Ligand-Sensitive but Not -Diagnostic: Evaluating Cr Valence-to-Core X-ray Emission Spectroscopy as a Probe of Inner-Sphere Coordination

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Supporting Information

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Fitted Experimental Data and DFT Calculated Spectra

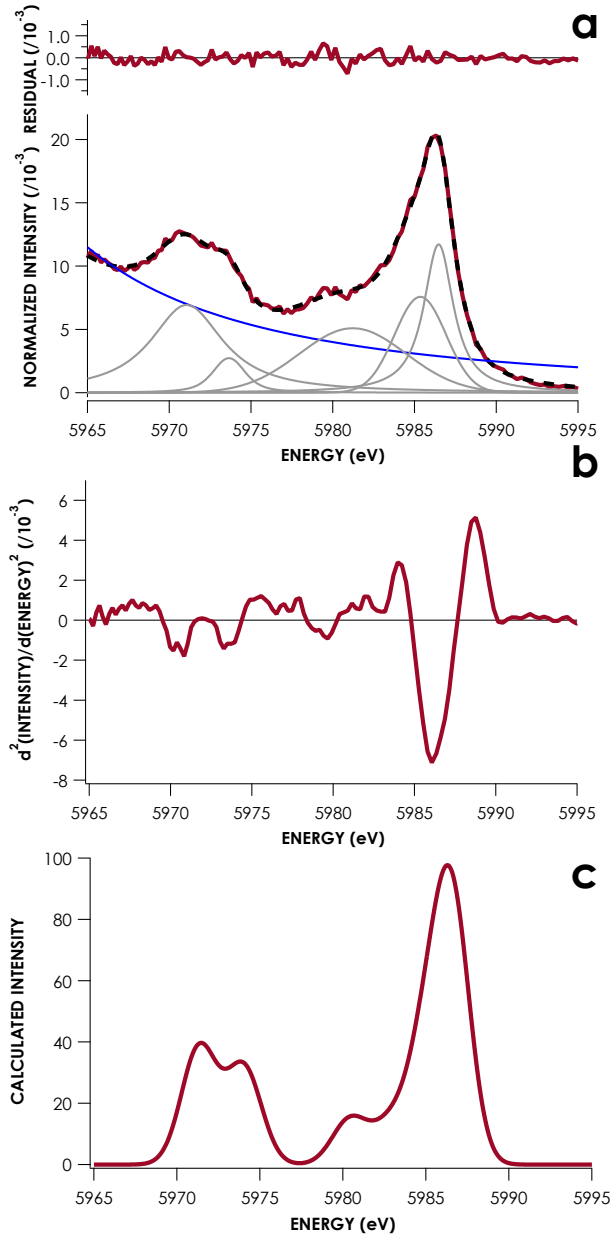

Figure S1. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of $Cr(\eta^6–C_6H_6)_2$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of $Cr(\eta^6–C_6H_6)_2$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

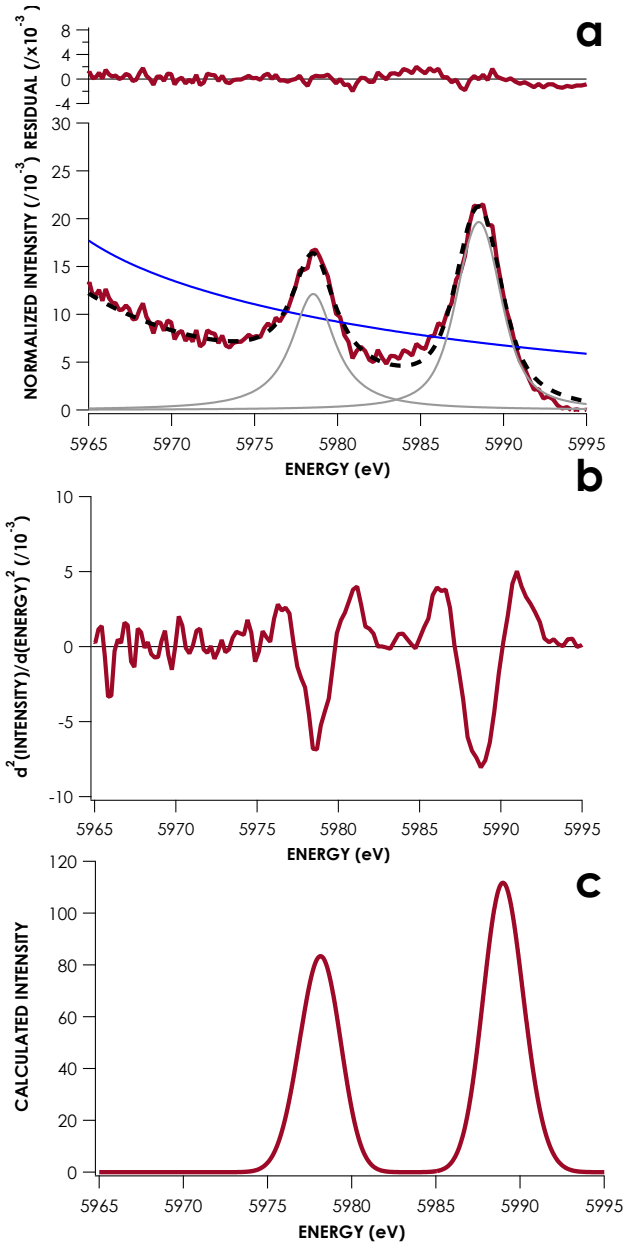

Figure S2. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of $(NH_4)_2[CrNCl_4]$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of $(NH_4)_2[CrNCl_4]$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

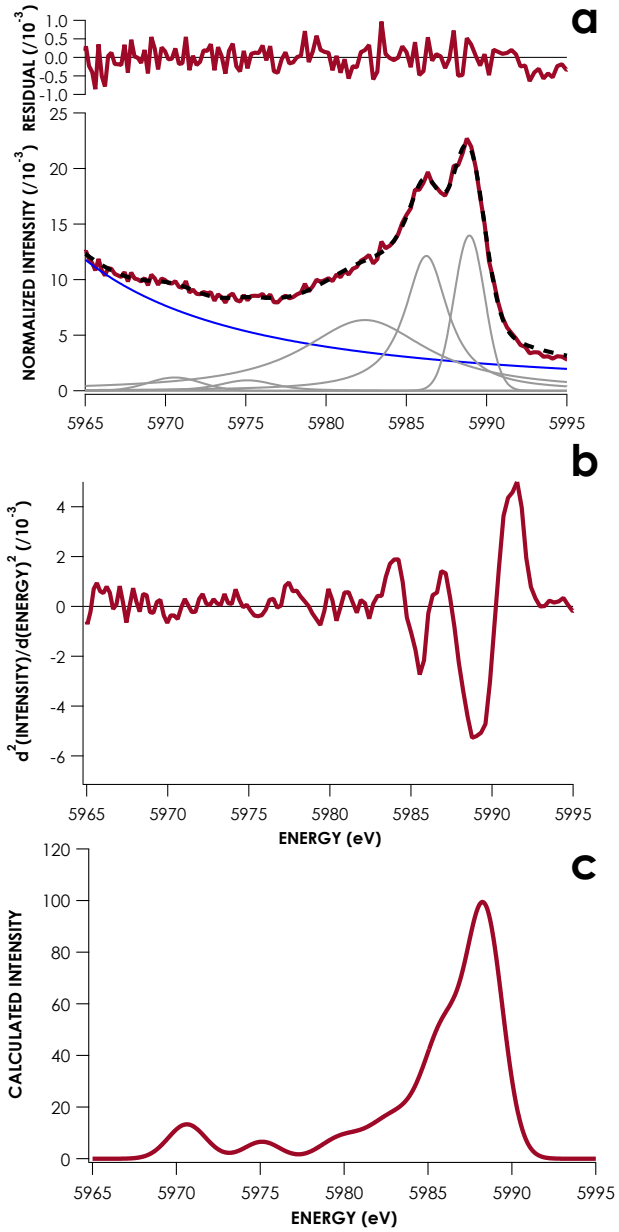

Figure S3. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of $[Cr(bpy)_3](PF_6)_3$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of $[Cr(bpy)_3](PF_6)_3$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

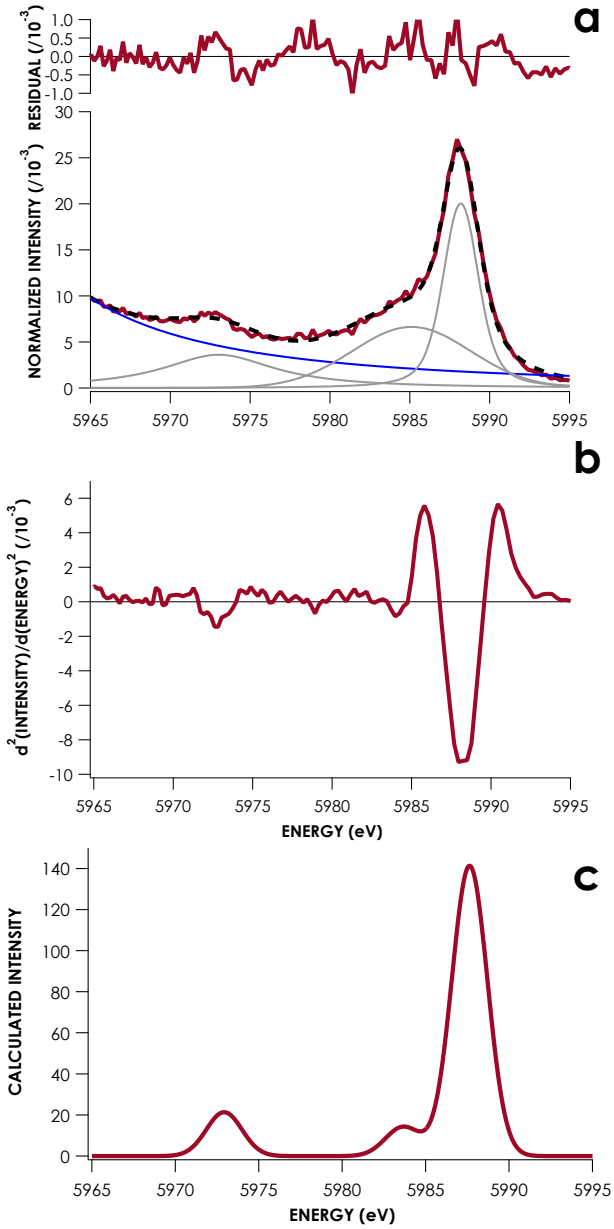

Figure S4. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of $[Cr(NH_3)_6](NO_3)_3$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of $[Cr(NH_3)_6](NO_3)_3$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

