

A Series of C_3 -Symmetric Heterobimetallic Cr/M (M = Fe, Co and Cu) Complexes.

Subramaniam Kuppuswamy,[†] Mark W. Bezpalko,[†] Tamara M. Powers,[‡] Matthew J. T. Wilding,[‡] Carl K. Brozek,[‡] Bruce M. Foxman,[†] Christine M. Thomas^{*,†}

[†]*Department of Chemistry, Brandeis University, 415 South Street, MS 015, Waltham, Massachusetts 02454, United States.* [‡]*Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02139.* ^{*}*Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139-4307 USA.*

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Figure S1. ^1H NMR spectrum of **1** in benzene- d_6 .

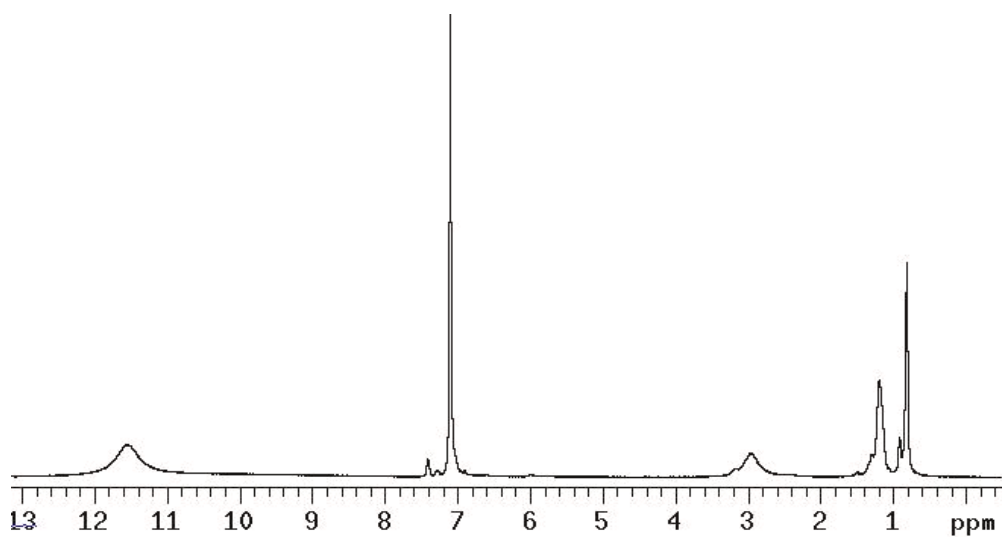


Figure S2. ^1H NMR spectrum of **2** in benzene- d_6 .

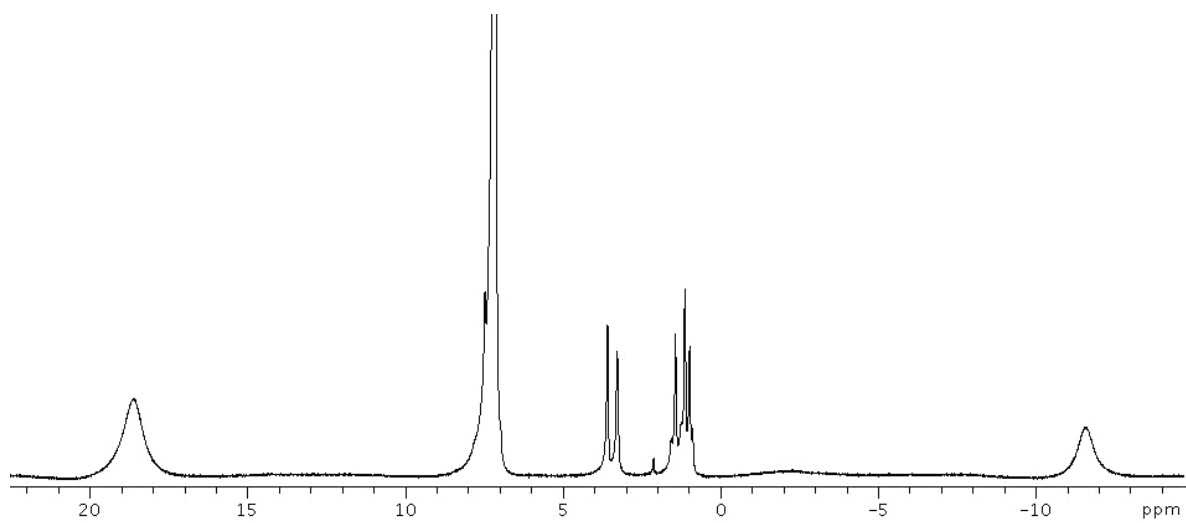


Figure S3. ^1H NMR spectrum of **3** in benzene- d_6 .

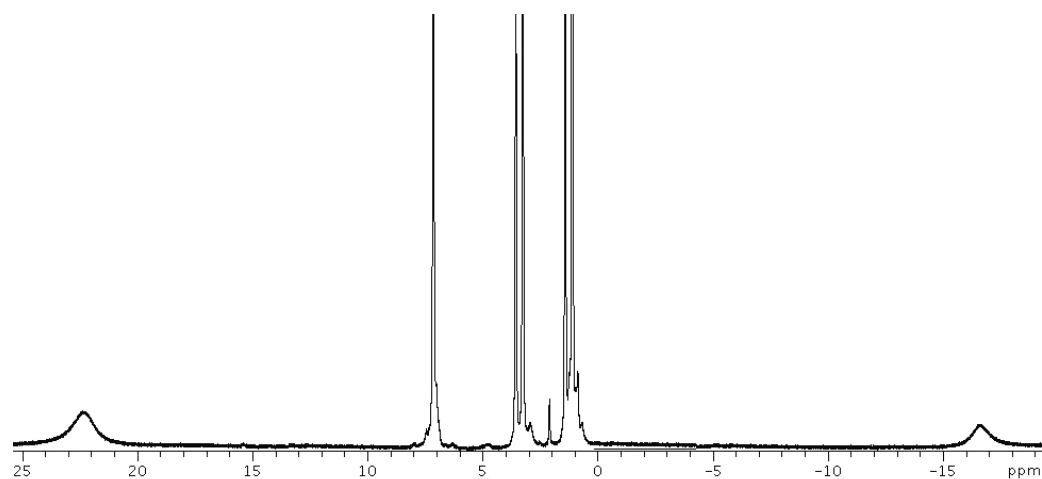


Figure S4. ^1H NMR spectrum of **4** in benzene- d_6 .

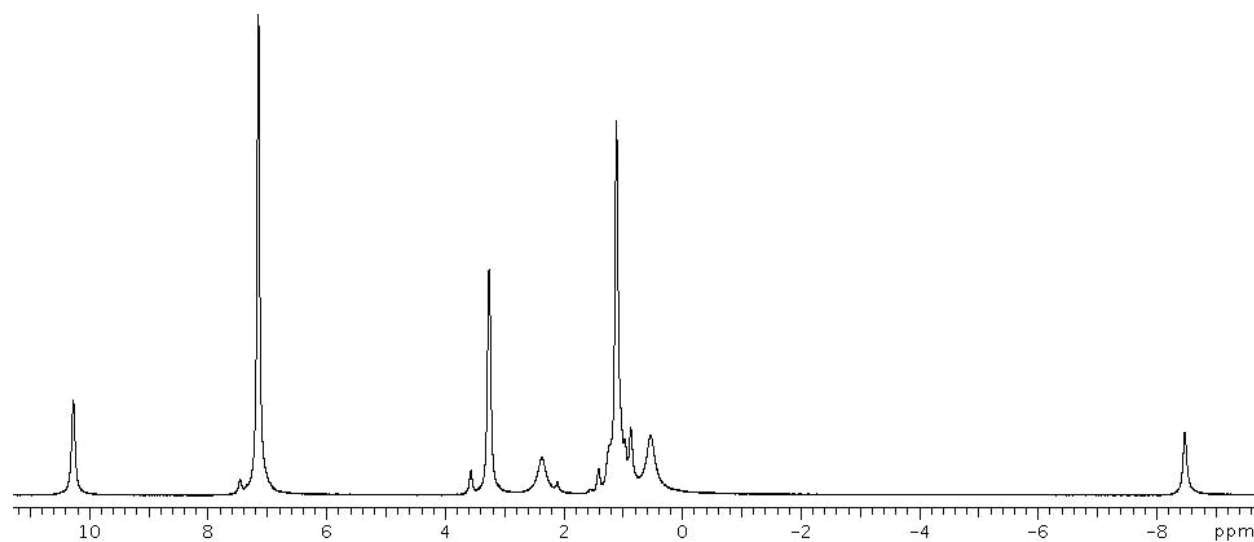


Figure S5. ^1H NMR spectrum of **5** in benzene- d_6 .

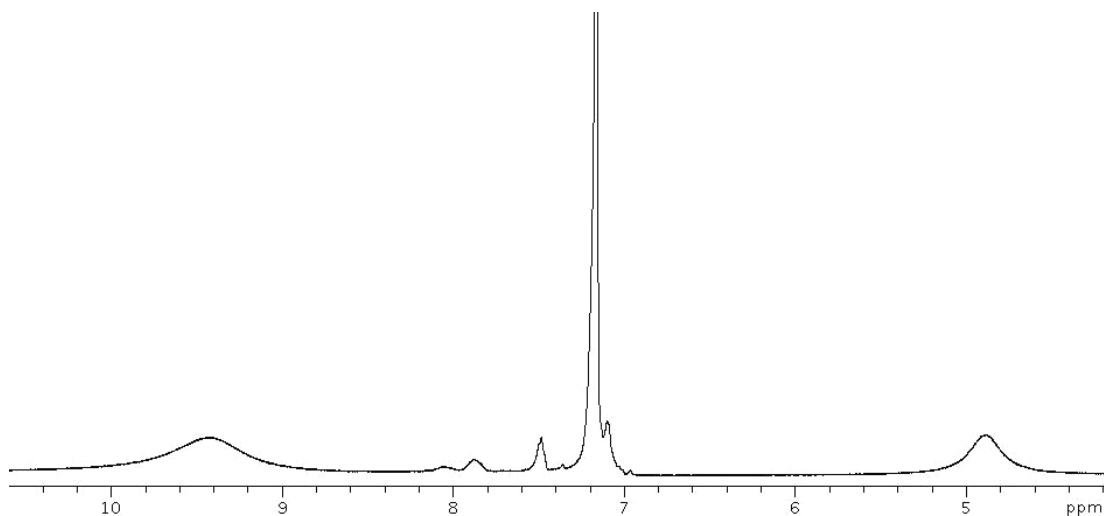


Figure S6. ^1H NMR spectrum of **6** in benzene- d_6 .

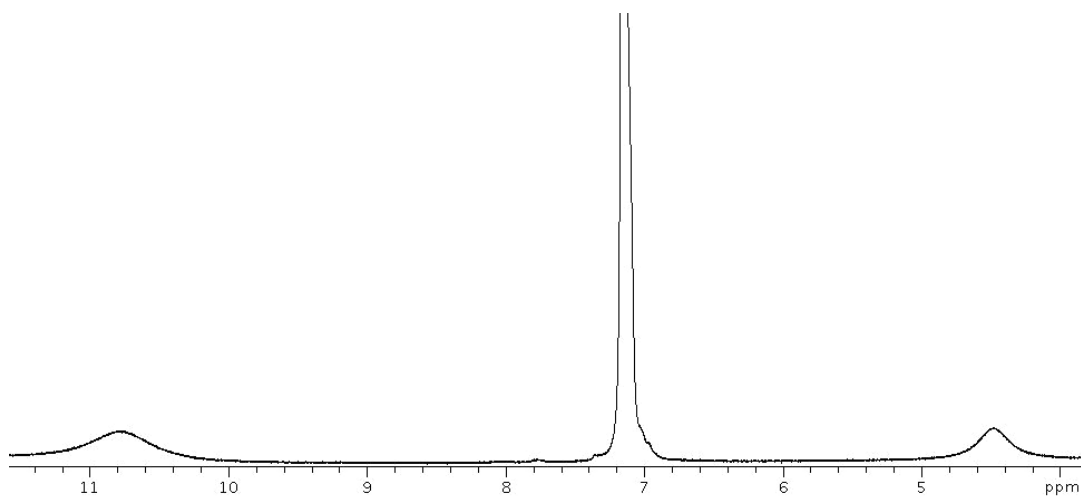


Figure S7. NIR spectra of complexes **2-6** in benzene-d₆.

