H	3.062872	-0.790995	0.758476
H	2.167147	-0.925909	-0.756069
H	3.421175	1.690759	0.276771
H	2.510510	1.503991	-1.223555
C	5.800550	-0.153323	0.017189
H	5.793314	0.938648	0.091159
H	5.633776	-0.576452	1.015740
H	6.797493	-0.449508	-0.325306
C	-4.002939	0.499714	-1.930528
H	-4.313351	1.225879	-1.173215
H	-3.597689	1.056549	-2.781064
H	-4.874009	-0.076436	-2.261586
C	-1.816085	-0.625628	3.059848
H	-2.641808	0.079822	2.930572
H	-2.147162	-1.465764	3.680519
H	-1.009961	-0.098517	3.578574
C	0.967052	3.299940	0.553489
H	0.831245	3.587263	-0.493209
H	0.104823	3.671760	1.115579
H	1.879203	3.766574	0.942045
C	-2.443601	-1.781835	-2.608307
H	-3.393972	-2.211370	-2.945335
H	-1.967072	-1.275023	-3.453673
H	-1.782318	-2.594314	-2.289568
C	0.039014	-2.447776	1.927429
H	0.865125	-1.956224	2.450072
H	-0.395549	-3.202295	2.593410
H	0.449835	-2.951414	1.046332
C	1.537702	1.278702	2.441391
H	1.750427	0.230859	2.673580
H	2.427969	1.877669	2.666279
H	0.721179	1.611101	3.090296
C	4.647844	-2.546844	-0.935188
H	4.559201	-2.818697	0.123995
H	3.856989	-3.055572	-1.496191
H	5.607326	-2.917296	-1.310550