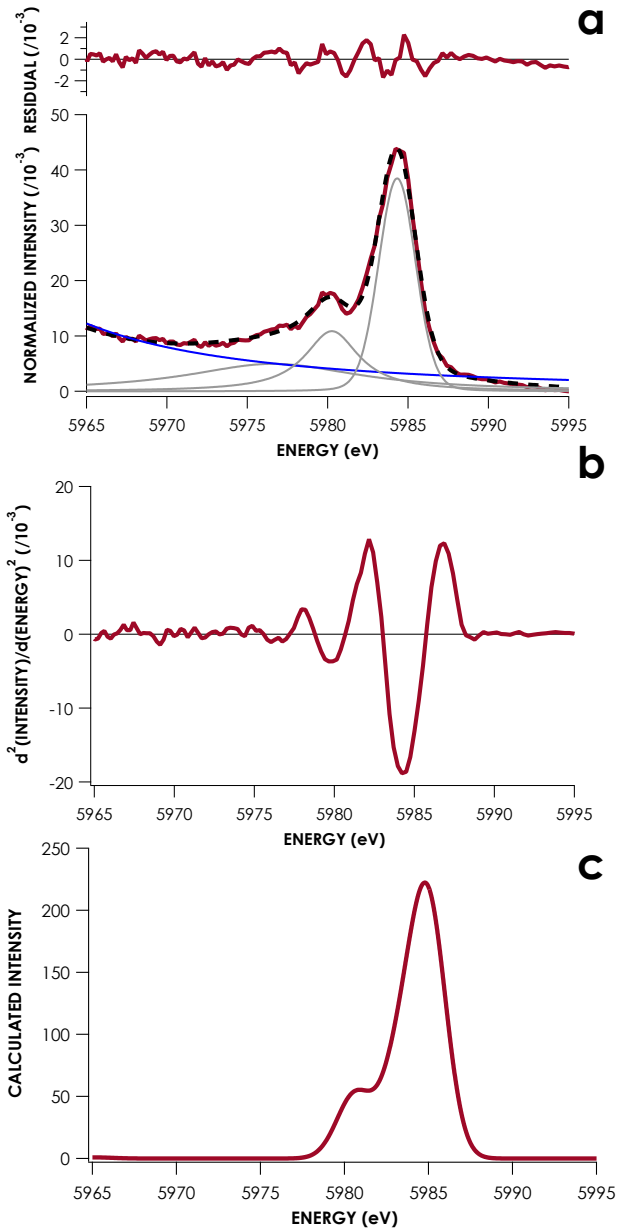

Figure S5. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of $Cr(CO)_6$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of $Cr(CO)_6$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

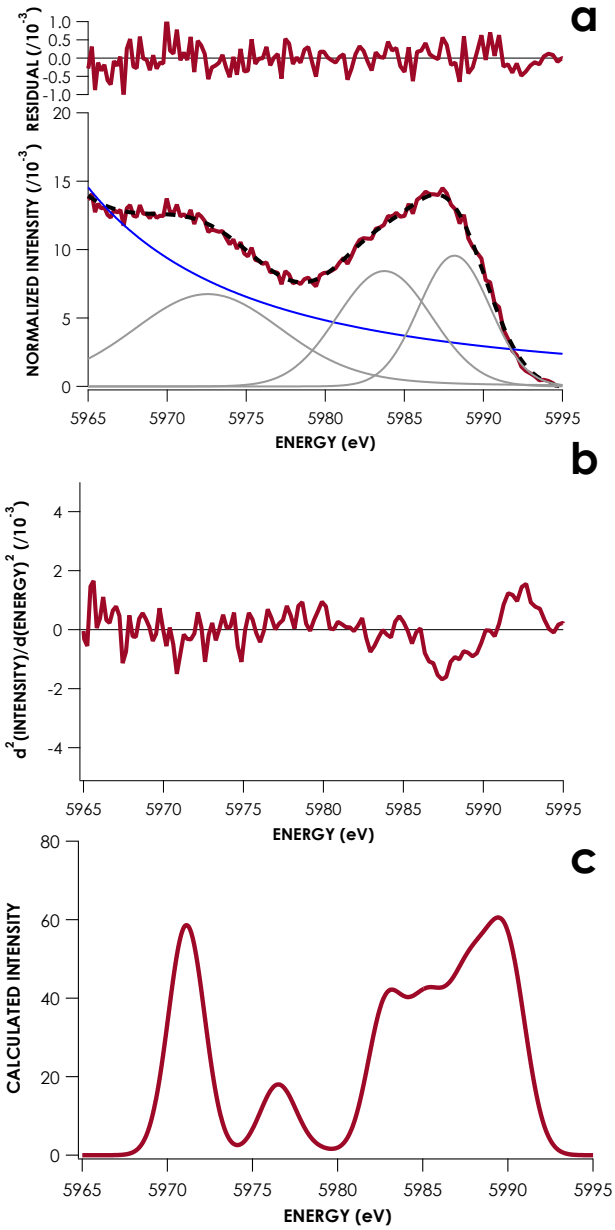

Figure S6. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of Cr(O*t*Bu)$_4$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of Cr(O*t*Bu)$_4$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

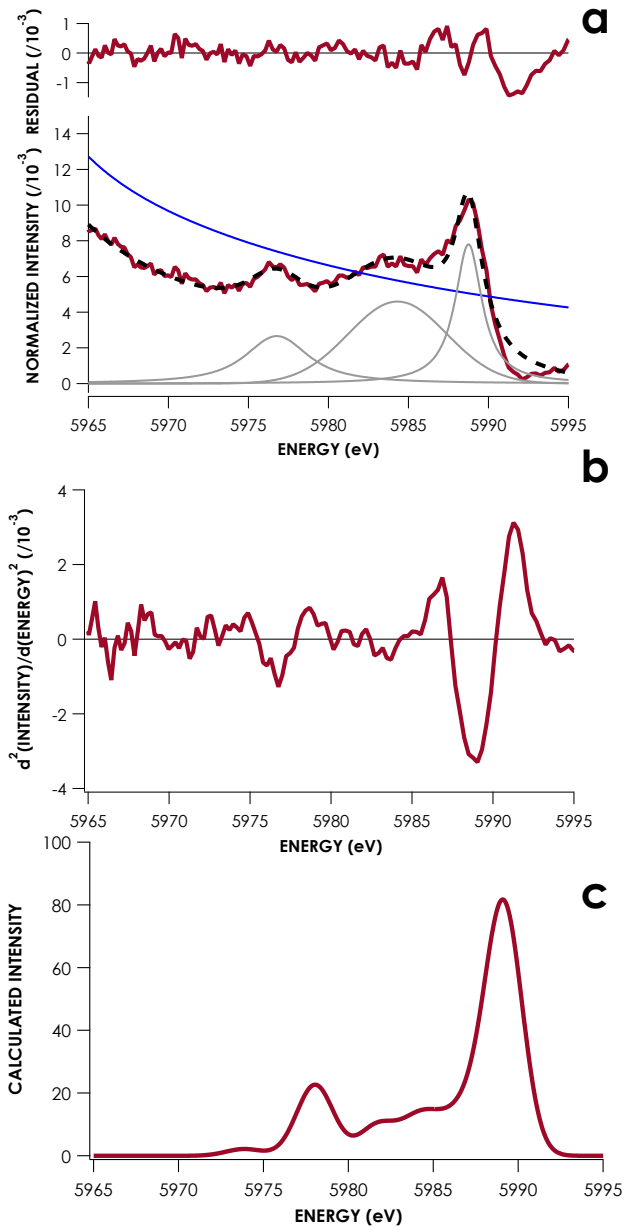

Figure S7. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of Np_4Cr. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of Np_4Cr. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

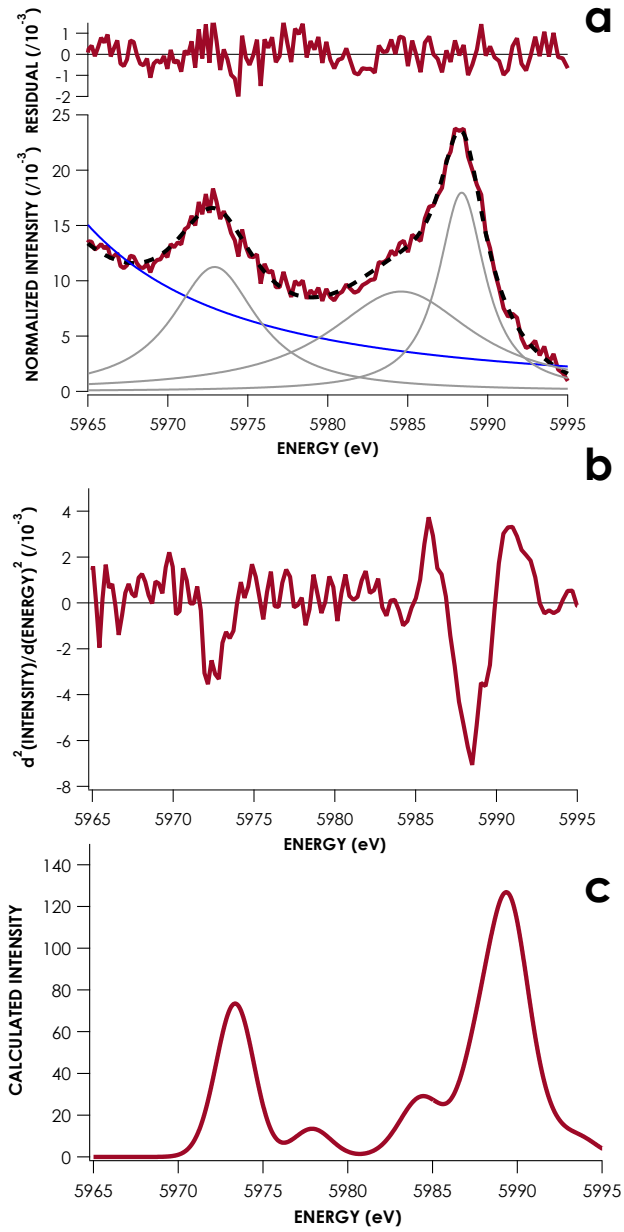

Figure S8. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of (tpfc)CrO. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of (tpfc)CrO. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

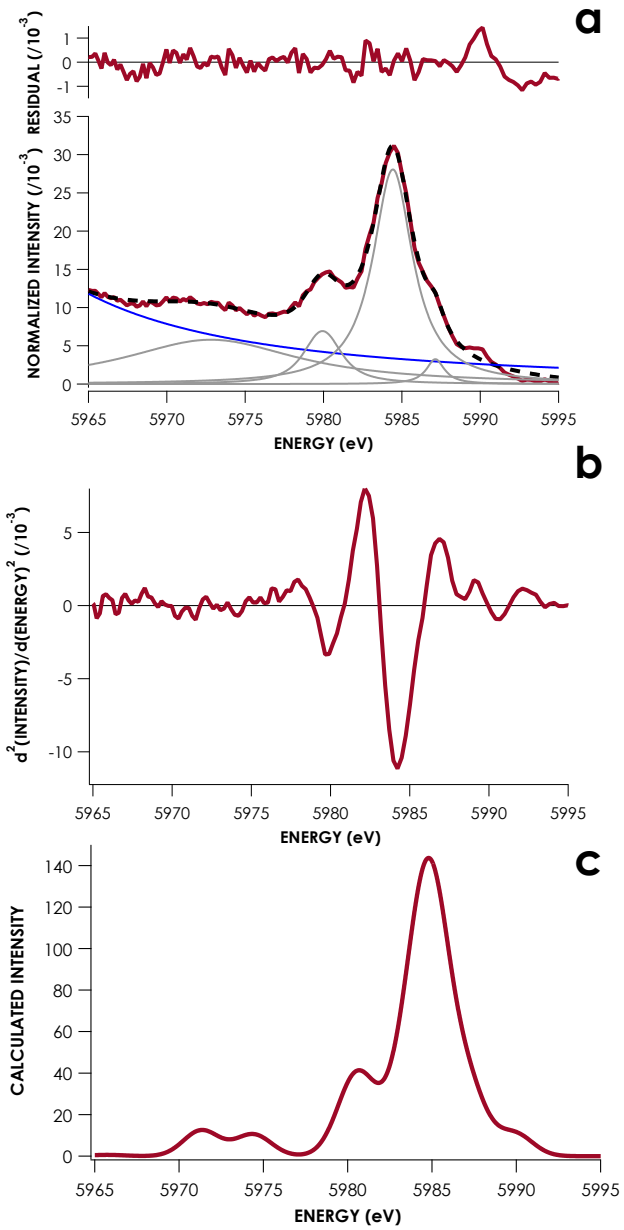

Figure S9. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of Cr(η^6–C_6H_6)$(CO)_3$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of Cr(η^6–C_6H_6)$(CO)_3$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