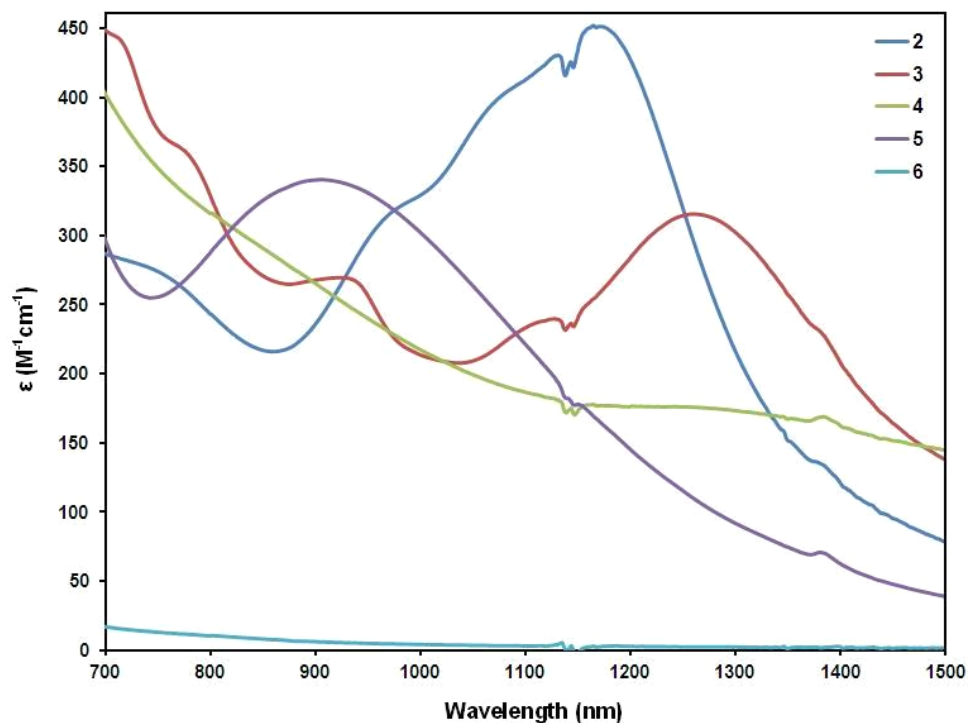


Figure S8. Solid state zero field Mössbauer spectrum of **2** at 110 K. The spectrum was fit to include a ~37% impurity. This impurity was present despite repeated attempts to collect this data on different samples of **2**.

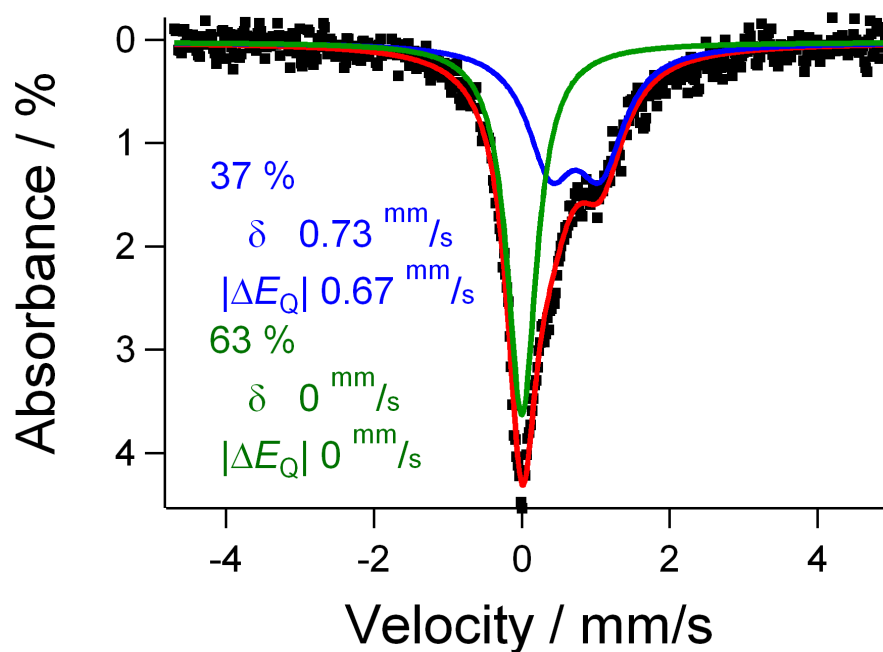


Figure S9. Cyclic voltammogram of **1** (2 mM in 0.4 M [ⁿBu₄N][PF₆] in THF, scan rate = 100 mV/s). Y axis is potential versus ferrocene/ferrocenium.

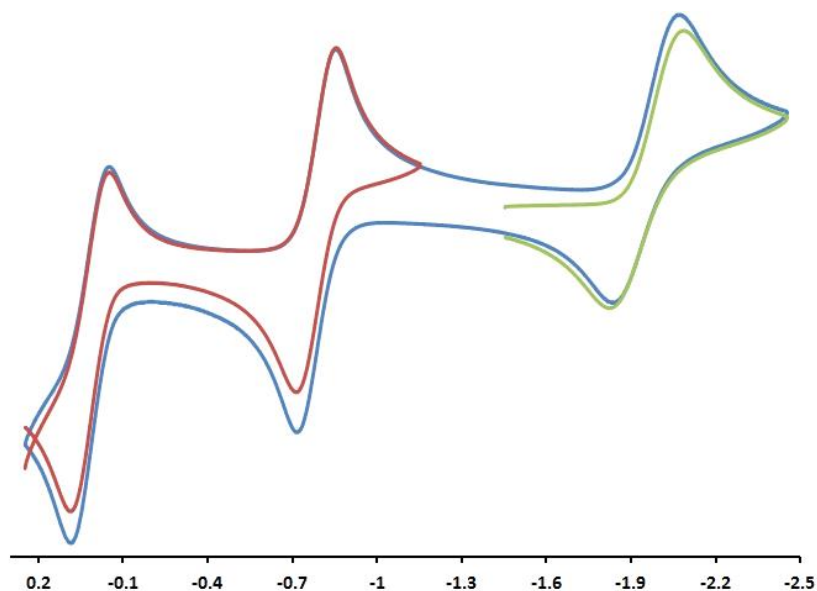


Figure S10. Cyclic voltammogram of **2** (2 mM in 0.4 M [ⁿBu₄N][PF₆] in THF, scan rate = 100 mV/s), shown in blue. Addition of a small amount of NaI leads to the CV shown in red, and addition of excess NaI leads to the CV shown in green. Y axis is potential versus ferrocene/ferrocenium.

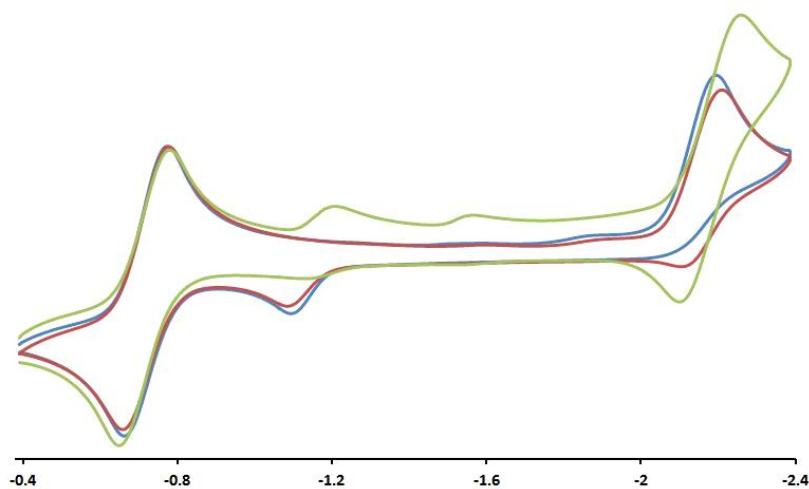


Figure S11. Cyclic voltammogram of **3** (2 mM in 0.4 M [ⁿBu₄N][PF₆] in THF, scan rate = 100 mV/s). Y axis is potential versus ferrocene/ferrocenium.

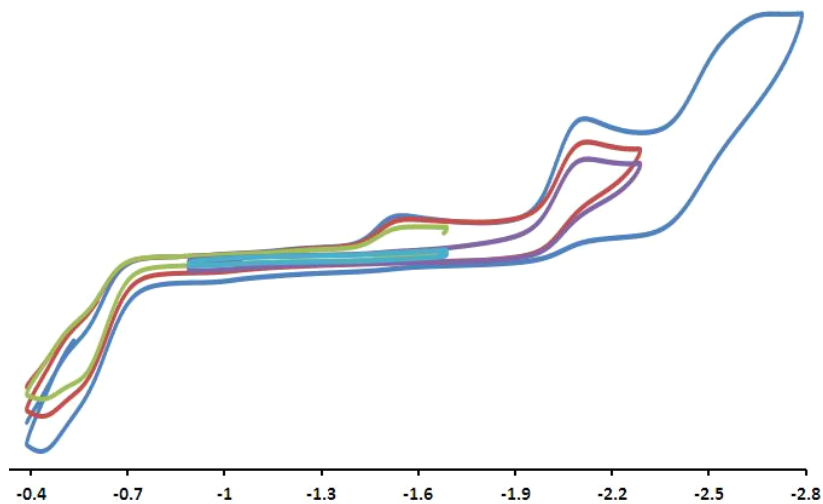


Figure S12. Cyclic voltammogram of **6** (2 mM in 0.4 M [ⁿBu₄N][PF₆] in THF, scan rate = 100 mV/s). Y axis is potential versus ferrocene/ferrocenium.

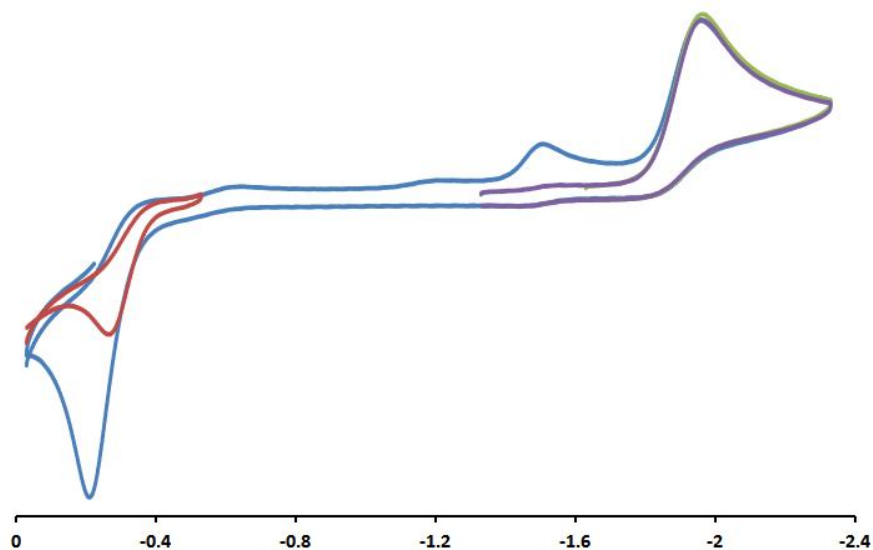
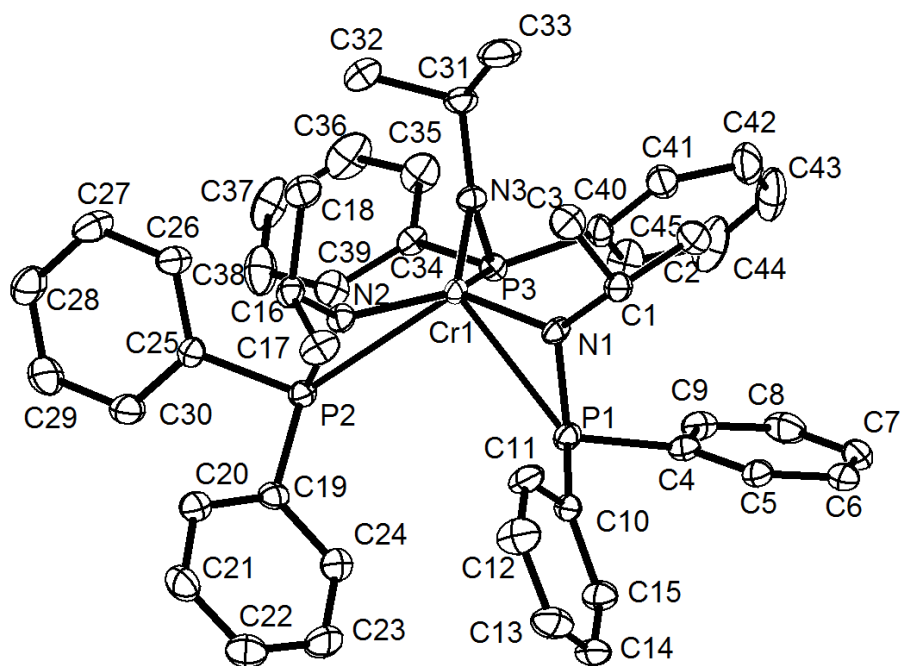


Table S1. X-ray data collection and refinement details for **1-6**.