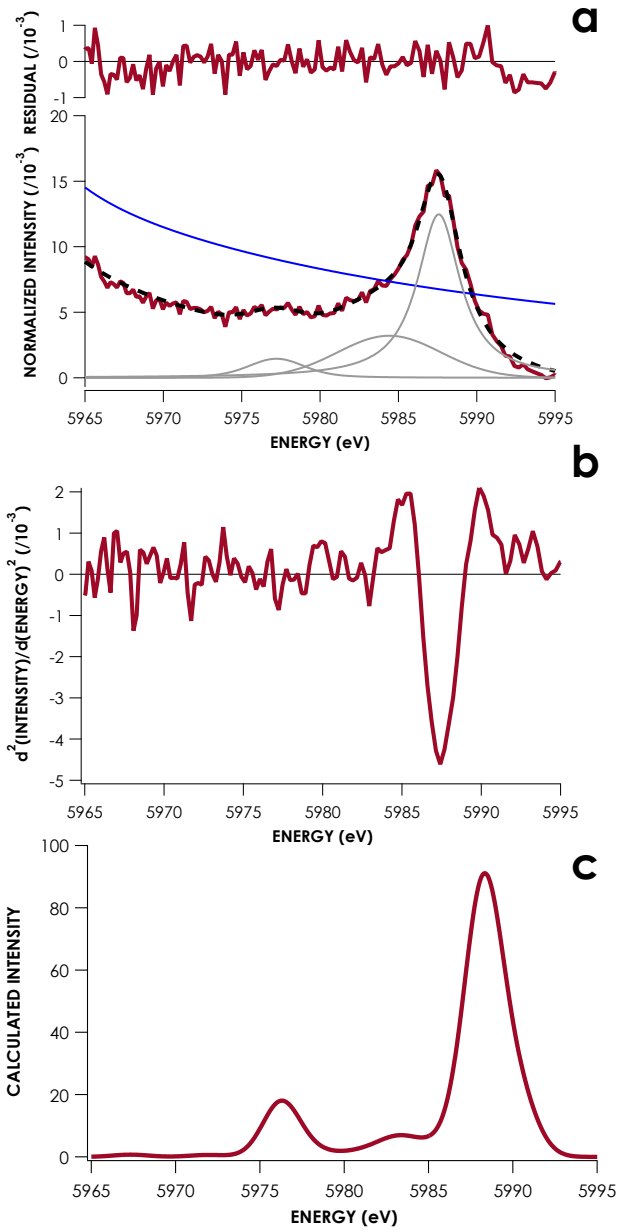

Figure S10. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of (PNP^{OMe})$CrCl_3$. Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of (PNP^{OMe})$CrCl_3$. (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

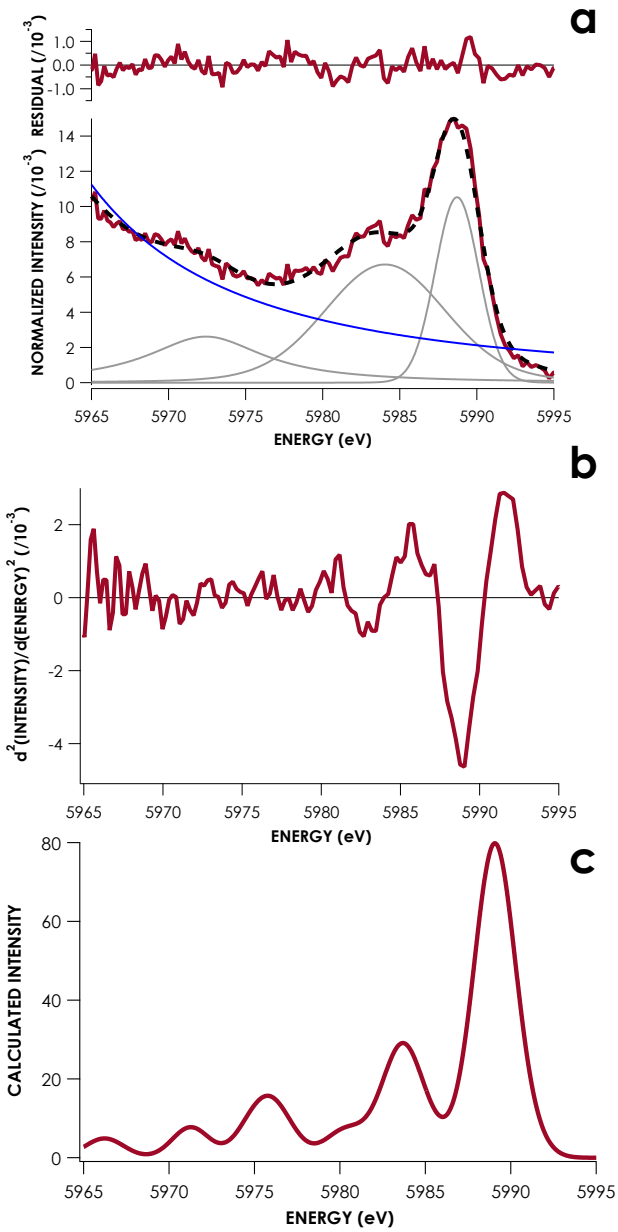

Figure S11. (a) Least-squares fit of pseudo-Voigt lineshapes to the V2C XES spectrum of Cr^{III}(14-TMC(O_2)(Cl). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks are gray, and the modeled Kß main line background is blue. (b) Savitsky-Golay smoothed second derivative V2C XES spectrum of Cr^{III}(14-TMC(O_2)(Cl). (c) DFT-calculated V2C XES spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

Example ORCA Input Files

Geometry Optimization

```
! BP86 def2-TZVP(-f) def2-TZV/J TightSCF SlowConv COSMO(CH2Cl2)
! Grid4 NoFinalGrid Normalprint OPT ZORA
! PAL4

%maxcore 4000

%SCF   Directresetfreq 1
     DIIS MaxEq 15
         end
     Shift Shift 0.5
          Erroff 0.1
          end
     MaxIter 500
     end

* xyz CHARGE SPIN_MULTIPLICITY
COORDINATES
*
```

Single Point + X-ray Emission Spectrum

```
!UKS BP86 def2-TZVP def2-TZVP/J COSMO
!ZORA TightSCF PAL4 Grid4 NoFinalGrid SP NormalPrint SCFConv7

%basis newgto Cr "CP(PPP)" end
           end

%method SpecialGridAtoms 24
            SpecialGridIntAcc 7
            end

%maxcore 4000

%xes CoreOrb ACCEPTOR ORBITAL (Cr 1s)
    OrbOp ACCEPTOR ORBITAL SPIN (Both alpha and beta = 0,1)
    end

* xyz CHARGE SPIN_MULTIPLICITY
COORDINATES
*
```

Geometry Optimized Coordinates

Cp_2Cr

Charge = 0
Spin Multiplicity = 3

C	0.309962	1.222881	-1.724656
C	1.164023	0.056899	-1.767425
C	0.310264	-1.102095	-1.840825
C	-1.044760	-0.653021	-1.847959
H	0.636621	-2.138236	-1.875688
C	-1.050276	0.768446	-1.775287
H	0.636001	2.258657	-1.686005
H	2.250363	0.055321	-1.785378
H	-1.935805	1.397169	-1.724973
H	-1.925454	-1.290982	-1.845371
C	-1.164235	0.007129	1.766043
C	-0.258801	1.129443	1.823698
C	1.075813	0.617604	1.838779
C	1.014783	-0.802913	1.787283
C	-0.362493	-1.194912	1.740607
H	-0.734229	-2.215556	1.709743
H	-2.249438	0.056044	1.784813
H	-0.537946	2.179364	1.851479
H	1.985518	1.213305	1.830696
H	1.870240	-1.472483	1.741224
Cr	-0.000722	0.003206	0.000062

$Cr(\eta^6\text{–}C_6H_6)_2$

Charge = 0
Spin Multiplicity = 1

C	0.848678	1.055556	-1.672122
C	-0.555837	1.277976	-1.639000
C	-1.449727	0.172848	-1.582089
C	-0.939322	-1.154452	-1.555370
C	0.465485	-1.376202	-1.587968
C	1.359749	-0.271595	-1.645478
H	-1.622823	-1.999997	-1.458952
H	-0.946079	2.296829	-1.606712
H	2.437751	-0.440501	-1.617929
C	0.994308	1.111744	1.548475
C	-0.396525	1.407962	1.577646
C	-1.347782	0.352286	1.638564

C	-0.907486	-0.999806	1.673742
C	0.483458	-1.296661	1.646622
C	1.434198	-0.240577	1.584224
H	0.819162	-2.334985	1.621924
H	-2.415309	0.577642	1.607315
H	1.721858	1.919266	1.448579
Cr	-0.000460	-0.000204	-0.000994
H	1.535354	1.904033	-1.663390
H	0.857341	-2.392520	-1.516311
H	-2.524670	0.346197	-1.504847
H	-0.735316	2.442510	1.497364
H	-1.636964	-1.811862	1.669614
H	2.499167	-0.468717	1.511274

$(NH_4)_2[CrNCl_4]$

Charge = 2
Spin Multiplicity = 2

Cr	-0.000000	-0.000139	0.088010
N	0.000005	-0.000100	1.621432
Cl	2.282650	-0.000180	-0.484622
Cl	-2.282651	-0.000184	-0.484625
Cl	-0.000004	-2.282870	-0.484525
Cl	0.000000	2.282473	-0.484669

$[Cr(bpy)_3](PF_6)_3$

Charge = 3
Spin Multiplicity = 4

N	0.539617	0.598526	-0.186982
N	-1.084085	0.310625	-2.239948
C	0.060594	1.763892	-0.717956
C	1.394325	0.652378	0.857917
C	1.808013	1.855203	1.419039
C	1.323855	3.048516	0.883302
C	0.441618	3.000810	-0.194373
C	-0.860993	1.602280	-1.851247
C	-1.917200	0.068931	-3.275753
C	-2.559772	1.089412	-3.967421
C	-1.479303	2.667005	-2.509523
C	-2.337355	2.409869	-3.577031
H	1.628049	4.009028	1.298297
H	2.498214	1.843890	2.260886

H	0.054658	3.922642	-0.623766
H	1.748789	-0.297704	1.252548
H	-1.294492	3.691392	-2.192716
H	-2.825047	3.233921	-4.097044
H	-3.220581	0.840770	-4.796114
H	-2.064642	-0.972107	-3.555740
N	1.597765	-1.139679	-2.282189
N	1.082232	-2.403485	-0.030576
C	2.615603	-1.918493	-1.806042
C	1.782898	-0.438590	-3.422163
C	2.975162	-0.480202	-4.136055
C	4.018490	-1.272083	-3.656573
C	3.835396	-1.997285	-2.480787
C	2.319242	-2.642199	-0.561941
C	0.724988	-3.028112	1.112929
C	1.572343	-3.908968	1.775623
C	3.211008	-3.518032	0.060037
C	2.835513	-4.158457	1.239304
H	4.966790	-1.326896	-4.190510
H	3.072381	0.102721	-5.050372
H	4.639320	-2.619305	-2.092567
H	0.947388	0.166136	-3.768770
H	4.192545	-3.701980	-0.372015
H	3.524137	-4.844360	1.731942
H	1.236472	-4.385663	2.694946
H	-0.266262	-2.808238	1.504307
N	-1.788901	-1.357725	0.049963
N	-0.996173	-2.730608	-2.053459
C	-2.621244	-2.373793	-0.330037
C	-2.126463	-0.591835	1.110462
C	-3.294347	-0.798636	1.835922
C	-4.148840	-1.832745	1.454089
C	-3.807366	-2.627099	0.361321
C	-2.168513	-3.152790	-1.490912
C	-0.503416	-3.391186	-3.124120
C	-1.147301	-4.490150	-3.681264
C	-2.858564	-4.250490	-2.009022
C	-2.344196	-4.926846	-3.113560
H	-5.072624	-2.022221	2.000029
H	-3.519168	-0.153618	2.683622
H	-4.462555	-3.438280	0.050522
H	-1.435362	0.203310	1.382631
H	-3.790963	-4.578617	-1.554177
H	-2.874699	-5.785336	-3.524556
H	-0.708149	-4.986892	-4.544764
H	0.429915	-3.020958	-3.543335