	1	2	3	4	5	6•0.75THF
chemic al	C ₄₅ H ₅₁ Cr ₁ N ₃ P ₃	C ₄₅ H ₅₁ Cr ₁ Fe ₁ I ₁ N ₃ P ₃	C ₄₅ H ₅₁ Co ₁ Cr ₁ I ₁ N ₃ P ₃	C ₄₈ H ₆₀ Cr ₁ Fe ₁ N ₃ P ₄	C ₄₈ H ₆₀ Co ₁ Cr ₁ N ₃ P ₄	C ₄₈ H ₅₇ Cr ₁ Cu ₁ I ₁ N ₃ O _{0.75} P ₃
fw	778.84	961.59	964.67	910.76	913.85	1023.37
T (K)	120 K	120 K	120 K	120 K	120 K	120 K
λ (Å)	0.71073 Å	0.71073	0.71073	0.71073	0.71073	0.71073
a (Å)	13.0611(5)	20.6666(3)	20.6768(2)	16.2739(3)	16.2999(6)	10.7036(3)
b (Å)	16.5349(7)	20.6666(3)	20.6768(2)	16.2739(3)	16.2999(6)	22.2854(6)
c (Å)	22.6345(9)	20.6666(3)	20.6768(2)	23.1328(5)	22.8438(9)	22.5333(6)
α (deg)	90	90	90	90	90	61.763(1)
β (deg)	90	90	90	90	90	81.327(1)
γ (deg)	90	90	90	120	120	87.515(1)
V (Å ³)	4888.2(3)	8826.9(2)	8839.95(15)	5305.69(18)	5256.2(3)	4678.8(2)
space group	P2 ₁ 2 ₁ 2 ₁	Pa-3	Pa-3	P-3c1	P-3c1	P-1
Z	4	8	8	4	4	4
D _{calcd} (g/cm ³)	1.058	1.447	1.450	1.140	1.155	1.453
μ _f (cm ⁻¹)	0.362	1.417	1.462	0.630	0.676	1.487
R1, wR2 ^a (I ≥ 2σ)	0.0385, 0.0874	0.0368, 0.0798	0.0295, 0.0749	0.0323, 0.0985	0.0306, 0.0968	0.0533, 0.1193

^aR1 = Σ(|F_o| - |F_c|) / Σ|F_o|, wR2 = {Σ[w(F_o² - F_c²)²] / Σ[w(F_o)²]}^{1/2}

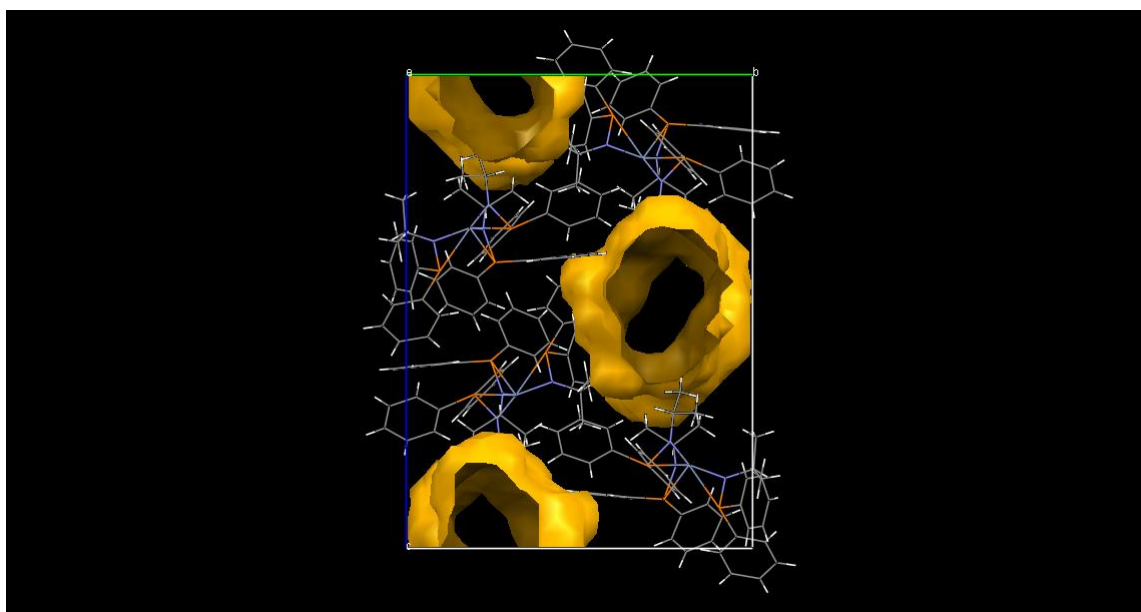
Figure S13. Fully labeled displacement ellipsoid (50%) representation of **1**. Hydrogen atoms have been omitted for clarity.



X-ray data collection, solution, and refinement details for 1. All operations were performed on a Bruker-Nonius Kappa Apex2 diffractometer, using graphite-monochromated MoK α radiation. All diffractometer manipulations, including data collection, integration, scaling, and absorption corrections were carried out using the Bruker Apex2 software.¹ Preliminary cell constants were obtained from three sets of 12 frames. Data collection was carried out at 120K, using a frame time of 40 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of two phi and two omega scan sets, with 0.5° steps in phi or omega; completeness was 99.9 %. A total of 1315 frames were collected. Final cell constants were obtained from the xyz centroids of 9416 reflections after integration.

From the systematic absences, the observed metric constants and intensity statistics, space group $P2_12_12_1$ was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using *SIR-92*,² and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.³ The asymmetric unit contains one Cr complex, and likely one molecule of pentane, modeled using the SQUEEZE procedure (see below) ($Z = 4$; $Z' = 1$). All non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and U_{iso} (H) in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints.⁴ During the structure solution, electron density difference maps revealed that there were considerable disordered solvent molecules which could not be successfully modeled. From the sample's history, the remaining solvate was likely pentane in a volume of 1045.8 Å³ per unit cell (21.4%). It appeared

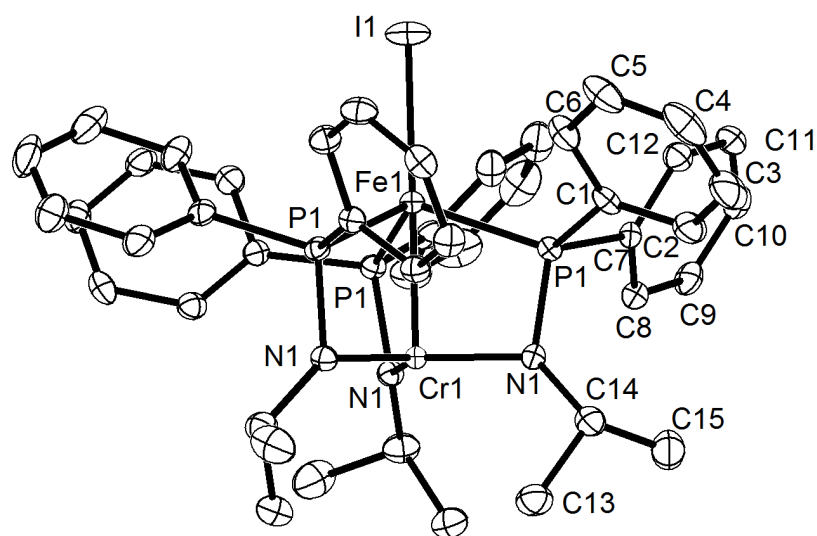
that the cavity area contained *ca.* four pentane molecules, located near the twofold screw axes at $(0, \frac{1}{4}, 0)$ and $(0, \frac{3}{4}, \frac{1}{2})$ as shown in the *bc* projection below.⁵



Mode

ling with or without restraints was unsuccessful, as was step by step acquisition of peaks using successive electron density difference maps. Thus, the structure factors were modified using the PLATON SQUEEZE^{6,7} technique, in order to produce a “solvate-free” structure factor set. PLATON reported a total electron density of 129 e⁻ per unit cell, likely representing four pentane molecules, consistent with our earlier observations. Use of the SQUEEZE technique resulted in a decrease of *ca.* 1.75 % in *R*. The absolute structure was established by using Flack parameter refinement (*x* = 0.019(2)). The final least-squares refinement converged to *R*₁ = 0.0385 (*I* > 2σ(*I*), 9556 data) and w*R*₂ = 0.0874 (*F*², 11530 data, 469 parameters). The final CIF is available as supporting material.

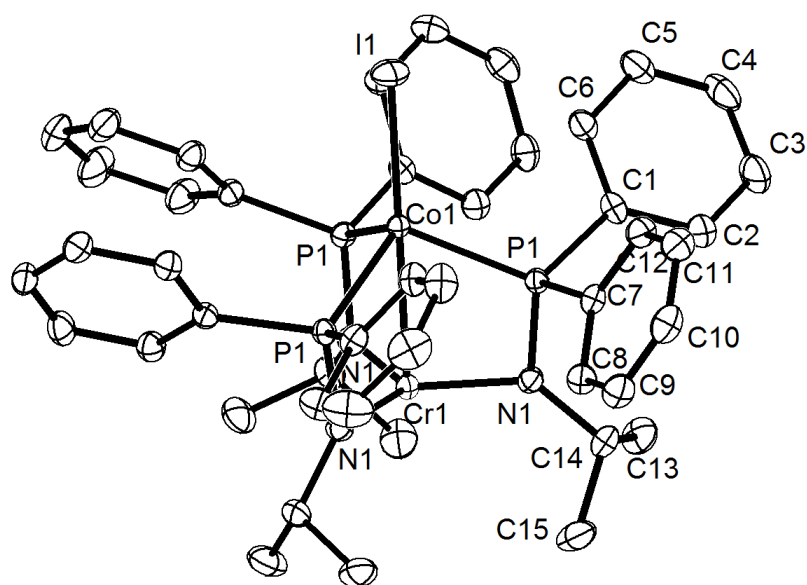
Figure S14. Fully labeled displacement ellipsoid (50%) representation of **2**. Hydrogen atoms have been omitted for clarity.



X-ray data collection, solution, and refinement details for 2. All operations were performed on a Bruker-Nonius Kappa Apex2 diffractometer, using graphite-monochromated MoK α radiation. All diffractometer manipulations, including data collection, integration, scaling, and absorption corrections were carried out using the Bruker Apex2 software. Preliminary cell constants were obtained from three sets of 12 frames. Data collection was carried out at 120K, using a frame time of 20 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of three omega scan sets, with 0.5° steps in omega; completeness was 99.8%. A total of 302 frames were collected. Final cell constants were obtained from the xyz centroids of 2518 reflections after integration.

From the systematic absences, the observed metric constants and intensity statistics, space group *Pa*-3 was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using the coordinates of the isomorphous Hf analogue (CMT20),⁸ and simply changing the identity of the Hf atom to Cr, Co atom to Fe and remove Cl atom. The asymmetric unit contains one complex ($Z = 8$; $Z' = 1$). The structure was solved using *SuperFlip*,⁹ and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.³ All non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and U_{iso} (H) in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints.⁴ The final least-squares refinement converged to $R_1 = 0.0368$ ($I > 2\sigma(I)$, 2281 data) and $wR_2 = 0.0798$ (F^2 , 3373 data, 163 parameters). The final CIF is available as supporting material.

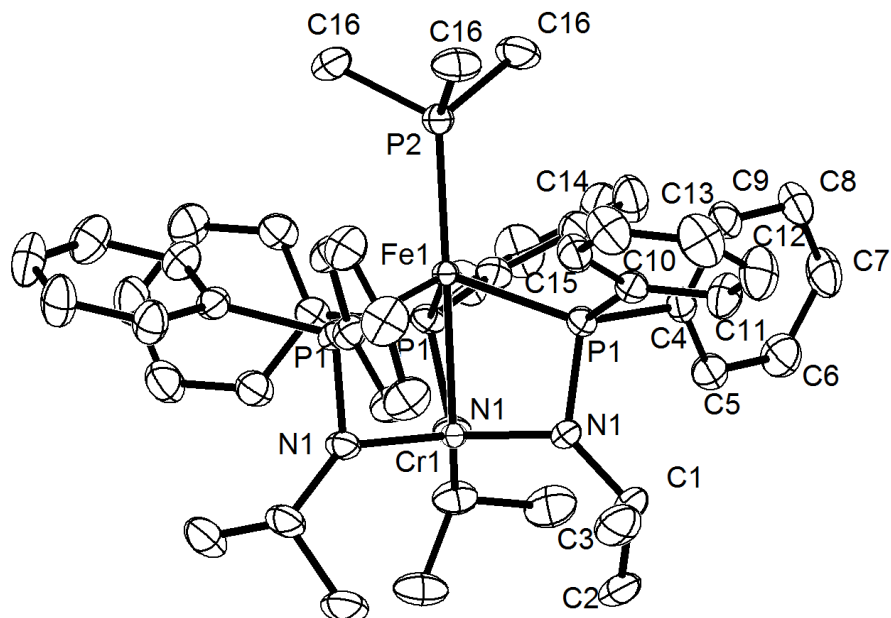
Figure S15. Fully labeled ellipsoid representation of **3**. Hydrogen atoms have been omitted for clarity.



X-ray data collection, solution, and refinement details for 3. All operations were performed on a Bruker-Nonius Kappa Apex2 diffractometer, using graphite-monochromated MoK α radiation. All diffractometer manipulations, including data collection, integration, scaling, and absorption corrections were carried out using the Bruker Apex2 software.¹ Preliminary cell constants were obtained from three sets of 12 frames. Data collection was carried out at 120K, using a frame time of 10 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of four omega scan sets, with 0.5° steps in omega; completeness was 99.7%. A total of 524 frames were collected. Final cell constants were obtained from the xyz centroids of 8910 reflections after integration.

From the systematic absences, the observed metric constants and intensity statistics, space group *Pa*-3 was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using the coordinates of the isomorphous Cr(1)-Fe(1) analogue (sk_782), and simply changing the identity of the Fe atom to Co. The structure was refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.³ The asymmetric unit contains one-third of the complex ($Z = 8$; $Z' = 0.333$). All non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and U_{iso} (H) in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints.⁴ The final least-squares refinement converged to $R_1 = 0.0295$ ($I > 2\sigma(I)$, 3587 data) and $wR_2 = 0.0749$ (F^2 , 4291 data, 163 parameters). The final CIF is available as supporting material.

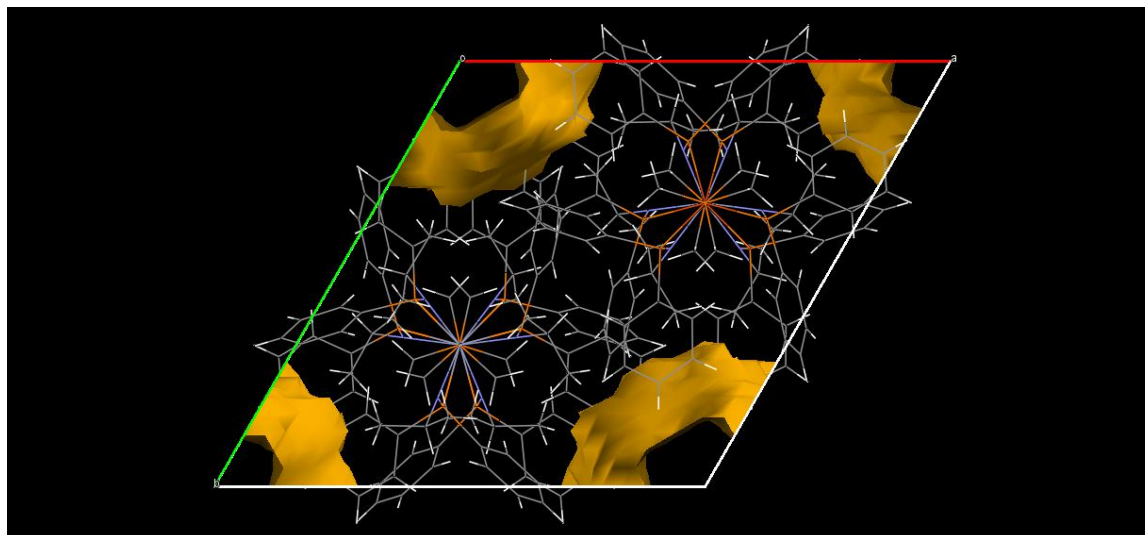
Figure S16. Fully labeled displacement ellipsoid representation of **4**. Hydrogen atoms have been omitted for clarity.



X-ray data collection, solution, and refinement details for 4. All operations were performed on a Bruker-Nonius Kappa Apex2 diffractometer, using graphite-monochromated MoK α radiation. All diffractometer manipulations, including data collection, integration, scaling, and absorption corrections were carried out using the Bruker Apex2 software.¹ Preliminary cell constants were obtained from three sets of 12 frames. Data collection was carried out at 120K, using a frame time of 10 sec and a detector distance of 65 mm. The optimized strategy used for data collection consisted of one phi and four omega scan sets, with 0.5° steps in phi or omega; completeness was 99.8%. A total of 1301 frames were collected. Final cell constants were obtained from the xyz centroids of 6427 reflections after integration.

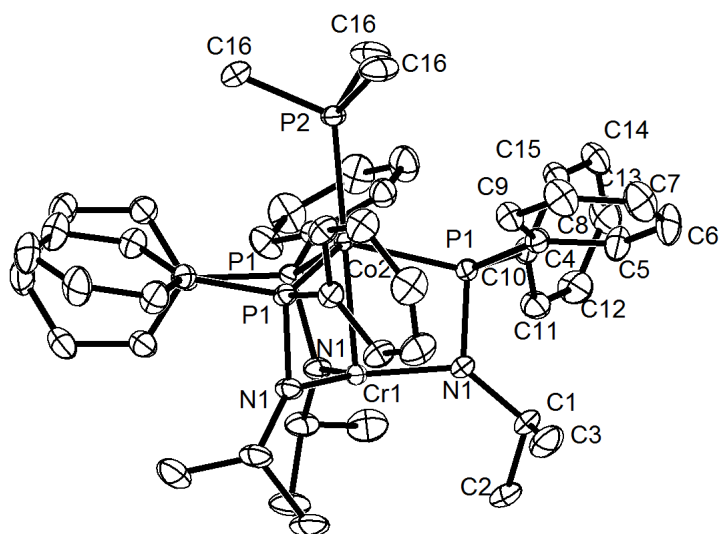
From the systematic absences, the observed metric constants and intensity statistics, space group *P*-3*c*1 was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using *SuperFlip*, and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.³ The structure is isomorphous with Co(*i*-PrNPh₂)₃Co-PMe₃ analogue (rm_147).¹⁰ The asymmetric unit contains one-third molecule of the complex, and likely a partial molecule of ether, modeled using the SQUEEZE procedure (see below) (for the complex *Z* = 4; *Z'* = 0.333). All non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and *U*_{iso} (H) in the range 1.2-1.5 times *U*_{eq} of the parent atom), after which the positions were refined with riding constraints.⁴ During the structure solution, electron density difference maps revealed that there were considerable disordered solvent molecules which could not be successfully modeled. From the sample's history, the remaining solvate was likely ether in a volume of 936.5 Å³ per unit cell

(17.7%). It appeared that the cavity area contained *ca* two ether molecules, located near the $\bar{3}$ position at (0, 0, 0) as shown in the *ab* projection below.⁵



Modeling with or without restraints was unsuccessful, as was step by step acquisition of peaks using successive electron density difference maps. Thus, the structure factors were modified using the PLATON SQUEEZE^{6,7} technique, in order to produce a “solvate-free” structure factor set. PLATON reported a total electron density of 65 e⁻ per unit cell, likely representing two ether molecules, consistent with our earlier observations. Use of the SQUEEZE technique resulted in a decrease of *ca.* 1.5 % in *R*. The final least-squares refinement converged to $R_1 = 0.0338$ ($I > 2\sigma(I)$, 12331 data) and $wR_2 = 0.0803$ (F^2 , 16125 data, 593 parameters). The final CIF is available as supporting material.

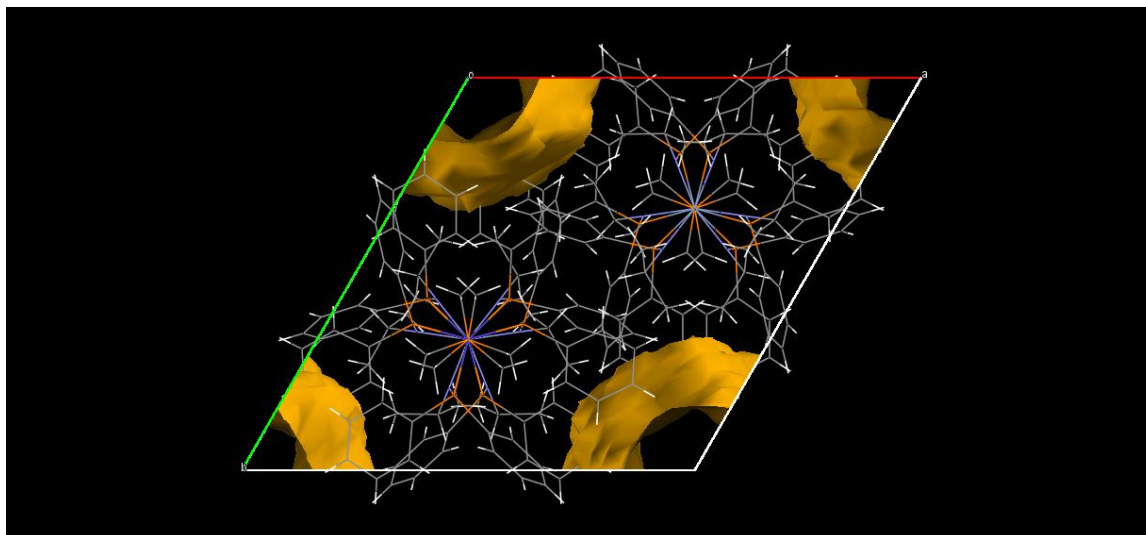
Figure S17. Fully labeled displacement ellipsoid representation of **5**. Hydrogen atoms have been omitted for clarity.



X-ray data collection, solution, and refinement details for 5. All operations were performed on a Bruker-Nonius Kappa Apex2 diffractometer, using graphite-monochromated MoK α radiation. All diffractometer manipulations, including data collection, integration, scaling, and absorption corrections were carried out using the Bruker Apex2 software.¹ Preliminary cell constants were obtained from three sets of 12 frames. Data collection was carried out at 120K, using a frame time of 20 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of two phi and three omega scan sets, with 0.5° steps in phi or omega; completeness was 99.7 %. A total of 1208 frames were collected. Final cell constants were obtained from the xyz centroids of 9735 reflections after integration.

From the systematic absences, the observed metric constants and intensity statistics, space group *P*-3 c 1 was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using the coordinates of the isomorphous Co(*i*PrNPh₂)₃Co-PMe₃ analogue (rm_147), and simply replacing the Co(1) atom by the new atom Cr(1). The structure was refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.³ The asymmetric unit contains one-third of the complex, and *ca.* 0.25-0.33 molecules of ether, modeled using the SQUEEZE procedure (see below) (for the complex *Z* = 4; *Z'* = 0.333). All non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and *U*_{iso} (H) in the range 1.2-1.5 times *U*_{eq} of the parent atom), after which the positions were refined with riding constraints.⁴ During the structure solution, electron density difference maps revealed that there were considerable disordered solvent molecules which could not be successfully modeled. From the sample's history, the

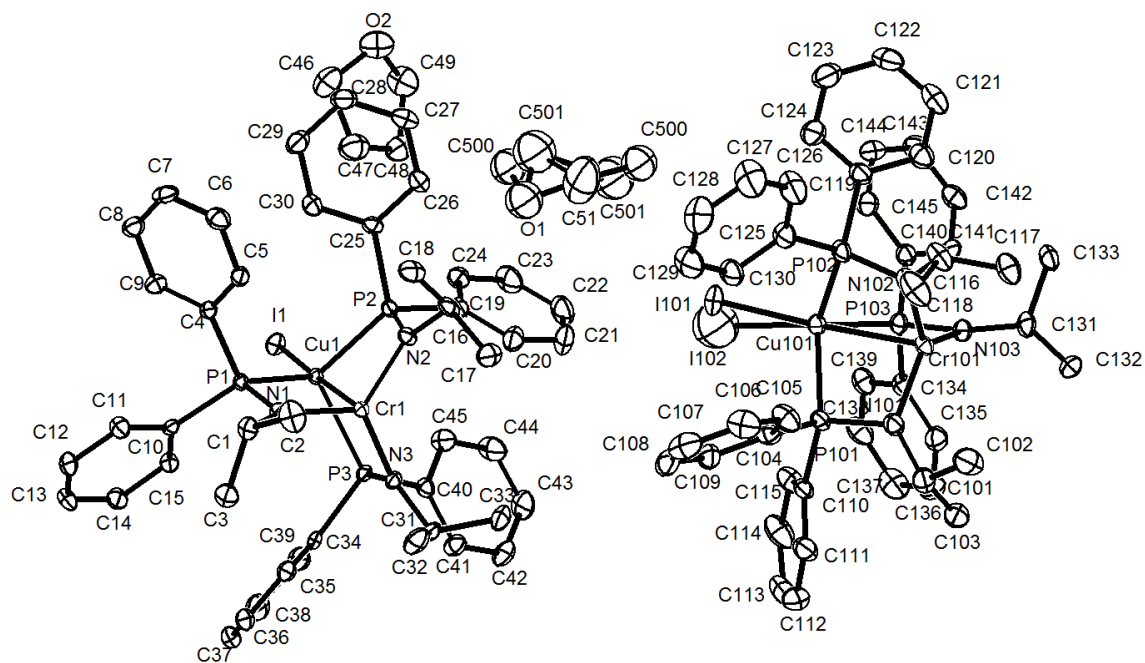
remaining solvate was likely diethyl ether in a volume of $923.6 \text{ \AA}^3$ per unit cell (17.6%). It appeared that the cavity area contained *ca.* three ether molecules, located near the -3 position at (0, 0, 0) as shown in the *ab* projection below.⁵



Mod

eling with or without restraints was unsuccessful, as was step by step acquisition of peaks using successive electron density difference maps. Thus, the structure factors were modified using the PLATON SQUEEZE^{6,7} technique, in order to produce a “solvate-free” structure factor set. PLATON reported a total electron density of 97 e^- per unit cell, likely representing three diethyl ether molecules, consistent with our earlier observations. Use of the SQUEEZE technique resulted in a decrease of *ca.* 1.9 % in *R*. The final least-squares refinement converged to $R_1 = 0.0306$ ($I > 2\sigma(I)$, 4031 data) and $wR_2 = 0.0968$ (F^2 , 5119 data, 172 parameters). The final CIF is available as supporting material.