Cr	-0.108551	-1.120194	-1.122198

$[Cr(NH_3)_6](NO_3)_3$

Charge = 3
Spin Multiplicity = 4

N	0.02057	-0.02103	-2.00858
H	0.74111	-0.69931	-2.34250
H	0.25923	0.91791	-2.39742
H	-0.89427	-0.32733	-2.40582
N	0.00979	2.00874	-0.01948
H	0.96106	2.38409	-0.22909
H	-0.64187	2.35360	-0.75915
H	-0.31809	2.40943	0.88635
N	0.00000	-0.00000	2.00880
H	0.32060	0.91259	2.39987
H	-0.94754	-0.21567	2.39015
H	0.66011	-0.73051	2.35717
N	2.00870	-0.01106	0.02178
H	2.35441	0.71745	0.68547
H	2.40131	0.20174	-0.92180
H	2.39109	-0.92573	0.34690
N	-0.03044	-2.00863	-0.00109
H	-0.26005	-2.38693	0.94439
H	-0.75973	-2.34616	-0.66811
H	0.87909	-2.41315	-0.31360
N	-2.00861	0.03193	-0.00142
H	-2.34737	0.69857	0.72765
H	-2.40577	-0.90903	0.21440
H	-2.39311	0.35818	-0.91482
Cr	0.00000	0.00000	0.00000

$Cr(CO)_6$

Charge = 0
Spin Multiplicity = 1

O	-3.057642	0.000092	0.000108
C	-1.903776	-0.000166	0.000157
O	0.000634	-3.057786	-0.001431
C	0.000345	-1.903920	-0.000706
O	-0.000829	3.057642	0.001155
C	-0.000297	1.903774	0.000646
O	0.000642	-0.000507	3.057717
C	0.000341	-0.000525	1.903850

O	3.057787	0.000086	0.000158
C	1.903920	0.000101	-0.000091
O	-0.000791	0.000705	-3.057711
C	-0.000280	0.000470	-1.903845
Cr	0.000067	-0.000067	0.000003

Cr(O*t*Bu)$_4$

Charge = 0
Spin Multiplicity = 3

O	-6.111430	-0.846778	-6.955099
C	-6.528860	0.364397	-7.643209
C	-6.339895	0.144965	-9.149666
C	-5.712526	1.570165	-7.162070
C	-8.012710	0.546079	-7.298962
H	-5.282598	-0.053256	-9.372871
H	-6.660002	1.034252	-9.712824
H	-6.937782	-0.713662	-9.487136
H	-6.055390	2.485786	-7.665760
H	-5.825781	1.708012	-6.077977
H	-4.645230	1.432906	-7.387443
H	-8.588084	-0.337325	-7.609808
H	-8.421006	1.426887	-7.815993
H	-8.142966	0.685504	-6.216442
O	-3.452901	-1.206614	-7.917022
C	-2.014002	-1.343052	-8.077735
C	-1.360247	-0.026369	-7.638594
C	-1.484535	-2.518256	-7.246807
C	-1.784424	-1.594682	-9.573498
H	-1.590737	0.176039	-6.583692
H	-1.737240	0.807502	-8.247788
H	-0.267797	-0.078104	-7.758501
H	-1.658524	-2.346751	-6.174964
H	-0.402691	-2.637662	-7.405078
H	-1.982554	-3.453737	-7.536795
H	-0.708219	-1.669175	-9.788245
H	-2.201168	-0.769973	-10.168689
H	-2.267976	-2.531021	-9.885906
O	-4.713964	-3.070939	-5.855422
C	-5.438632	-4.200872	-6.414443
C	-5.282665	-4.245108	-7.939396
C	-6.914925	-4.058036	-6.022197
C	-4.820728	-5.449629	-5.772495
H	-4.222467	-4.313113	-8.219475
H	-5.709409	-3.342696	-8.400270

H	-5.806624	-5.121004	-8.349184
H	-7.017906	-4.037425	-4.927882
H	-7.501523	-4.904059	-6.410366
H	-7.326229	-3.125421	-6.432205
H	-3.758862	-5.536668	-6.042815
H	-5.343409	-6.354973	-6.114610
H	-4.899728	-5.395666	-4.677534
O	-3.665545	-0.523363	-5.163521
C	-3.947700	-0.455568	-3.738722
C	-5.459944	-0.434715	-3.484363
C	-3.300735	0.846351	-3.248645
C	-3.300073	-1.674088	-3.068035
H	-5.927691	0.419473	-3.992921
H	-5.661764	-0.349533	-2.406549
H	-5.928743	-1.359447	-3.849987
H	-3.758717	1.714499	-3.743303
H	-2.224106	0.845021	-3.469888
H	-3.432238	0.954209	-2.161923
H	-3.476695	-1.656843	-1.982188
H	-3.722651	-2.600745	-3.479950
H	-2.214788	-1.673540	-3.243266
Cr	-4.487433	-1.411983	-6.475482

Np_4Cr

Charge = 0
Spin Multiplicity = 3

Cr	5.785179	2.022917	11.173250
C	4.341590	1.239885	10.009535
H	3.444076	1.319989	10.652003
H	4.277616	2.069884	9.275085
C	4.326439	-0.115995	9.267862
C	4.036039	-1.265930	10.249778
H	3.070998	-1.112648	10.757292
H	4.813616	-1.349131	11.022269
H	3.987921	-2.228073	9.716267
C	3.191229	-0.080529	8.216931
H	2.219082	0.114148	8.695053
H	3.122011	-1.042122	7.682507
H	3.368226	0.710931	7.472674
C	5.656219	-0.382136	8.538736
H	5.893059	0.431379	7.836381
H	5.602223	-1.319186	7.962385
H	6.493447	-0.472652	9.246987
C	4.959459	3.564364	12.160630

C	3.864001	3.608749	13.249680
C	2.592729	2.861020	12.809986
C	3.496287	5.091656	13.498013
C	4.370968	3.009148	14.573026
C	7.284177	2.740712	10.042710
H	8.079848	2.855781	10.806780
H	7.519627	1.812049	9.480630
C	7.322065	3.956911	9.089373
C	6.163573	3.927778	8.076558
H	6.153926	2.984925	7.508846
H	6.260963	4.754151	7.355057
H	5.188830	4.033969	8.575549
C	7.272899	5.274215	9.884469
H	8.100335	5.328070	10.608953
H	6.329870	5.377419	10.439290
H	7.361360	6.137745	9.206820
C	8.656333	3.911147	8.306657
H	8.727328	2.993919	7.702282
H	9.515999	3.932517	8.993715
H	8.740888	4.775037	7.627401
C	6.522711	0.597114	12.379330
H	5.655154	0.511928	13.069004
H	6.491930	-0.299056	11.728322
C	7.844729	0.597917	13.181322
C	8.079903	1.942209	13.894915
H	7.246561	2.184653	14.569726
H	8.182331	2.767852	13.174700
H	9.002271	1.905389	14.495977
C	9.032767	0.296760	12.249042
H	8.904642	-0.678370	11.753849
H	9.974359	0.265298	12.819139
H	9.138917	1.061594	11.466712
C	7.770896	-0.518661	14.249074
H	7.598573	-1.499693	13.780699
H	6.949810	-0.331498	14.957930
H	8.710643	-0.574469	14.822495
H	5.868733	4.083815	12.526843
H	4.613735	4.128767	11.267027
H	4.378288	5.667846	13.816610
H	2.729442	5.177010	14.285125
H	3.098948	5.557217	12.583117
H	5.267674	3.538791	14.928997
H	4.625749	1.945285	14.462250
H	3.598775	3.090961	15.353936
H	2.224445	3.233229	11.841576
H	1.790139	2.998167	13.551569

H	2.775728	1.780769	12.713283

(tpfc)CrO

Charge = 0
Spin Multiplicity = 2

Cr	0.721957	3.335475	-0.279416
F	-2.264414	8.110980	0.887891
F	-2.391222	10.807721	1.102685
F	-0.220413	12.343730	0.445596
F	2.089831	11.151696	-0.416534
F	2.240723	8.454883	-0.610036
F	2.270909	3.741095	-5.244510
F	2.107993	3.799573	-7.951171
F	-0.302304	3.405225	-9.190485
F	-2.555741	2.964874	-7.697311
F	-2.408191	2.923624	-4.990052
F	2.246890	-1.791739	-0.582078
F	2.091400	-4.486892	-0.374113
F	-0.222289	-5.670842	0.490618
F	-2.392221	-4.127569	1.134487
F	-2.261597	-1.433021	0.902898
N	0.157407	4.552116	1.122960
N	0.129303	4.736678	-1.502373
N	0.118519	1.930510	-1.493995
N	0.168964	2.120833	1.129806
C	0.080166	4.042729	2.407830
C	-0.001395	6.290697	2.574557
C	0.092718	5.929012	1.192277
C	0.069031	6.704828	0.025849
C	0.062753	6.113280	-1.248993
C	-0.073013	6.797265	-2.498335
H	-0.172879	7.872782	-2.611065
C	-0.090198	5.856205	-3.497833
H	-0.196442	6.033394	-4.563803
C	0.035849	4.569799	-2.884522
C	0.022501	3.328281	-3.535751
C	0.044489	2.090245	-2.879371
C	-0.045077	0.799407	-3.489436
H	-0.119603	0.616265	-4.557116
C	-0.034078	-0.137102	-2.485870
H	-0.112768	-1.214608	-2.596318
C	0.070957	0.553234	-1.236894
C	0.074369	-0.034394	0.039686
C	0.096311	0.745183	1.203737

C	-0.004618	0.389337	2.587151
H	-0.074599	-0.624322	2.971600
C	-0.017751	1.561371	3.332260
H	-0.105344	1.650424	4.411241
C	0.083721	2.636241	2.411504
C	-0.005631	8.187935	0.136101
C	-1.169118	8.834290	0.575038
C	-1.254244	10.222177	0.684584
C	-0.151360	11.006835	0.346554
C	1.023370	10.397328	-0.095458
C	1.082518	9.007237	-0.193158
C	-0.063291	3.331846	-5.027388
C	1.067395	3.552373	-5.823716
C	1.001913	3.581373	-7.217005
C	-0.224938	3.380268	-7.850576
C	-1.371343	3.153655	-7.087855
C	-1.277303	3.132776	-5.696110
C	-0.001153	-1.517062	0.156283
C	1.086633	-2.339847	-0.165085
C	1.025283	-3.729292	-0.059361
C	-0.151190	-4.334658	0.383663
C	-1.253632	-3.546400	0.714629
C	-1.166514	-2.159396	0.596364
C	-0.014968	5.121797	3.324382
H	-0.066593	7.306156	2.955015
H	-0.098126	5.037399	4.404066
O	2.293427	3.335942	-0.348420

$Cr(\eta^6–C_6H_6)(CO)_3$

Charge = 0
Spin Multiplicity = 1

C	1.258639	0.964488	1.797169
C	-0.094649	1.348299	1.874382
C	-1.116169	0.355613	1.902898
C	-0.773285	-1.009829	1.852793
C	0.595562	-1.398017	1.774822
C	1.605634	-0.416550	1.746760
H	0.857309	-2.452036	1.700749
H	-2.162721	0.654157	1.927701
H	2.037557	1.722734	1.739842
Cr	0.158537	0.014303	0.091815
H	-0.362663	2.403331	1.877686
H	-1.554360	-1.767887	1.838539
H	2.649269	-0.710864	1.651307

C	-0.303532	-1.375635	-1.004104
C	1.528188	0.398355	-1.058619
C	-0.913232	1.094063	-0.922907
O	-0.601352	-2.262355	-1.709400
O	2.400983	0.646776	-1.799604
O	-1.596137	1.784031	-1.578789