Figure S18. Fully labeled displacement ellipsoid representation of **6•0.75THF**. All hydrogen atoms have been omitted for clarity.



X-ray data collection, solution, and refinement details for 6•0.75THF. All operations were performed on a Bruker-Nonius Kappa Apex2 diffractometer, using graphite-monochromated MoK α radiation. All diffractometer manipulations, including data collection, integration, scaling, and absorption corrections were carried out using the Bruker Apex2 software.¹ Preliminary cell constants were obtained from three sets of 12 frames. Data collection was carried out at 120K, using a frame time of 40 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of three phi and four omega scan sets, with 0.5° steps in phi or omega; completeness was 99.6%. A total of 2473 frames were collected. Final cell constants were obtained from the xyz centroids of 9894 reflections after integration. From the systematic absences, the observed metric constants and intensity statistics, space group *P*-1 was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using the coordinates of the isomorphous V-Fe-I analogue (sk_803), and simply changing V atoms to Cr and Fe atoms to Cu. The structure was refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.³ The asymmetric unit contains two molecules of the complex and 1.5 THF solvate molecules (for the complex, *Z* = 4; *Z'* = 2). The second molecule of the complex was numbered similarly to the first, with atom sequence numbers exactly 100 greater than those of the reference molecule. All ordered non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and *U*_{iso} (H) in the range 1.2-1.5 times *U*_{eq} of the parent atom), after which the positions were refined with riding constraints. One of the two THF solvate molecules was disordered about a center of symmetry; occupancies of atoms O(1), C(500), and C(501) (required

to be 0.5) were fixed in the refinement. One of the terminal I atoms was found to be disordered and was modeled as a two-component disorder. Occupancies of major and minor component atoms, I(101) and I(102), respectively, were constrained to sum to 1.0; the major component occupancy refined to a value of 0.904(3). Vibration and distance restraints were applied to the Cu(101)-I(102) (minor component) bond; details of the restraints appear in the CIF file. All the modeled disordered components were refined using isotropic displacement parameters. The final least-squares refinement converged to $R_1 = 0.0533$ ($I > 2\sigma(I)$, 17671 data) and $wR_2 = 0.1193$ (F^2 , 22585 data, 1044 parameters). The final CIF is available as supporting material.

Full reference for Gaussian 09

Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Figure S19. Calculated frontier molecular orbital diagram for complex **2**.

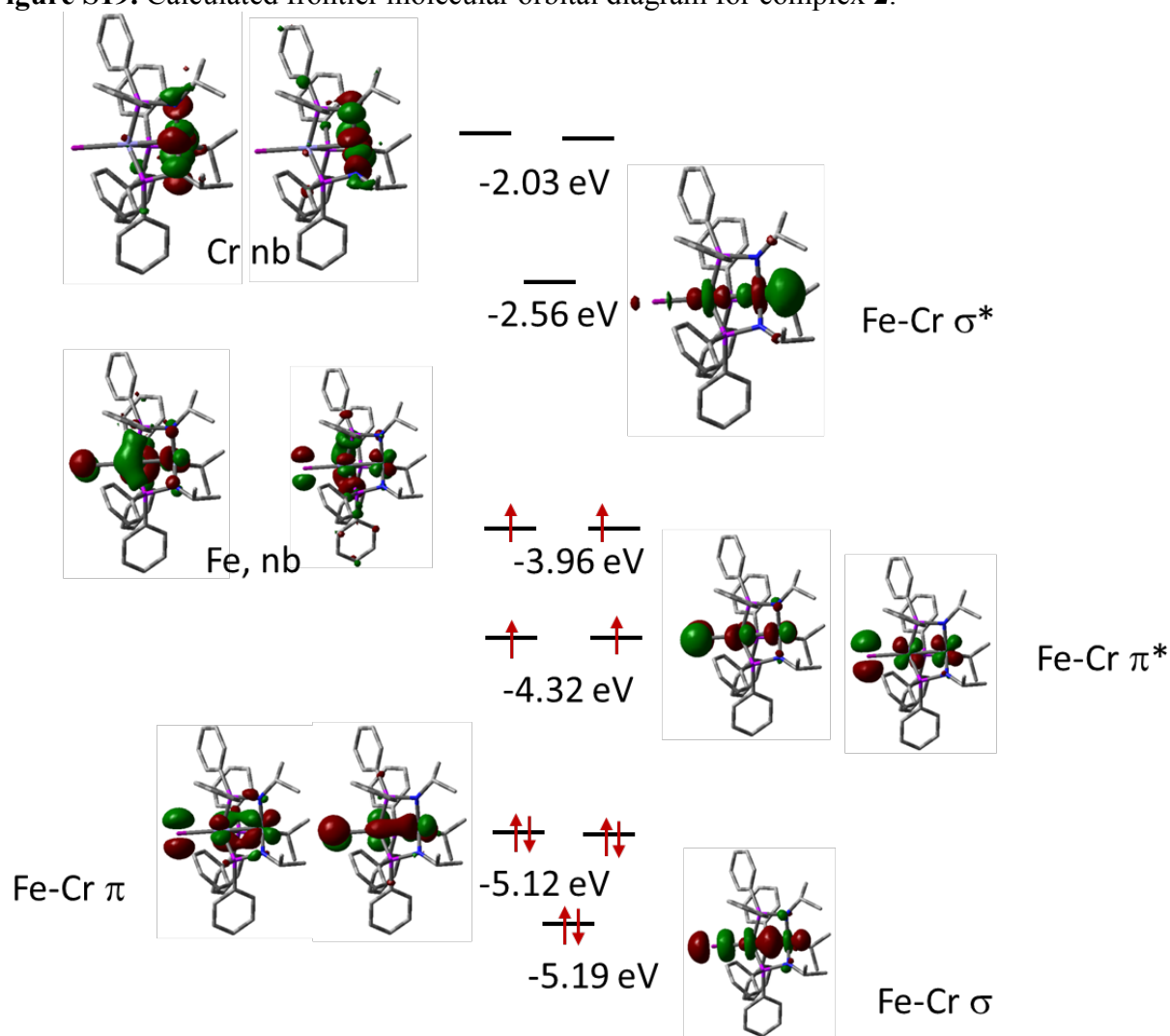
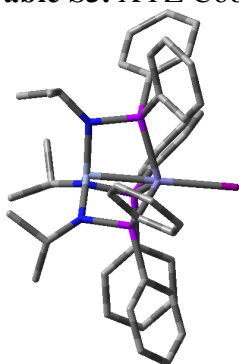


Table S2. Experimental (X-ray) and calculated (DFT geometry optimization) interatomic distances (Å) in complex **2** using three different spin states (the optimized geometry with $S = 2$ is the best match with the X-ray derived geometry).

	Experiment	calculated		
		$S = 2$	$S = 1$	$S = 0$
Cr-Fe	2.37	2.39	2.42	1.93
Cr-N	1.88	1.88	1.88	1.88
Fe-P	2.27	2.28	2.27	2.26
Fe-I	2.57	2.58	2.57	2.71
Relative energies (kcal/mol)		0	11.2	28.1

Table S3. XYZ Coordinates of optimized structure of **2**



Symbol	X	Y	Z
Fe	-0.00087	-0.00078	-0.65653
P	-0.59883	2.063283	0.118896
P	-1.48815	-1.55029	0.119649
P	2.086528	-0.51335	0.11772
N	-0.38419	1.836796	1.802949
N	1.783816	-0.58708	1.801733
C	4.222716	0.742188	-1.28831
N	-1.39893	-1.25088	1.803811
C	4.874542	-3.57917	-0.52533
C	2.880985	-4.08905	-1.85509
C	-1.1015	-3.35069	-0.08988
C	5.214572	1.729614	-1.48653
C	0.313413	3.572686	-0.46628
C	2.260977	-2.90914	-1.37924
C	-2.35134	2.629267	-0.09137
C	-3.25153	-1.51479	-0.46444
C	3.682078	1.725776	0.88759
C	-0.33658	-4.04869	0.882596
C	0.014329	-5.40377	0.686618
C	-0.05066	4.886172	-0.05374
C	-3.33776	2.321677	0.883745
C	-1.48121	-4.0303	-1.2817
C	-0.37934	-6.07762	-0.49433
C	2.10456	4.538483	-1.84942
C	-5.93139	-1.40415	-1.41775
C	0.665046	6.010498	-0.52158
C	-5.07388	3.367128	-0.49733
C	-4.20723	-2.48626	-0.05132
C	-3.65107	-0.50096	-1.37354
C	-4.68659	2.695502	0.686957
C	4.257955	-2.39794	-0.05662
C	2.741973	-0.96877	2.875285

C	-4.98355	-0.44634	-1.84755
C	1.391701	3.41178	-1.37444
C	1.747909	5.838369	-1.42098
C	4.679952	2.707667	0.692746
C	2.938378	-2.05678	-0.46927
C	-2.2062	-1.88922	2.879344
C	-5.53905	-2.42795	-0.51828
C	2.443564	-0.18226	4.173296
C	-4.10147	3.657171	-1.48665
C	-1.12284	-5.38307	-1.48094
C	-2.75086	3.291233	-1.28664
C	5.452074	2.712613	-0.49362
C	3.452154	0.722459	-0.09144
C	-3.51401	-1.10159	3.154631
C	-0.53101	2.856932	2.877039
C	2.71663	-2.4957	3.146835
C	0.806375	3.592816	3.152423
C	-1.06845	2.20592	4.173087
C	4.184896	-4.43019	-1.4261
C	-1.37301	-2.02503	4.17554
H	4.051153	-0.01511	-2.06262
H	5.891496	-3.82917	-0.19922
H	2.343713	-4.73238	-2.56124
H	5.802456	1.728022	-2.41244
H	1.26051	-2.63509	-1.73284
H	3.069838	1.738675	1.795669
H	-0.00905	-3.52238	1.785598
H	0.600558	-5.92955	1.450094
H	-0.90698	5.034113	0.616227
H	-3.04552	1.779938	1.789747
H	-2.05984	-3.50496	-2.05097
H	-0.10708	-7.12879	-0.64682
H	2.931537	4.394584	-2.55411
H	-6.96347	-1.36287	-1.78657
H	0.373131	7.016321	-0.1958
H	-6.12026	3.657011	-0.65047
H	-3.9072	-3.30189	0.618581
H	-2.91322	0.228045	-1.72764
H	-5.43457	2.455685	1.452455
H	4.813447	-1.73077	0.614499
H	3.761999	-0.69006	2.532916
H	-5.27229	0.341408	-2.5527

H	1.655285	2.408129	-1.72697
H	2.299286	6.711501	-1.79045
H	4.848605	3.471533	1.461539
H	-2.47702	-2.91156	2.537504
H	-6.26442	-3.18317	-0.19192
H	3.157628	-0.46225	4.97107
H	2.517437	0.907029	4.005842
H	1.423117	-0.41332	4.53658
H	-4.39196	4.170921	-2.4111
H	-1.42731	-5.89344	-2.40275
H	-2.0073	3.524049	-2.05829
H	6.226044	3.474404	-0.64527
H	-4.14271	-1.64049	3.89031
H	-3.27462	-0.10457	3.57004
H	-4.0976	-0.96307	2.229508
H	-1.27877	3.604096	2.533702
H	3.498641	-2.77104	3.881387
H	1.73442	-2.78963	3.562156
H	2.889016	-3.06776	2.220205
H	0.655689	4.407336	3.887799
H	1.219147	4.027716	2.227187
H	1.548201	2.885473	3.568343
H	-1.18139	2.963696	4.97175
H	-2.05047	1.729731	4.002898
H	-0.36221	1.434053	4.536686
H	4.666034	-5.3435	-1.79657
H	-1.97085	-2.50396	4.974238
H	-1.06233	-1.02591	4.538916
H	-0.46683	-2.63345	4.005963
I	-0.0024	-0.0011	-3.23694
Cr	0.000466	-0.00043	1.736808

Figure S20. Calculated frontier molecular orbital diagram for complex **3**.