(PNP^{OMe})$CrCl_3$

Charge = 0
Spin Multiplicity = 4

Cr	-5.369237	-1.472526	-3.141832
C	-6.734499	2.195053	0.110627
C	-7.912874	2.898579	0.397652
C	-6.771458	1.086618	-0.771192
C	-9.124378	2.499102	-0.173861
C	-8.003064	0.709593	-1.331589
C	-9.178194	1.402387	-1.033475
H	-7.892559	3.753554	1.071067
H	-10.031331	3.058136	0.062513
H	-10.122380	1.089525	-1.479441
H	-8.030812	-0.139472	-2.015204
P	-5.362381	0.031592	-1.256925
C	-3.969201	-3.111432	0.919004
C	-4.792790	-1.510567	2.551717
C	-5.150116	-0.648067	1.514060
C	-4.329660	-2.243619	-0.116623
C	-4.200597	-2.736401	2.246278
C	-4.914971	-0.992504	0.176576
H	-3.521184	-4.079947	0.711746
H	-3.919015	-3.424463	3.044513
H	-5.617803	0.308952	1.740945
H	-4.981280	-1.228340	3.587677
O	-5.521796	2.512091	0.648784
C	-5.450023	3.631330	1.551878
O	-4.133105	-2.561171	-1.457795
C	-6.007450	4.123035	-3.277329
H	-5.246949	4.451511	-5.611658
H	0.107752	-2.995740	-3.517640
H	1.933284	-1.285685	-3.496262
O	-5.124601	2.992025	-3.337468
C	-0.128574	-1.933193	-3.458652
C	-4.650878	3.542022	-5.661120
C	0.887461	-0.976944	-3.452592
C	-4.526144	2.717146	-4.531466

C	-1.458660	-1.512312	-3.404022
H	-4.132654	3.855756	-7.725513
C	-4.018379	3.202063	-6.859071
H	-2.261221	-2.247295	-3.455099
C	0.583830	0.385668	-3.400786
H	1.391531	1.115452	-3.403143
C	-1.798899	-0.152939	-3.336603
C	-0.752874	0.810208	-3.345695
C	-3.735248	1.546256	-4.605859
C	-3.251461	2.039577	-6.949597
P	-3.582703	0.275533	-3.295682
C	-3.119589	1.224727	-5.824380
O	-1.119142	2.119710	-3.295705
C	-0.086002	3.119487	-3.354444
H	-2.760766	1.765654	-7.883880
N	-3.933703	0.860425	-1.719148
C	-3.107232	1.757640	-0.902077
H	-2.048357	1.551980	-1.094495
H	-3.312225	1.570365	0.157138
H	-3.321775	2.809646	-1.133223
H	-2.524286	0.312484	-5.895916
Cl	-6.665635	-0.191091	-4.469598
Cl	-4.543027	-2.828810	-4.834442
Cl	-7.091724	-2.825974	-2.391189
H	-6.425962	4.111752	-2.265745
H	-6.821033	4.030477	-4.012196
H	-5.461782	5.065131	-3.441369
C	-3.709233	-3.931652	-1.726829
H	-3.694395	-4.022219	-2.815954
H	-4.437015	-4.633441	-1.300942
H	-2.708801	-4.095629	-1.307629
H	-4.399379	3.696168	1.852369
H	-6.079455	3.464157	2.438349
H	-5.749927	4.562773	1.049670
H	-0.610866	4.079616	-3.330744
H	0.491377	3.035224	-4.286895
H	0.588453	3.043574	-2.488346

Cr(14-TMC)(O_2)(Cl)

Charge = 1
Spin Multiplicity = 1

Cr	-3.002459	-0.632836	0.521661
C	-2.939294	-3.222246	2.163918
C	-1.412254	-3.186029	2.081816

H	-3.247334	-3.759828	3.076157
H	-3.339953	-3.774530	1.305435
N	-3.608650	-1.874395	2.192551
H	-1.065212	-4.203250	2.319879
H	-0.980716	-2.543897	2.863645
C	-0.846460	-2.848726	0.701706
H	-1.380234	-3.428579	-0.061140
H	0.216938	-3.137504	0.655714
N	-0.940184	-1.398519	0.316888
C	0.129145	-0.654540	1.042110
C	-0.715067	-1.275004	-1.164394
H	0.348960	-1.451687	-1.394633
C	-1.105371	0.103421	-1.667321
H	-1.300878	-2.057098	-1.656913
H	-0.422862	0.855419	-1.253546
N	-2.504507	0.531583	-1.282476
H	-1.000121	0.143564	-2.763150
C	-2.461951	2.023412	-1.215241
C	-3.499087	0.132770	-2.342521
H	-3.235998	0.678321	-3.265330
C	-4.966694	0.442989	-2.007754
H	-3.366648	-0.936070	-2.540533
H	-5.119728	1.529754	-1.946933
C	-5.637192	-0.259338	-0.816325
H	-5.542405	0.130021	-2.893096
N	-5.061200	0.073226	0.536626
H	-5.596772	-1.348498	-0.936329
H	-6.700745	0.035312	-0.801261
C	-5.351254	1.506634	0.841070
C	-5.745898	-0.724231	1.624232
C	-3.434651	-1.297750	3.557636
C	-5.073806	-2.054371	1.907399
H	-6.798873	-0.891468	1.347567
H	-5.745432	-0.097005	2.523785
H	-5.563925	-2.535007	2.770370
H	-5.161868	-2.721790	1.041678
H	0.109340	0.405109	0.776819
H	1.109438	-1.086802	0.783162
H	-0.030223	-0.728530	2.121722
H	-3.924853	-0.324244	3.630447
H	-2.372082	-1.152025	3.771596
H	-3.868907	-1.992082	4.295042
H	-3.454898	2.436102	-1.027367
H	-2.096453	2.417425	-2.177396
H	-1.797907	2.333789	-0.404210
H	-4.948991	2.161396	0.066072

H	-4.895298	1.778639	1.796353
H	-6.443263	1.647777	0.887259
O	-3.304502	-2.090210	-0.603998
O	-4.277470	-2.972125	-0.819288
Cl	-2.312825	1.131429	1.907589

$Cr(NH_3)_5F^{2+}$

Charge = 2
Spin Multiplicity = 4

Cr	0.74118146661262	0.08364303918359	0.04725868899772
N	0.42249485452371	2.16267458976049	0.04245746693107
H	1.34902746403788	2.60304199075659	-0.00251400913367
H	-0.03797564004979	2.54981688376349	0.87285670687141
H	-0.10586861540561	2.52676759609711	-0.75727120048221
N	0.90397524184209	0.09986735315892	2.14331695156440
H	1.90576965357372	0.12907361116063	2.36658018034184
H	0.48891561442709	0.91515232679931	2.60625880102682
H	0.52120355075747	-0.71621976558744	2.63199510521327
F	2.55869284299547	0.40313057012878	-0.06059768260481
N	1.15993251533410	-1.97781161005293	0.03736490625325
H	0.94729637806880	-2.47738103488875	0.90723158999462
H	0.71673094834710	-2.52341440840465	-0.70918246138790
H	2.17325397030157	-2.06948672900388	-0.10093841287583
N	0.67352569945985	0.06685327111115	-2.05561892775122
H	1.63469503006874	0.22192111165007	-2.38202315045595
H	0.36433719331293	-0.81164634684834	-2.48454170708904
H	0.10415173913219	0.80054341578124	-2.49028072118536
N	-1.34078462719318	-0.28071807267530	0.18193794698317
H	-1.56792679281034	-1.19284881594899	0.59299188269674
H	-1.83837408088973	0.40775304434119	0.75707446009639
H	-1.81549440644669	-0.26875202028229	-0.72754641400474

$Cr(NH_3)_5Cl^{2+}$

Charge = 2
Spin Multiplicity = 4

Cr	0.76347871744668	0.10084634393916	0.05259048380341
N	0.31053234886958	2.15697084941670	0.04653848555858
H	1.17629780907339	2.67819769625598	-0.13462130976803
H	-0.05549629060028	2.51810922302614	0.93428696080316
H	-0.36222222077168	2.45615550983560	-0.66765700927834
N	0.88377625678064	0.09781731295018	2.15222615032631
H	1.68770209938149	-0.46121695590985	2.45899845308667

H	1.05853247639815	1.03560379777759	2.52980518964822
H	0.06774738519946	-0.26308470463045	2.65867296146328
Cl	3.01058632280593	0.58084380024237	-0.04096287613047
N	1.18310084434448	-1.96113414891644	0.03142371179211
H	0.99492860499963	-2.44608196581838	0.91564414824556
H	0.68873713545725	-2.49801053937406	-0.68939704844461
H	2.18518611243713	-2.08827831917519	-0.15219355675141
N	0.67971435301997	0.06775218063510	-2.05122150324737
H	1.64333726894937	0.04569791475243	-2.40492489108297
H	0.20081395713223	-0.73867138631925	-2.46666925658514
H	0.24786537742657	0.89563179431258	-2.47562685908563
N	-1.30365391669907	-0.32160512169559	0.16442705372321
H	-1.51104808928958	-1.24946710561064	0.55057270960559
H	-1.81873685583684	0.34267292290621	0.75296847028124
H	-1.77242969652452	-0.29680909860018	-0.74809046796337

$Cr(NH_3)_5Br^{2+}$

Charge = 2
Spin Multiplicity = 4

Cr	0.75945544757051	0.10368400062999	0.04913281926185
N	0.26100880348577	2.14873847591009	0.05292315831482
H	1.10433605728844	2.70050672901809	-0.14378073812992
H	-0.09631012544112	2.49474617010853	0.95022555670728
H	-0.43683974487073	2.42725842170242	-0.64569857723851
N	0.88664291899572	0.11348944458146	2.14831985961736
H	1.55017338410801	-0.59403603039117	2.48258282436790
H	1.26091124802568	1.00444691548940	2.49304005373106
H	0.01297226600399	-0.05034617432620	2.66072468182716
Br	3.15533151517656	0.66149019283849	-0.05956475293592
N	1.20255527382885	-1.95378390762564	0.02566692935779
H	0.91200809204966	-2.46759316666775	0.86483385626684
H	0.79975875088408	-2.46730160651828	-0.76584806066367
H	2.21965619518493	-2.07587746929291	-0.04416976608845
N	0.67805948833879	0.06901866450625	-2.05331318184145
H	1.59403909567661	-0.21242704804680	-2.42136738055990
H	-0.01056606714233	-0.56694196147389	-2.47082787575034
H	0.49376233475772	0.98869297404572	-2.46849249268887
N	-1.29998737571533	-0.35303886272317	0.17302686213265
H	-1.48918513436238	-1.27740797866097	0.57655911321062
H	-1.82659116757593	0.31178511544725	0.75074376299328
H	-1.77244125626751	-0.35313289855092	-0.73793665189159

$Cr(NH_3)_5I^{2+}$

Charge = 2
Spin Multiplicity = 4

Cr	0.71972871142121	0.08565646497933	0.02567693963302
N	0.34081392319482	2.15541919420519	0.06787150510489
H	1.24489166023520	2.64230846299511	0.05828332541328
H	-0.15006541868822	2.48608227248723	0.90617862224766
H	-0.18522386906173	2.53101557711712	-0.72921550760262
N	0.84936702538621	0.09855026532210	2.11902630124166
H	1.51514673031899	-0.60399887291397	2.45814712660796
H	1.19500460491408	0.99730530498227	2.47202130959291
H	-0.03072488072541	-0.08206889953993	2.61545066127241
I	3.32957447703816	0.62424659572903	-0.13162655812869
N	1.19469019674721	-1.96505005010364	0.03852015387913
H	0.87620408041505	-2.47874230774931	0.86780120257533
H	0.86391798189067	-2.50573080561316	-0.76854711928657
H	2.21813063131154	-2.04769320230127	0.02870111742352
N	0.62274403145568	0.08136138655476	-2.07821936231095
H	1.55609707510658	0.27952556432675	-2.45796349106681
H	0.33422189633852	-0.80940043476429	-2.49856691372953
H	0.00062431467030	0.78997393222911	-2.48340197519562
N	-1.34173567242461	-0.34490462056919	0.19799037006538
H	-1.51842716785305	-1.21743221327773	0.70774469443106
H	-1.85715815544596	0.38308269842684	0.70473335811102
H	-1.81908217624524	-0.44752631252231	-0.70380576027843