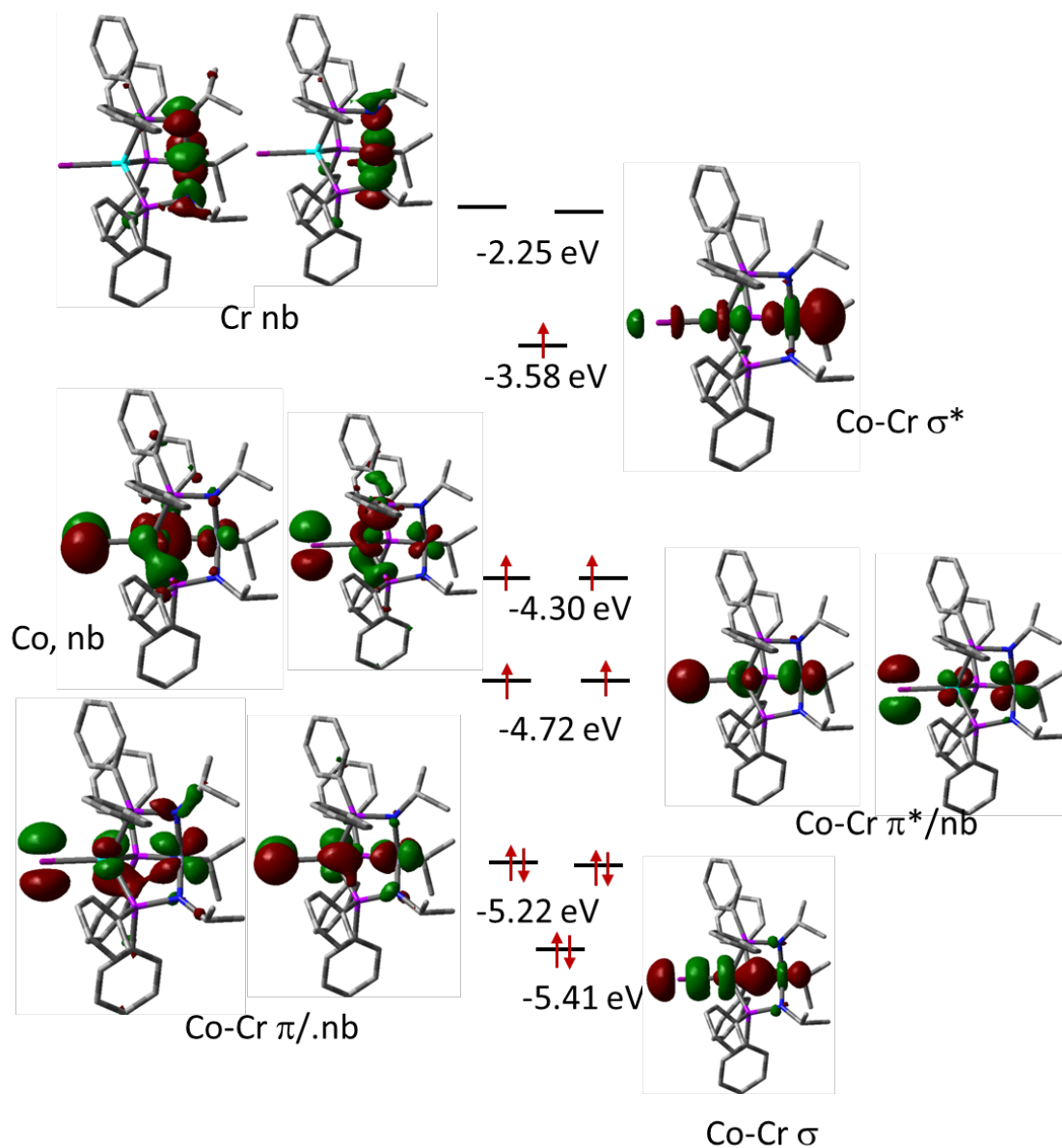
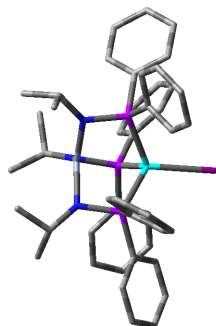


Table S4. Experimental (X-ray) and calculated (DFT geometry optimization) interatomic distances (Å) in complex **3** using three different spin states (the optimized geometry with $S = 5/2$ is the best match with the X-ray derived geometry).

	Experiment	calculated		
		$S = 1/2$	$S = 3/2$	$S = 5/2$
Cr-Co	2.68	2.39	2.34	2.71
Co-P1	2.27	2.24	2.23	2.31
Co-I	2.54	2.59	2.58	2.57
Cr-N1	1.88	1.88	1.88	1.89
Relative energy (kcal/mol)		3.0	3.8	0

Table S5. XYZ Coordinates of optimized structure of **3**



Symbol	X	Y	Z
P	-0.72262	1.983048	0.164888
P	-1.35748	-1.61586	0.163612
P	2.079179	-0.3664	0.16412
N	-0.50124	1.819109	1.859865
N	1.826115	-0.47757	1.859258
C	4.103189	1.030871	-1.2693
N	-1.32447	-1.34295	1.859216
C	5.064648	-3.22637	-0.54113
C	3.11226	-3.83644	-1.88837
C	-0.84627	-3.38384	-0.05913
C	5.02761	2.079087	-1.47945
C	0.078549	3.543915	-0.44861
C	2.413921	-2.713	-1.38536
C	-2.51004	2.420875	-0.05817
C	-3.10912	-1.69966	-0.45202
C	3.535434	1.973313	0.918179
C	-0.04535	-4.03691	0.914781
C	0.396043	-5.36437	0.711828
C	-0.3681	4.834501	-0.04485
C	-3.47472	2.062402	0.920398
C	-1.17149	-4.07722	-1.25909
C	0.056845	-6.0533	-0.47703
C	1.776835	4.614799	-1.87186
C	-5.77023	-1.77905	-1.46207
C	0.261336	5.99953	-0.53609
C	-5.2745	2.967012	-0.47829
C	-4.0085	-2.72563	-0.04371
C	-3.55482	-0.72912	-1.38627
C	-4.8455	2.340717	0.716144
C	4.36961	-2.10116	-0.04554
C	2.854719	-0.80686	2.887304

C	-4.87738	-0.76863	-1.88842
C	1.150258	3.447786	-1.37351
C	1.33943	5.892075	-1.45093
C	4.465326	3.017608	0.710229
C	3.030098	-1.83962	-0.45227
C	-2.12111	-2.07143	2.887717
C	-5.33082	-2.76142	-0.53864
C	2.580849	-0.01785	4.189156
C	-4.32164	3.308275	-1.47038
C	-0.72346	-5.40188	-1.4647
C	-2.95	3.037153	-1.26365
C	5.216974	3.073643	-0.48763
C	3.354446	0.960423	-0.06064
C	-3.45866	-1.34306	3.17958
C	-0.7321	2.873671	2.88807
C	2.892786	-2.33044	3.173994
C	0.568061	3.667843	3.177045
C	-1.28035	2.240293	4.188197
C	4.435198	-4.10011	-1.46378
C	-1.29721	-2.23164	4.186849
H	3.967927	0.265508	-2.0429
H	6.096059	-3.41436	-0.21894
H	2.620322	-4.49573	-2.61253
H	5.600806	2.115868	-2.41375
H	1.399299	-2.49808	-1.73911
H	2.940017	1.94425	1.836858
H	0.236862	-3.49725	1.824973
H	1.009164	-5.8563	1.476672
H	-1.22309	4.93285	0.635405
H	-3.14782	1.558219	1.836053
H	-1.77789	-3.58559	-2.02913
H	0.398834	-7.0831	-0.63477
H	2.599722	4.518994	-2.58931
H	-6.79469	-1.81076	-1.85229
H	-0.09458	6.986482	-0.21637
H	-6.3377	3.183239	-0.63689
H	-3.67131	-3.51203	0.6428
H	-2.85921	0.039639	-1.74156
H	-5.5769	2.0627	1.484675
H	4.88043	-1.41415	0.640463
H	3.846689	-0.49363	2.496969
H	-5.20049	-0.01264	-2.61308

H	1.476221	2.461972	-1.72388
H	1.823631	6.796611	-1.83846
H	4.597237	3.788925	1.478717
H	-2.34626	-3.08652	2.496025
H	-6.01162	-3.5582	-0.21522
H	3.325333	-0.27871	4.965543
H	2.625481	1.072189	4.01413
H	1.573903	-0.2654	4.578548
H	-4.64383	3.788492	-2.40228
H	-0.98711	-5.92444	-2.3922
H	-2.2224	3.309265	-2.03752
H	5.938605	3.883301	-0.6489
H	-4.07429	-1.93005	3.88887
H	-3.25458	-0.35511	3.634097
H	-4.03933	-1.19009	2.254556
H	-1.49897	3.576174	2.496981
H	3.709215	-2.57231	3.882217
H	1.935423	-2.64946	3.627813
H	3.050564	-2.90671	2.247034
H	0.368887	4.494896	3.886234
H	0.989236	4.093551	2.250954
H	1.322348	2.997204	3.63045
H	-1.42848	3.014079	4.965587
H	-2.24595	1.733779	4.010036
H	-0.56271	1.491685	4.577406
H	4.977269	-4.9696	-1.85487
H	-1.89278	-2.74824	4.963694
H	-1.00734	-1.23674	4.57793
H	-0.37596	-2.81445	4.007124
I	-0.00273	0.001712	-3.35061
Cr	0.00075	0.000252	1.922947
Co	0.000926	0.001121	-0.78344

Figure S21. Calculated frontier molecular orbital diagram for complex **4**.

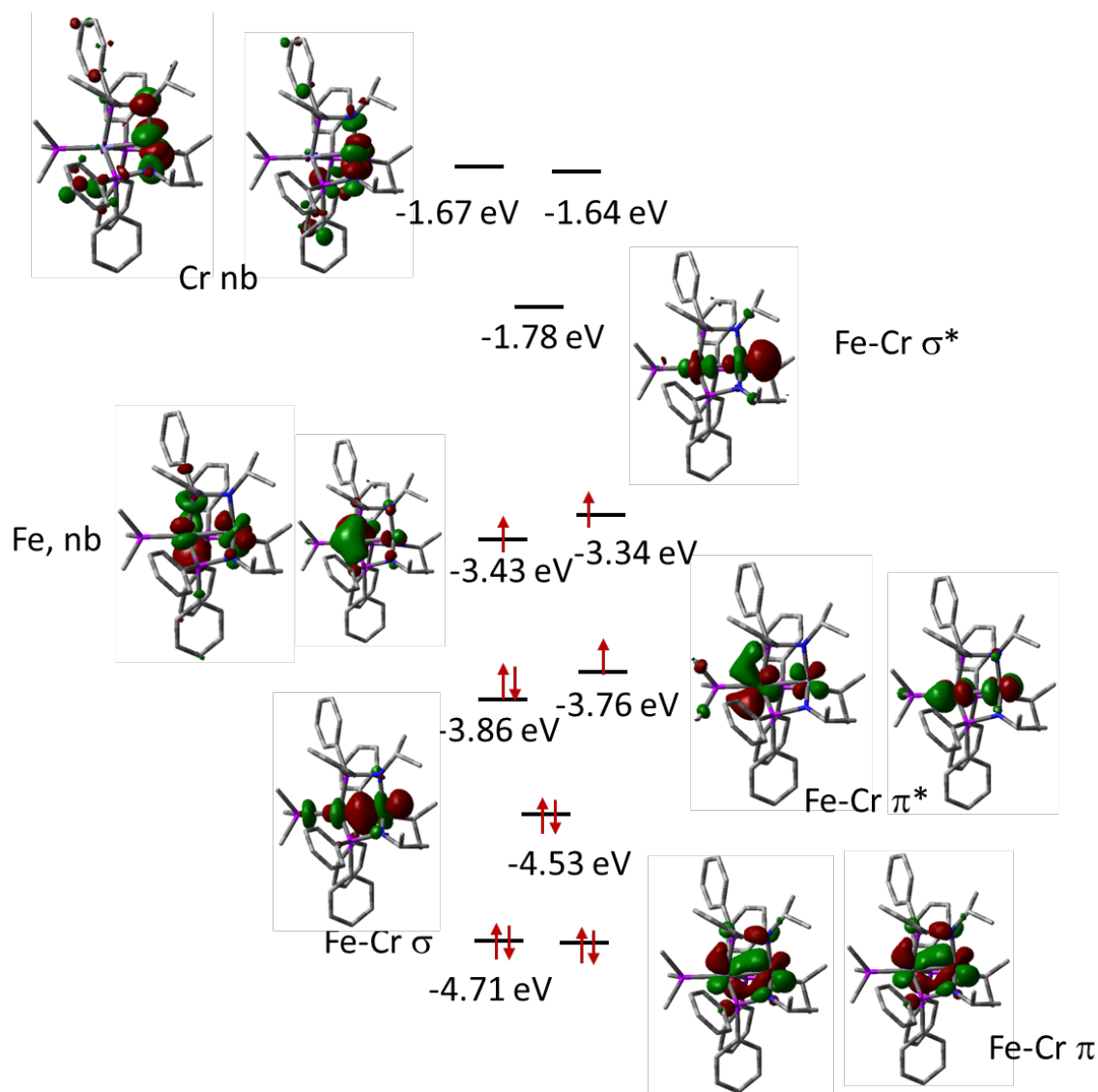
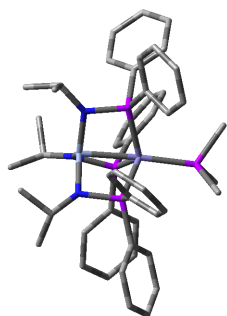


Table S6. Experimental (X-ray) and calculated (DFT geometry optimization) interatomic distances (Å) in complex **4** using three different spin states (the optimized geometry with $S = 3/2$ is the best match with the X-ray derived geometry).

	experiment	calculated		
		$S = 1/2$	$S = 3/2$	$S = 5/2$
Cr-Fe	2.38	2.41	2.38	2.65
Cr-N	1.86	1.88	1.88	1.89
Fe-P	2.25	2.23	2.23	2.30
Fe-P _{PMe3}	2.26	2.23	2.24	2.36
Relative energies (kcal/mol)		0	1.2	10.4

Table S7. XYZ Coordinates of optimized structure of **4**



Symbol	X	Y	Z
Fe	0.008846	0.101108	-0.70887
P	-0.1521	-2.03233	-0.0389
P	1.982067	0.855215	0.009963
P	-1.83188	1.137046	0.01166
N	-0.32652	-1.80667	1.666621
N	-1.48077	1.192065	1.701201
C	-4.41436	0.723383	-1.18084
N	1.782032	0.647881	1.708845
C	-3.48015	4.95732	-0.67451
C	-1.32706	4.842496	-1.83416
C	2.246386	2.691765	-0.19102
C	-5.68541	0.112996	-1.28367
C	-1.52586	-3.17407	-0.60719
C	-1.15967	3.51253	-1.38187
C	1.29106	-3.21502	-0.15402
C	3.686272	0.253823	-0.4822
C	-4.01287	-0.4635	0.917582
C	1.626665	3.590718	0.719657
C	1.753603	4.988987	0.561252
C	-1.60869	-4.54779	-0.24134
C	2.342112	-3.13426	0.802037
C	2.977644	3.236226	-1.28497
C	2.491097	5.519757	-0.52468
C	-3.62044	-3.433	-1.88362
C	6.229477	-0.72336	-1.32997
C	-2.68231	-5.35178	-0.68717
C	3.616489	-4.86862	-0.37595
C	4.888318	0.886064	-0.05371
C	3.782278	-0.86932	-1.34367
C	3.487095	-3.95476	0.697806
C	-3.30853	3.628019	-0.22591
C	-2.28301	1.859851	2.759558

C	5.041952	-1.35657	-1.76616
C	-2.54452	-2.63259	-1.43264
C	-3.69272	-4.79624	-1.51234
C	-5.28437	-1.07179	0.817557
C	-2.14438	2.885387	-0.57364
C	2.730428	1.043884	2.78231
C	6.148739	0.401092	-0.4698
C	-2.25777	1.036772	4.070528
C	2.586981	-4.94862	-1.34596
C	3.098078	4.635765	-1.45122
C	1.437018	-4.13182	-1.23458
C	-6.12984	-0.78539	-0.2813
C	-3.56135	0.453286	-0.07167
C	3.710798	-0.10583	3.136747
C	-0.4797	-2.85461	2.707915
C	-1.77987	3.304629	3.021055
C	-1.9741	-3.15034	3.004578
C	0.252044	-2.44382	4.008163
C	-2.48922	5.569261	-1.48299
C	1.957755	1.495681	4.044787
H	-4.09304	1.426494	-1.95929
H	-4.38509	5.512283	-0.39782
H	-0.54936	5.307581	-2.45149
H	-6.33071	0.346237	-2.14008
H	-0.25293	2.953707	-1.64466
H	-3.35286	-0.70532	1.757013
H	1.033713	3.180694	1.544112
H	1.269155	5.662761	1.278495
H	-0.82454	-4.99671	0.38072
H	2.261476	-2.41052	1.619494
H	3.472823	2.567255	-1.99896
H	2.59114	6.604787	-0.64823
H	-4.40059	-2.98903	-2.51344
H	7.207208	-1.09727	-1.65742
H	-2.72805	-6.40858	-0.39614
H	4.50416	-5.50745	-0.45617
H	4.840546	1.772317	0.59123
H	2.860453	-1.36268	-1.67183
H	4.281736	-3.87471	1.449845
H	-4.09108	3.161317	0.384852
H	-3.337	1.914136	2.409882
H	5.091616	-2.23046	-2.42667

H	-2.48795	-1.57176	-1.7035
H	-4.52492	-5.42026	-1.8603
H	-5.6121	-1.77378	1.594243
H	3.322581	1.911509	2.417169
H	7.063879	0.902537	-0.13137
H	-2.85569	1.536314	4.857229
H	-2.6668	0.022705	3.912711
H	-1.21894	0.940679	4.44248
H	2.670965	-5.65389	-2.18247
H	3.673526	5.033201	-2.29673
H	0.640707	-4.22595	-1.98239
H	-7.11771	-1.25521	-0.35716
H	4.459883	0.236543	3.877931
H	3.153566	-0.95431	3.577414
H	4.244213	-0.46558	2.241192
H	-0.00354	-3.78531	2.328917
H	-2.42907	3.816499	3.758632
H	-0.75096	3.276161	3.427364
H	-1.77148	3.89638	2.090471
H	-2.07001	-3.99938	3.709977
H	-2.52247	-3.39835	2.080615
H	-2.44898	-2.26376	3.46662
H	0.159167	-3.23649	4.775558
H	1.325002	-2.26372	3.818755
H	-0.191	-1.51676	4.422354
H	-2.62312	6.599745	-1.83375
H	2.659589	1.788027	4.849474
H	1.330627	0.665358	4.424966
H	1.301681	2.356133	3.82276
Cr	-0.00095	0.034665	1.669805
P	0.004695	-0.00097	-2.95
C	1.277101	1.025233	-3.85835
H	2.287859	0.6953	-3.55775
H	1.173067	0.924181	-4.95716
H	1.166136	2.089976	-3.58405
C	-1.51864	0.535559	-3.89621
H	-1.74994	1.588211	-3.65127
H	-1.37284	0.443156	-4.99124
H	-2.38132	-0.08672	-3.59651
C	0.298299	-1.64514	-3.78317
H	-0.50917	-2.34762	-3.50975
H	0.317694	-1.53009	-4.88499

H	1.259833	-2.07237	-3.44829
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Figure S22. Calculated frontier molecular orbital diagram for complex **5**.

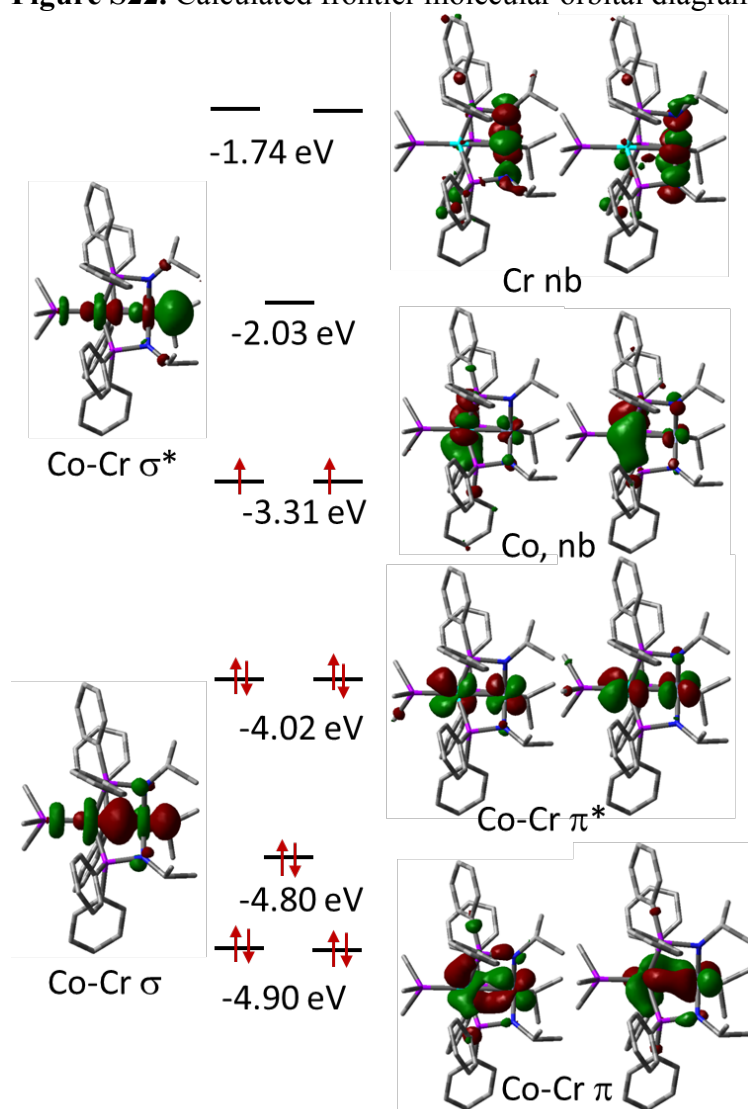
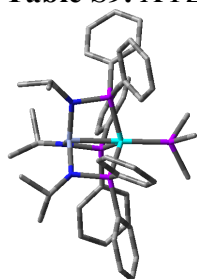


Table S8. Experimental (X-ray) and calculated (DFT geometry optimization) interatomic distances (Å) in complex **5** using three different spin states (the optimized geometry with $S = 1$ and $S = 0$ both match well with the X-ray derived geometry, but the paramagnetic nature of **5** is apparent from the ^1H NMR data).

	Experiment	Calculated		
		$S = 0$	$S = 1$	$S = 2$
Cr-Co	2.3316(5)	2.36	2.36	2.64
Co-P	2.1753(4)	2.21	2.21	2.27
Cr-N	1.8658(12)	1.86	1.87	1.89
Co-P _{PMe3}	2.1878(7)	2.2	2.21	2.26
P-N	1.6898(13)	1.72	1.73	1.72
Relative energy (kcal/mol)		28.5	0	12.1

Table S9. XYZ Coordinates of optimized structure of **5**



Symbol	X	Y	Z
P	1.85344	1.005513	-0.04126
P	-1.81071	1.085752	-0.04444
P	-0.04446	-2.10505	-0.02782
N	1.701436	0.786907	1.668214
N	-0.17064	-1.84823	1.679429
C	1.641455	-3.97886	-1.38651
N	-1.53544	1.083282	1.666285
C	-2.29751	-5.6385	-0.52338
C	-3.57282	-3.79365	-1.50223
C	-3.51929	0.35381	-0.21344
C	2.805962	-4.75982	-1.56455
C	3.594061	0.476202	-0.5009
C	-2.53519	-2.89663	-1.1539
C	2.083638	2.846968	-0.22293
C	-2.23252	2.853311	-0.51358
C	2.445474	-3.26927	0.807643
C	-4.08073	-0.44965	0.816366
C	-5.34585	-1.05987	0.654405
C	4.742215	1.259907	-0.18675
C	1.639869	3.745172	0.785392
C	-4.25965	0.51414	-1.42138
C	-6.07348	-0.89059	-0.54848
C	5.083636	-1.21269	-1.50659
C	-2.76636	5.57215	-1.21322
C	6.039923	0.813266	-0.52361
C	2.306943	5.676172	-0.57527
C	-3.48921	3.453375	-0.20969
C	-1.25362	3.642012	-1.17088
C	1.755877	5.143836	0.615308
C	-1.26292	-4.73923	-0.18003
C	-0.39788	-2.87191	2.732632
C	-1.51545	4.988271	-1.52028
C	3.786083	-0.76311	-1.16458
C	6.215714	-0.42657	-1.18817