$Cr(NH_3)_5(THF)^{3+}$

Charge = 3
Spin Multiplicity = 4

Cr	0.71417640179943	-0.02080688147422	-0.00672645924544
N	0.82234544915761	2.07445278138765	0.07467116318130
H	1.59288136735381	2.45084004202986	-0.49062046625631
H	0.96257866066818	2.46151773953719	1.01555922930979
H	-0.02094086349337	2.54167512223002	-0.27963921206039
N	0.54926374036580	-0.17272332819515	2.07839478823295
H	1.43536855428883	-0.45156072676403	2.51604196989072
H	0.26631829420114	0.69317916164127	2.55201385227309
H	-0.13613360957882	-0.87412142659594	2.38347228172545
O	2.73972088174090	-0.13724823911244	0.12622956873186
N	0.58983778351577	-2.11348619930544	-0.14135204391161
H	0.92233687641572	-2.59152217734681	0.70467642132619
H	-0.36348403936704	-2.46434961625097	-0.29087381410105
H	1.13977040423171	-2.51332330090569	-0.91099342123496
N	0.82323708140307	0.11457160154073	-2.09675139870949

H	1.79313867253680	0.13157736000845	-2.43374798561671
H	0.37043916368973	-0.66167796697079	-2.59338388599195
H	0.39303092967908	0.96560222378703	-2.47809066127580
N	-1.36358353194307	0.11580767127513	-0.09990261691825
H	-1.84996856768000	-0.70566934931019	0.27881288575296
H	-1.73868768970645	0.91213614687683	0.42956933553751
H	-1.72590161696912	0.22682933122506	-1.05429357008713
C	3.62148678944230	0.85656496952081	0.81885994406928
C	3.59598783295407	-1.22913660154991	-0.44024540943409
C	5.01680387058942	-0.71192243206404	-0.31115046825284
H	3.27499718519747	-1.39998269987994	-1.47463766307557
H	3.42333335675486	-2.12403490957015	0.17108129517293
C	4.95438377709110	0.14809858418903	0.96077046198788
H	3.14357042118119	1.11677171877446	1.77012153688480
H	3.69088036741212	1.73891897709230	0.16914717578673
H	4.96912354224895	-0.47917493592904	1.86231634112408
H	5.77807625066091	0.86946031690817	1.02199482661781
H	5.29096768884944	-0.10336199256160	-1.18317679165114
H	5.72884457530847	-1.54139096423762	-0.22483720978262

$Cr(NH_3)_5O^+$

Charge = 1
Spin Multiplicity = 4

Cr	0.75699822316616	0.03402442364285	-0.09092642788347
N	0.78014520453398	2.16753208108311	0.01671709761595
H	1.79422973485382	2.31070675843425	-0.06901377838432
H	0.48059560024257	2.60764984951618	0.89148466293868
H	0.32485904796840	2.69252106729181	-0.73541118953248
N	0.90339367948223	-0.08500736081340	2.03658227960710
H	1.92768114275096	-0.07900798648501	2.11930558879678
H	0.54377287756274	0.69937998909291	2.58802796198494
H	0.55954850047895	-0.93430617696951	2.49376407339465
O	2.52374783240336	0.04861730675954	-0.18486435567962
N	0.81017051991937	-2.09903056885993	-0.21258122667811
H	0.47198216107891	-2.63960928574104	0.58873520660581
H	0.40920275586339	-2.54162869019239	-1.04437249681996
H	1.83040745562930	-2.21478582875754	-0.25898194777639
N	0.69270927551197	0.14570888706501	-2.22435529768663
H	1.70648150883837	0.12379947963739	-2.39368604672659
H	0.27189074043016	-0.63296613734020	-2.73936694764923
H	0.32711281632383	1.00118883068104	-2.65229574988896
N	-1.49580597515014	0.02363188201443	0.03139330601865
H	-1.88600821829310	-0.89017958893472	0.28151720294779
H	-1.86824387364290	0.67856511523627	0.72577064618239

H	-1.94581100995233	0.27861595363896	-0.85314256138697

$Cr(NH_3)_5(O\mathit{t}Bu)^{2+}$

Charge = 2
Spin Multiplicity = 4

Cr	0.72424905841409	0.28174740475803	0.04449053636154
N	0.04824921847192	2.23614627600457	-0.39386818665669
H	0.87851742747072	2.83708206725587	-0.43453004815763
H	-0.59505019925989	2.66687356380230	0.27827218359089
H	-0.41077436422121	2.32763383463763	-1.30600954869885
N	0.58086960021569	0.67310345893536	2.11351883036547
H	1.44940666274768	0.44029804314953	2.60644129138035
H	0.39821747081825	1.65777483423453	2.33416833936466
H	-0.15946762335909	0.14515618596835	2.58877131928452
O	2.49731279304454	0.81531897119410	-0.21906663560675
N	1.35093998756552	-1.69275117177214	0.46796400759217
H	1.23895385691610	-1.99869370960099	1.44013000158390
H	0.91530987346011	-2.42633463921011	-0.10086528461834
H	2.35642469267608	-1.73024310878233	0.26865002437580
N	0.79126861014757	-0.17936856783635	-2.02536124638811
H	1.76606102810354	0.02775283512761	-2.27299681879395
H	0.61759540952016	-1.15511941122458	-2.28694150840824
H	0.20300131232155	0.38430940643391	-2.64734959594553
N	-1.33179071162095	-0.36816595782233	0.09947583024748
H	-1.47464066226173	-1.24626070397654	0.61002872182039
H	-1.96562386428501	0.30811747498877	0.53859723710713
H	-1.72212722189322	-0.53401317156003	-0.83399721605581
C	3.64176121014728	1.32296275293009	0.48532569316587
C	3.31815731088918	2.66210210217608	1.16765520427658
C	4.72578582325818	1.54561224111372	-0.58399632871735
H	4.37792498505772	2.27224274530060	-1.33170662162250
H	4.95460647622449	0.60013290382764	-1.09538044630600
H	5.65131362885771	1.92917758752490	-0.13035375198921
H	2.97468041199562	3.39781255711930	0.42503049083704
H	4.21287575377949	3.07619363629677	1.65476524426875
H	2.54612925471041	2.55433543583235	1.94299365443945
C	4.15189109483756	0.29950667698434	1.51414036646336
H	5.07112068095603	0.66151067937230	1.99673377977682
H	4.38465141555480	-0.65776664704815	1.02468013895582
H	3.42085959873910	0.11344341386491	2.31530034270697

$Cr(NH_3)_5N$

Charge = 0
Spin Multiplicity = 4

Cr	0.63055026650039	0.03009640393609	-0.08929957505596
N	0.78533487497830	2.18558706877452	0.03447387903036
H	1.80857131672082	1.92614051176462	-0.04343556076054
H	0.60227957739664	2.68480366019934	0.90811122283928
H	0.50323270703031	2.79029811365082	-0.74033251429839
N	0.90386809908484	-0.09555306948483	2.04987219843889
H	1.91727306268925	-0.05579370355688	1.76265788032055
H	0.67158543079506	0.68912820001307	2.66325401310083
H	0.70974168703327	-0.96115427913957	2.55885464833965
N	2.43968076789218	0.04981898261607	-0.19710681240310
N	0.79988694086174	-2.11862079033401	-0.21991723663752
H	0.58569008568058	-2.72285706692229	0.57692988596782
H	0.54175532522418	-2.62005440404073	-1.07308455028275
H	1.82468388508129	-1.86420305971544	-0.23741607384039
N	0.65992419354392	0.15858331626474	-2.24832492668407
H	1.69911225119156	0.13847955081795	-2.05864793108053
H	0.38193089128972	-0.62959589396270	-2.83781863269761
H	0.40053723899568	1.02056875034449	-2.73399984614227
N	-1.69083868366951	0.02122049216654	0.04530428241066
H	-2.07195010061719	-0.85742243974454	0.40675439017517
H	-2.05298618903754	0.75940624510307	0.65503042281879
H	-2.13076362866548	0.16654341124965	-0.86755916355885

$Cr(NH_3)_5(N\mathit{t}Bu)^{1+}$

Charge = 1
Spin Multiplicity = 4

Cr	0.86171309501623	-0.02864180688965	0.00357987372756
N	0.80971142896008	2.07454480881247	0.42226348301698
H	1.81457601204293	2.26121019900229	0.30699564607504
H	0.52948480090084	2.39807139264591	1.35311886099304
H	0.30338358805837	2.66169133788256	-0.24719037172733
N	0.74095794252292	-0.48852948147224	2.07508252401347
H	1.48072586243113	-1.14203896174786	2.35049307708029
H	0.86388162374139	0.33051468724808	2.67811713085821
H	-0.14493167240434	-0.91682941308885	2.36370095033213
N	2.69239679048665	0.04018672865431	-0.21146800055485
N	0.86845597982707	-2.12379172979041	-0.45002939377509
H	0.69043076198916	-2.78726377811390	0.30985125556363
H	0.30658860414403	-2.44002819457897	-1.24607016617197
H	1.86153368813406	-2.20050586635227	-0.70684669140424
N	0.86749960093660	0.41145564805528	-2.13721633085589

H	1.90394489954211	0.40153479824804	-2.07529235640805
H	0.55672545128506	-0.29009758856487	-2.81458533322860
H	0.55439106707805	1.32221026831714	-2.48363953058249
N	-1.41665387192222	-0.03229947787407	-0.02858929298259
H	-1.84765962005877	-0.94706540227554	0.13762348836650
H	-1.84969632666225	0.60411694857009	0.64788631093537
H	-1.76148185909172	0.26812408753042	-0.94514800138505
C	3.90652428845497	-0.10754168909829	0.55556098564338
C	3.99702323273803	0.87789419160440	1.75615380077622
H	3.18773587823169	0.69754283956517	2.48014405905113
H	3.90837689313440	1.91547290798739	1.39718016284689
H	4.95306176870898	0.78727389487079	2.30050363746373
C	4.10651885585060	-1.54921041201891	1.10740468922831
H	4.09748955513742	-2.27344017930989	0.27801022989537
H	3.29973202976783	-1.82738026464812	1.80448208898188
H	5.06041040075719	-1.66288991293848	1.65125220841536
C	5.10908411672867	0.19353587218773	-0.37479312918542
H	5.02627057009679	1.21973382688080	-0.76251788166244
H	5.09302442904568	-0.49441677963244	-1.23309980302485
H	6.07775013439037	0.08895650033187	0.14323181968439

$Cr(NH_3)_5(Py)^{3+}$

Charge = 3
Spin Multiplicity = 4

Cr	0.51450975747307	-0.12031220663238	0.08824818051844
N	0.68547045102313	1.97210472742844	0.00268383193940
H	1.55851109093728	2.27627456986862	-0.44494105523175
H	0.66599830692151	2.44692368264840	0.91302799035534
H	-0.06494429335350	2.41738929412504	-0.53893103329911
N	0.37315992822022	-0.13278034414500	2.18502877007466
H	1.16559923051305	-0.61312785576905	2.62809568452772
H	0.33214350934899	0.79329412757338	2.62677702495743
H	-0.46211785562130	-0.62352232602656	2.52630324019742
N	2.58621317926967	-0.30998987426984	0.19533995831659
N	0.30052307191429	-2.21129497747909	0.17235692532264
H	-0.52416816105308	-2.51671260593861	0.70293294550068
H	0.20934918432314	-2.67289511606923	-0.74028997197947
H	1.09619554063599	-2.66882027806745	0.63380643513167
N	0.59391784702180	-0.11696274861466	-2.01244193599976
H	1.53507178922830	0.07535820765642	-2.37645635171616
H	0.30251930027639	-0.99790061862229	-2.45210080287900
H	-0.00565304164008	0.59860371203802	-2.44041733841598
N	-1.57966717817879	0.09535777344959	-0.00835747803839
H	-2.09117262771206	-0.79112447836824	0.07305642542168