C	3.608961	-4.05414	0.635041
C	-1.36777	-3.352	-0.48936
C	-2.31544	1.809579	2.702113
C	-3.75367	4.798573	-0.55276
C	0.317354	-2.46329	4.043454
C	2.74112	4.7924	-1.59592
C	-5.52098	-0.10175	-1.58922
C	2.632193	3.394	-1.41952
C	3.796509	-4.80434	-0.55083
C	1.438086	-3.22525	-0.19379
C	-1.77054	3.243303	2.940765
C	2.703404	1.120822	2.713236
C	-1.90902	-3.10329	2.998425
C	3.670717	-0.06204	2.985849
C	1.994727	1.547457	4.021658
C	-3.45807	-5.16829	-1.18921
C	-2.32383	1.010827	4.028446
H	0.872406	-3.97724	-2.1701
H	-2.19617	-6.7027	-0.27647
H	-4.46591	-3.41324	-2.01235
H	2.935216	-5.33925	-2.48749
H	-2.62693	-1.83273	-1.39082
H	2.317129	-2.6733	1.716616
H	-3.51568	-0.59773	1.742464
H	-5.76063	-1.67097	1.465708
H	4.623177	2.230177	0.310155
H	1.192801	3.338853	1.698747
H	-3.86218	1.147814	-2.22548
H	-7.05571	-1.36185	-0.67323
H	5.203124	-2.17538	-2.01735
H	-2.97208	6.61481	-1.48454
H	6.909809	1.432973	-0.27308
H	2.398958	6.760903	-0.70652
H	-4.27182	2.864839	0.283367
H	-0.28219	3.196226	-1.40127
H	1.410793	5.81715	1.409759
H	-0.36344	-5.12299	0.316453
H	0.045689	-3.82855	2.382527
H	-0.73928	5.574558	-2.02582
H	2.91416	-1.37683	-1.40874
H	7.222049	-0.77181	-1.45502
H	4.370693	-4.07478	1.424167

H	-3.36408	1.891802	2.344324
H	-4.72856	5.239363	-0.31052
H	0.159353	-3.22693	4.829067
H	1.404163	-2.34325	3.886219
H	-0.08897	-1.50269	4.417399
H	3.175409	5.190599	-2.52177
H	-6.07595	0.04421	-2.52487
H	3.001679	2.723517	-2.20671
H	4.697664	-5.4146	-0.68386
H	-2.41209	3.785737	3.662931
H	-0.74629	3.194641	3.356662
H	-1.73991	3.817519	2.00034
H	3.301835	1.983205	2.349124
H	-2.05228	-3.92467	3.72809
H	-2.362	-2.18503	3.417811
H	-2.44168	-3.36362	2.069318
H	4.462787	0.240818	3.698765
H	4.14975	-0.40485	2.054024
H	3.114258	-0.91051	3.42717
H	2.737312	1.802953	4.801983
H	1.344448	2.425325	3.857462
H	1.369368	0.717764	4.406556
H	-4.2597	-5.86615	-1.46046
H	-2.90122	1.548508	4.804873
H	-1.28922	0.880952	4.403293
H	-2.77176	0.010444	3.890559
Cr	-0.00171	0.014347	1.658526
Co	-0.00077	0.001113	-0.69748
P	0.00018	-0.01145	-2.91512
C	-0.02594	1.623526	-3.8168
H	0.813102	2.256542	-3.47692
H	0.053862	1.475789	-4.91273
H	-0.9669	2.157494	-3.59303
C	1.429565	-0.81079	-3.81004
H	2.359142	-0.25107	-3.60202
H	1.569266	-1.84687	-3.45356
H	1.255126	-0.82608	-4.90457
C	-1.40422	-0.85496	-3.8114
H	-2.37439	-0.45803	-3.46535
H	-1.32376	-0.70521	-4.90567
H	-1.3855	-1.93787	-3.59576

Figure S23. Calculated frontier molecular orbital diagram for complex **6**.

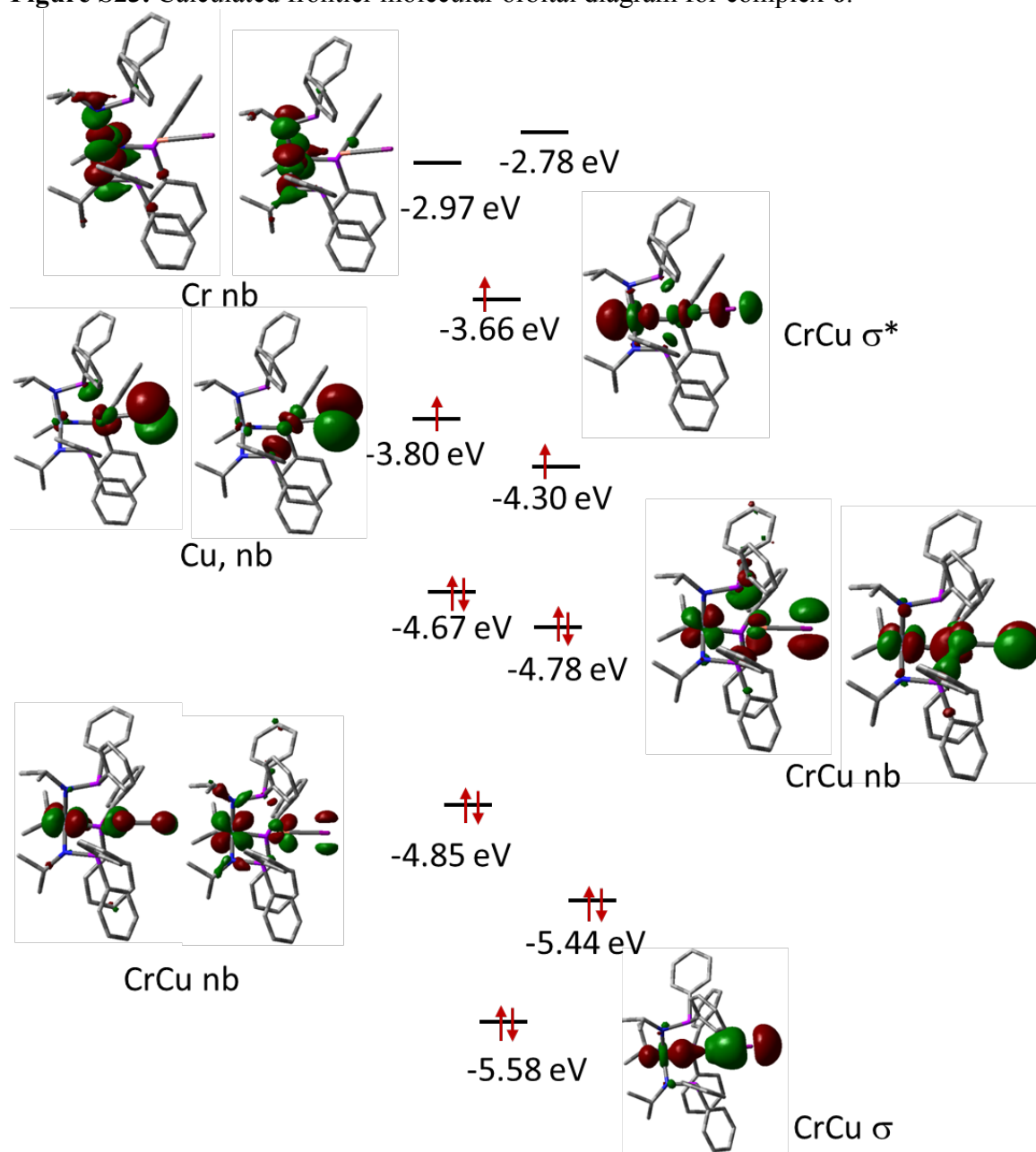
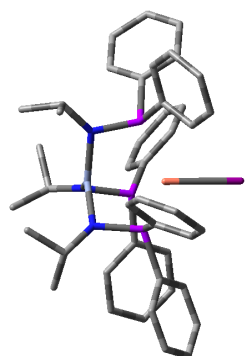


Table S10. Experimental (X-ray) and calculated (DFT geometry optimization) interatomic distances (Å) in complex **6**.

	experimental	calculated
Cr-Cu	2.63	2.67
Cu-P1	2.32	2.36
Cr-N1	1.87	1.89
Cu-I	2.55	2.60

Table S11. XYZ Coordinates of optimized structure of **6**



Symbol	X	Y	Z
P	2.050544	0.740021	0.149532
P	-1.66647	1.405082	0.150111
P	-0.3839	-2.14534	0.151297
N	1.825048	0.495119	1.838785
N	-0.48363	-1.82648	1.840498
C	0.957237	-4.21761	-1.24495
N	-1.33888	1.334944	1.838979
C	-3.38618	-4.98579	-0.54422
C	-3.91187	-2.98597	-1.85988
C	-3.44876	0.955257	-0.03752
C	1.9831	-5.16935	-1.44281
C	3.570637	-0.13144	-0.45007
C	-2.74746	-2.3523	-1.36423
C	2.553087	2.507967	-0.04082
C	-1.67288	3.156203	-0.45174
C	1.899523	-3.66405	0.947717
C	-4.12368	0.193653	0.953303
C	-5.46352	-0.21273	0.759184
C	4.883484	0.252513	-0.0542
C	2.218502	3.478632	0.940536
C	-4.13159	1.273335	-1.24589
C	-6.14248	0.120443	-0.43723
C	4.541891	-1.8967	-1.86063
C	-1.60357	5.817722	-1.45172
C	6.011031	-0.44309	-0.54344
C	3.183322	5.255758	-0.44713
C	-2.65899	4.102897	-0.05281
C	-0.66874	3.551437	-1.37384
C	2.539139	4.84109	0.742974
C	-2.2206	-4.35666	-0.05406
C	-0.86513	-2.81948	2.888118

C	-0.63427	4.876542	-1.86975
C	3.411086	-1.204	-1.36617
C	5.841687	-1.52348	-1.44667
C	2.920915	-4.62121	0.750835
C	-1.89796	-3.02701	-0.44851
C	-2.00785	2.16451	2.88479
C	-2.62044	5.426656	-0.54351
C	-0.08148	-2.54815	4.193398
C	3.498854	4.297374	-1.44233
C	-5.46868	0.859334	-1.44149
C	3.185074	2.93374	-1.24379
C	2.96553	-5.37973	-0.4433
C	0.897269	-3.46357	-0.03849
C	-1.22375	3.47635	3.147449
C	2.877212	0.662058	2.884916
C	-2.3923	-2.79455	3.155417
C	3.619364	-0.6727	3.152557
C	2.252083	1.205869	4.190667
C	-4.23748	-4.29888	-1.44716
C	-2.16321	1.35393	4.192565
H	0.2033	-4.06427	-2.0262
H	-3.62401	-6.01026	-0.23311
H	-4.55285	-2.4529	-2.57107
H	2.012831	-5.7459	-2.37518
H	-2.47756	-1.34822	-1.71312
H	1.880509	-3.06319	1.863273
H	-3.59373	-0.08488	1.870423
H	-5.97323	-0.79403	1.537134
H	5.027852	1.107467	0.618128
H	1.698832	3.164404	1.852084
H	-3.62103	1.843862	-2.03083
H	-7.18171	-0.19496	-0.58805
H	4.400626	-2.71832	-2.57182
H	-1.57805	6.843757	-1.83829
H	7.01711	-0.13777	-0.23121
H	3.432266	6.31254	-0.60031
H	-3.46905	3.802496	0.623491
H	0.060364	2.812847	-1.72762
H	2.280161	5.577555	1.513336
H	-1.55191	-4.9093	0.617675
H	-0.58485	-3.82967	2.52058
H	0.144564	5.162771	-2.58551

H	2.406764	-1.47083	-1.71615
H	6.717802	-2.05897	-1.83204
H	3.683492	-4.76933	1.525083
H	-3.02341	2.424933	2.517383
H	-3.38525	6.146839	-0.22839
H	-0.37337	-3.27122	4.978699
H	1.00829	-2.62947	4.031112
H	-0.30257	-1.52887	4.566915
H	3.990494	4.609007	-2.37173
H	-5.98253	1.115678	-2.37576
H	3.434778	2.201989	-2.02128
H	3.757678	-6.1223	-0.59603
H	-1.77132	4.11795	3.865078
H	-0.23305	3.241121	3.580236
H	-1.07227	4.044052	2.214381
H	3.611738	1.409396	2.516002
H	-2.6729	-3.5881	3.875151
H	-2.68083	-1.81783	3.587633
H	-2.96291	-2.94768	2.224409
H	4.446957	-0.51831	3.872125
H	4.037352	-1.09034	2.221647
H	2.918062	-1.41095	3.585225
H	3.02408	1.310185	4.976687
H	1.782109	2.192605	4.029577
H	1.476666	0.507383	4.562545
H	-5.13858	-4.79042	-1.8335
H	-2.63771	1.972078	4.978335
H	-1.16985	1.032172	4.562846
H	-2.78339	0.453363	4.034761
I	-0.0052	-0.00101	-3.37172
Cr	0.000222	0.001182	1.905951
Cu	-0.00104	-0.00013	-0.76776

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