H	-1.95738482841009	0.69591911782819	0.73420674399378
H	-1.91609377164392	0.50905435616711	-0.88574026989523
C	3.31460453197233	0.46865699689750	1.03484402207057
C	3.24707908274306	-1.21387398328416	-0.57169461644423
C	4.62689306672046	-1.36475401647557	-0.52542797258867
C	4.69659908278821	0.37132543534559	1.13255990443345
C	5.36932474054380	-0.56020099908847	0.34045421998954
H	5.10379040754849	-2.10673947533949	-1.16415945160900
H	6.45339397250465	-0.65764575519062	0.39685925938039
H	5.22952213263913	1.02243590534052	1.82392829733863
H	2.77143513821055	1.18978657229975	1.64451111909369
H	2.65023741483528	-1.83334681928590	-1.24045270046693

$Cr(NH_3)_5(CH_3)^{2+}$

Charge = 2
Spin Multiplicity = 4

Cr	0.97369901493871	0.13277342978170	0.07236490084751
N	0.50636495583729	2.19517476323682	0.07177059990547
H	1.35950507809377	2.75982790590599	0.00173164923782
H	0.02554586801884	2.51735251630383	0.91860399647414
H	-0.09298846344444	2.49200317089138	-0.70586256956996
N	1.05324820998134	0.11494057829772	2.18464930570321
H	1.86750387914238	-0.41535424946810	2.51280335717931
H	1.16804052777771	1.05141734778133	2.58670894595835
H	0.23984004326052	-0.29281635410182	2.65855820882173
C	2.99398184000028	0.60692128807829	0.00434037303388
N	1.35554439072828	-1.94923547639383	0.08668901054129
H	0.94999203045371	-2.44607884618344	0.88724872343265
H	1.01198213391499	-2.44432993254828	-0.74335524803099
H	2.36325587218364	-2.13610295927221	0.12356016514882
N	0.95987963998181	0.08535464193879	-2.04056244295115
H	1.79842738332590	-0.38835504265479	-2.39312829732996
H	0.16044581484612	-0.39217073960977	-2.47113360416506
H	0.98469641366676	1.01935781529271	-2.46353602810535
N	-1.22028286398436	-0.28052114469229	0.11921876211446
H	-1.46092585015099	-1.27743642194874	0.11416272438214
H	-1.69167470608874	0.10277138716422	0.94564825809392
H	-1.72543669528328	0.11851883824914	-0.67940068895467
H	3.32299765684536	1.09182235065554	0.93875018740105
H	3.62818017445402	-0.28176927016779	-0.15245281120837
H	3.19888765150036	1.30770440346362	-0.82297747796024

$Cr(NH_3)_5(\eta^1\text{-}C_6H_5)^{2+}$
Charge = 2
Spin Multiplicity = 4

Cr	0.50675232919723	-0.13708373522067	0.09155277322175
N	-1.70904234125911	0.01081849463970	-0.00211231280279
H	-2.19215241453572	-0.63693724865145	0.62939570812481
H	-2.07194577297892	0.93796052304326	0.24480969717392
H	-2.09558492287305	-0.18405938894483	-0.93214461648886
C	3.32850117549489	0.53920405120608	1.04528726433227
C	3.28059523878787	-1.21900682436089	-0.58474703672462
C	4.67576591135183	-1.32661267808168	-0.51985079944354
C	4.72372416012286	0.44118795361810	1.12114822515408
C	5.40314835353458	-0.49492003414917	0.33639653381092
H	5.19362460330710	-2.06171225861181	-1.13953399392114
H	6.48985363969216	-0.57539811699897	0.39140217676900
H	5.27917056439358	1.09727104281112	1.79461083569721
H	2.84653270877239	1.29307643878423	1.67757620075721
H	2.75801509633377	-1.89575629269969	-1.26946408700903
N	0.63732611814882	1.97346995382218	0.07203339484750
H	1.53762342338063	2.26556390795770	-0.32376932582352
H	0.59026383230875	2.41048554320617	0.99884330761880
H	-0.08572451481772	2.44277109882311	-0.48450970283660
N	0.36837590504193	-0.15199797507912	2.19881295722352
H	0.09654551661547	-1.06135403610906	2.58746715299492
H	1.27975328123112	0.06021107403300	2.62055400433464
H	-0.29638191317242	0.52242372793057	2.59350769828707
C	2.56258429877964	-0.28550910571568	0.19348055395382
N	0.33126152464342	-2.24308576415113	0.09603285837797
H	-0.53429029654831	-2.60185585776134	0.51418485743700
H	0.37174241665540	-2.66988866202203	-0.83592283444113
H	1.10350049779409	-2.66364564468737	0.62431612140887
N	0.57639298541599	-0.09938036314778	-2.02165302626158
H	1.54381173937522	-0.21219225460303	-2.34495163994927
H	0.03220203179857	-0.83470332991441	-2.48580736491398
H	0.24891682400794	0.78113376103487	-2.43333558090922

$Cr(NH_3)_5(CO)^{3+}$

Charge = 3
Spin Multiplicity = 4

Cr	0.75889290804765	0.09781233895187	0.06008090940528
N	0.30911384076998	2.14243887913896	0.03476087637355
H	1.02061797782627	2.72490952224298	-0.42422110819674
H	0.19252978857495	2.55155748720721	0.96971329628017

H	-0.56769967063973	2.34637452022796	-0.46111174363626
N	0.86676798666945	0.10401699112775	2.15224726694185
H	1.54163027235476	-0.56947553290506	2.53530405175849
H	1.13915539830891	1.00976042425171	2.55374470324727
H	-0.03038732497328	-0.12969428435739	2.59535943915251
C	2.80846509866311	0.56805851695329	0.04203492683074
N	1.22077619007448	-1.94237850861625	0.01410048834059
H	1.22777039736664	-2.38591990942222	0.94070735867444
H	0.54926790626158	-2.48503518642916	-0.54327796672243
H	2.13969785552980	-2.15880799235955	-0.39193833363739
N	0.74676062049358	0.07791331708863	-2.03289197800606
H	1.65153628308668	-0.16935035063694	-2.45249797026270
H	0.07871333002421	-0.59691433926453	-2.42604879445510
H	0.49815099743846	0.98354849691668	-2.44879354999494
N	-1.26092165186929	-0.33432126894294	0.14629321950431
H	-1.46229176966210	-1.27352738967780	0.51219405399409
H	-1.78464403858134	0.31223983971931	0.74989554738886
H	-1.73103716287889	-0.29191354759189	-0.76664324373631
O	3.90762476711411	0.82409797637736	0.04674855075577

$Cr(NH_3)_5(NHC)^{3+}$ (NHC = 1,3-dimethylimidazolium-2-yl)

Charge = 3
Spin Multiplicity = 4

Cr	1.18507276417926	0.18321463844488	0.04515774269874
N	0.76940137078452	2.25258905084140	0.04601848478154
H	1.56817840768165	2.81692566443780	-0.26540540702797
H	0.47893933260346	2.65052100153357	0.94658298697847
H	0.00698388279768	2.49463008830798	-0.59824412914441
N	1.10455034760799	0.01613160107345	2.14486767911039
H	1.99843313760228	-0.27347384825001	2.55668744896488
H	0.83519349598322	0.87440016775948	2.63837847346930
H	0.42604481039747	-0.68652696870799	2.46180658470272
C	3.28928215715618	0.51667110159733	0.04780540111437
N	1.43430721599041	-1.91233149476906	0.03141520654661
H	0.83282258655961	-2.38691412949244	0.71534425515410
H	1.21671354410624	-2.37037328718490	-0.86118099700586
H	2.38765840400885	-2.20376582654857	0.27522324133275
N	1.07465648824198	0.33090706850349	-2.05646578744855
H	1.83429759321665	0.89569858874829	-2.45251416231293
H	1.10074668820964	-0.56285272587977	-2.56008064852946
H	0.21184609328252	0.78542454674022	-2.37898260330050
N	-0.93791583907623	-0.14922663141449	0.06400662776534
H	-1.22085132824804	-1.02507346184486	0.51834908427867

H	-1.45897060017311	0.58425198693769	0.55856761746457
H	-1.36263675322012	-0.19637514001314	-0.86923017423555
N	4.02089817146374	1.31126341067279	0.89536632618897
N	4.23291109502190	-0.01174186666446	-0.79827178783831
C	5.49900752876821	0.44159014711920	-0.48460376122624
C	5.36575242772409	1.27324405656003	0.58396700694829
H	6.10487591533246	1.83152502373846	1.14631572722895
H	6.37585705726359	0.14005226738864	-1.04538542984058
C	4.01833268317983	-0.88177777879264	-1.95854409508972
H	3.14435183961950	-1.51778287228671	-1.80932019635973
H	4.89374103445826	-1.52879804367383	-2.07345258401674
H	3.89919423450548	-0.28434382521309	-2.87109232368663
C	3.54509048368155	2.07006647071388	2.05591331092549
H	2.51701301257894	2.40378933974265	1.90517091112114
H	4.17622854337208	2.95670986337538	2.17281318776625
H	3.61622217333827	1.46369181649937	2.96779678252162

Compounds for the calculated V2C library are indexed alphabetically by CCSD entry identifier.

ABEXOU[1]

Tricarbonyl-(η^6-N,N-diethyl-2-methyl-6-(α-hydroxyethyl)benzamide)-chromium(0)
Charge = 0
Spin Multiplicity = 1

Cr	0.034939	-0.065817	0.027347
O	3.091472	1.846053	0.488219
O	-0.886411	3.043463	2.064277
O	2.399268	-1.897975	0.249559
O	-1.702292	-2.492769	0.321394
O	0.135340	0.031870	3.027419
N	2.983175	3.281232	-1.285179
C	1.085969	1.757727	-0.829233
C	-0.050878	2.183156	-0.077400
C	-1.334354	1.656866	-0.392788
C	-1.478552	0.700756	-1.416705
C	-0.349758	0.258191	-2.149920
C	0.943616	0.755022	-1.849453
C	2.470672	2.299900	-0.485951
C	2.254233	3.937395	-2.383059
C	2.940882	3.839955	-3.747561
C	4.301317	3.835771	-0.921321
C	4.210024	5.002614	0.064838
C	0.068458	3.252052	1.012705
C	-0.080254	4.658143	0.426852
C	2.125212	0.253596	-2.637059

C	1.481971	-1.175438	0.158116
C	-1.025941	-1.541836	0.208617
C	0.086917	0.026813	1.858701
H	-2.195541	1.951447	0.203106
H	-2.458708	0.273875	-1.624418
H	-0.463766	-0.510161	-2.913055
H	1.252936	3.493721	-2.435559
H	2.118047	5.000492	-2.122125
H	3.903298	4.368332	-3.764851
H	2.295350	4.305919	-4.505288
H	3.116129	2.796443	-4.040137
H	4.794741	4.153036	-1.848814
H	4.891705	3.019165	-0.489520
H	3.754069	4.681466	1.010924
H	5.219599	5.380077	0.282214
H	3.621937	5.836436	-0.344680
H	1.055331	3.147138	1.485328
H	0.034635	5.402576	1.226501
H	0.674922	4.861588	-0.342556
H	-1.073226	4.779828	-0.034097
H	-1.673340	3.584247	1.867058
H	3.056942	0.302129	-2.060805
H	2.256727	0.857123	-3.547595
H	1.962621	-0.784797	-2.951682

ABORCR10[2]

π-(exo-2-Acetoxybenzonorbornenyl)-exo-tricarbonyl-chromium(0)
Charge = 0
Spin Multiplicity = 1

Cr	3.778074	2.792599	0.589582
C	0.748340	3.032594	2.263796
C	1.870443	2.217437	1.650412
C	1.628078	2.183409	0.252006
C	-2.641219	1.975027	3.216576
C	-3.668076	2.757714	3.990616
C	4.160974	4.100834	1.809321
C	5.566077	2.703819	0.222597
C	3.645254	4.091681	-0.689007
C	-0.498631	2.106313	2.148187
C	-0.781263	2.065814	0.616909
C	0.350315	2.966876	0.020684
C	2.453816	1.413333	-0.604489
C	3.516345	0.671941	-0.038676
C	3.754720	0.700268	1.366827

C	2.939169	1.479005	2.218658
C	0.460094	4.046514	1.126662
O	-1.577528	2.758298	2.887377
O	-2.728218	0.795866	2.910632
O	4.417884	4.941683	2.584689
O	6.712663	2.654855	-0.016255
O	3.564563	4.927716	-1.507004
H	0.924908	3.416178	3.273542
H	-4.499206	2.102422	4.268007
H	-4.040535	3.591858	3.379465
H	-3.213167	3.189818	4.892530
H	-0.342721	1.114251	2.586476
H	-0.775166	1.044824	0.216610
H	-1.763179	2.510677	0.407573
H	0.172504	3.306476	-1.004554
H	2.296488	1.408091	-1.682406
H	4.178938	0.099831	-0.684850
H	4.598795	0.151269	1.780388
H	3.147941	1.523791	3.286808
H	-0.479488	4.593779	1.276851
H	1.286336	4.749090	0.965739

ABUKIS[3]

Methyl-(perfluorophenyl)-(η^5-pentamethylcyclopentadienyl)-(pyridine)-chromium(III)
Charge = 0
Spin Multiplicity = 4

Cr	-1.13281	-1.03274	10.68737
F	2.02907	-0.35151	10.00410
F	4.01542	-1.79562	9.05834
F	3.71331	-4.46949	8.59537
F	1.31862	-5.63487	9.14187
F	-0.73703	-4.18854	10.03241
N	-2.59834	-1.73161	9.33442
C	-3.32935	-2.81774	9.62608
H	-3.12878	-3.28315	10.40619
C	-4.34818	-3.27979	8.84880
H	-4.82403	-4.03813	9.10081
C	-4.66294	-2.61666	7.69350
H	-5.36013	-2.90792	7.15125
C	-3.92046	-1.51276	7.35654
H	-4.10590	-1.04680	6.57501
C	-2.90125	-1.10124	8.18337
H	-2.40144	-0.35679	7.93702
C	0.51656	-2.16850	10.00551

C	1.77093	-1.66559	9.75067
C	2.82776	-2.38903	9.29619
C	2.66866	-3.73143	9.05551
C	1.47592	-4.32245	9.32026
C	0.42708	-3.54330	9.79456
C	-0.41297	-0.08977	12.58653
C	-0.48903	-1.48979	12.80315
C	-1.79894	-1.89179	12.69838
C	-2.59926	-0.74995	12.40672
C	-1.72416	0.36298	12.34726
C	0.80551	0.76180	12.68139
H	0.75138	1.30936	13.46858
H	0.86613	1.32197	11.90411
H	1.58327	0.20172	12.73519
C	0.66170	-2.38992	13.20524
H	0.77669	-2.35562	14.15808
H	1.46611	-2.09225	12.77342
H	0.46980	-3.29218	12.93907
C	-2.35305	-3.26387	13.01552
H	-1.87370	-3.92753	12.51433
H	-3.28354	-3.29549	12.77908
H	-2.25447	-3.44039	13.95420
C	-4.10044	-0.70977	12.29771
H	-4.48701	-0.78614	13.17268
H	-4.40190	-1.43802	11.74979
H	-4.37021	0.12132	11.89987
C	-2.10229	1.81408	12.15896
H	-3.01842	1.87224	11.87863
H	-1.53630	2.20840	11.49070
H	-1.99251	2.28354	12.99004
C	-0.70036	0.60545	9.49016
H	-0.32551	0.30443	8.65908
H	-0.06885	1.17176	9.93897
H	-1.50632	1.09817	9.31743

ACBCRA10[4]

mer-Bromo-tricarbonyl-(N,N-diethylaminocarbyne)-triphenylphosphine-chromium
Charge = 0
Spin Multiplicity = 4

Cr	8.207665	2.152304	4.957990
C	8.180543	1.977180	6.863518
O	8.200561	1.934980	8.014261
C	8.023209	2.353020	3.064538
O	7.913398	2.560265	1.936250

C	7.090626	3.692503	5.062346
O	6.492336	4.676277	5.116893
C	9.415068	0.681524	4.870451
O	10.219918	-0.146638	4.837727
C	9.611607	3.235444	5.037515
N	10.600827	4.036155	5.165611
C	10.676588	4.918193	6.383582
C	11.822751	4.540143	7.310575
C	11.717955	4.169297	4.172784
C	11.475134	3.451129	2.858635
P	6.184191	0.651867	4.879751
C	4.663720	1.679960	4.822163
C	4.080481	2.024628	3.592108
C	2.988142	2.895247	3.551810
C	2.474250	3.435320	4.734003
C	3.061679	3.108546	5.959964
C	4.154985	2.241704	6.006081
C	6.057345	-0.485519	3.433529
C	4.839399	-1.143010	3.179456
C	4.741541	-2.062258	2.135251
C	5.856931	-2.345407	1.338598
C	7.070869	-1.704371	1.590982
C	7.170011	-0.778140	2.634052
C	5.945762	-0.505108	6.296683
C	7.065793	-1.123308	6.873622
C	6.908244	-2.085873	7.873101
C	5.628792	-2.437123	8.311598
C	4.507702	-1.827271	7.741213
C	4.661488	-0.869518	6.736027
H	9.708993	4.837863	6.893029
H	10.776268	5.944635	6.003741
H	11.732660	3.502397	7.658080
H	11.785799	5.199355	8.188848
H	12.801878	4.673607	6.833615
H	11.837942	5.250948	4.017509
H	12.623473	3.792948	4.667752
H	10.590461	3.841147	2.338937
H	11.368982	2.367074	2.993241
H	12.347370	3.621522	2.213663
H	4.466163	1.607928	2.661165
H	2.538290	3.148166	2.590792
H	1.618937	4.111553	4.700356
H	2.669315	3.529111	6.886798
H	4.603913	2.002352	6.971309
H	3.960891	-0.938856	3.792136
H	3.790110	-2.560839	1.945112

H	5.777439	-3.065921	0.523404
H	7.946502	-1.920071	0.977587
H	8.126744	-0.291306	2.816878
H	8.072111	-0.866566	6.543378
H	3.505255	-2.095236	8.077948
H	3.774869	-0.408428	6.301549
H	5.505495	-3.184227	9.096778
H	7.789199	-2.557018	8.310638

ACEMIG[5]

(η^6-*t*-Butyl((2,3-diethyl-4,7-dimethoxy-5-phenyl-5,6-dihydronaphthalen-1-yl)oxy)dimethylsilane)-tricarbonyl-chromium(0)
Charge = 0
Spin Multiplicity = 1

Cr	-0.028350	0.015187	0.058574
Si	-1.077510	1.353275	-3.974377
O	-0.503691	-0.134245	-3.352339
O	4.456242	0.974786	-2.975113
O	1.250308	-2.825437	1.180308
O	-2.565074	1.600709	0.180595
O	-0.171854	0.104065	3.046865
O	1.418725	2.633056	0.247561
C	-0.095866	-0.663481	-2.166063
C	-1.021731	-1.435124	-1.390752
C	-0.559012	-2.176943	-0.266514
C	0.822406	-2.078128	0.100153
C	1.742397	-1.251501	-0.601253
C	3.250369	-1.241173	-0.322760
H	3.652103	-2.075563	-0.928602
C	3.917373	0.045171	-0.860400
H	3.675517	0.895127	-0.200041
H	5.008710	-0.077395	-0.831268
C	3.483245	0.369809	-2.252709
C	2.222283	0.099888	-2.670725
H	1.870065	0.379147	-3.659152
C	1.282576	-0.581182	-1.795319
C	4.136832	1.364639	-4.326452
H	3.851075	0.486504	-4.923541
H	5.050572	1.811767	-4.729566
H	3.324893	2.106414	-4.331837
C	1.779988	-4.116968	0.796386
H	1.024927	-4.709199	0.256554
H	2.048225	-4.620717	1.730971
H	2.675128	-4.009840	0.167129

C	-1.477611	-3.129819	0.482777
H	-0.861344	-3.917540	0.932339
H	-2.123603	-3.629485	-0.253159
C	-2.350706	-2.516762	1.588530
H	-1.732406	-2.118109	2.402211
H	-3.013280	-3.287859	2.008475
H	-2.977343	-1.697772	1.210199
C	-2.444229	-1.584010	-1.879232
H	-2.781693	-0.635987	-2.311106
H	-3.107967	-1.794132	-1.031786
C	-2.572917	-2.697530	-2.935227
H	-1.945994	-2.483461	-3.811084
H	-3.615625	-2.780623	-3.272431
H	-2.268988	-3.674424	-2.532554
C	-2.862935	1.660205	-3.469328
H	-3.548919	0.879362	-3.825866
H	-3.191112	2.616399	-3.906391
H	-2.969212	1.748997	-2.379282
C	-0.029068	2.782751	-3.355856
H	0.037059	2.765609	-2.258931
H	-0.501738	3.733543	-3.645513
H	0.993135	2.774461	-3.756230
C	-0.945878	1.096724	-5.865936
C	0.509343	0.805958	-6.280962
H	0.888255	-0.118447	-5.820378
H	1.187615	1.630769	-6.014038
H	0.570059	0.677673	-7.375829
C	-1.421061	2.388084	-6.567627
H	-1.353104	2.264065	-7.662354
H	-0.803072	3.258009	-6.297693
H	-2.468463	2.628034	-6.330640
C	-1.837896	-0.079790	-6.311053
H	-2.897949	0.089833	-6.070412
H	-1.529433	-1.025557	-5.841610
H	-1.766052	-0.212623	-7.404733
C	3.745620	-1.455428	1.102895
C	3.361501	-0.615536	2.158431
H	2.610168	0.156194	1.987478
C	3.916105	-0.767919	3.430577
H	3.597277	-0.109576	4.240577
C	4.877249	-1.757044	3.669031
H	5.311300	-1.874000	4.663433
C	5.281226	-2.587848	2.621196
H	6.036699	-3.357381	2.790058
C	4.720971	-2.432339	1.348859
H	5.051864	-3.078969	0.532226

C	-1.572225	0.972615	0.108164
C	-0.107776	0.041060	1.875072
C	0.864345	1.599614	0.159813

ACOYEW[6]

(η^6-8-ethylidene-3,4-dimethoxy-5-methyl-2-trimethylsilyl-5,6,7,8-tetrahydronaphthyl)-tricarbonyl-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	-0.025874	0.035604	0.052380
Si	-2.102300	-2.985732	1.115843
C	-0.403468	1.370340	-3.129423
C	1.079713	1.225225	-3.497762
C	1.424171	-0.186501	-3.975511
C	0.874212	-1.292368	-3.086177
C	-0.485968	-1.832617	-1.005890
C	-1.568895	-1.614555	-0.116827
C	-2.274978	-0.380910	-0.243592
C	-1.851408	0.616704	-1.170395
C	-0.778544	0.340450	-2.084043
C	-0.131859	-0.931713	-2.059728
C	1.208636	-2.587562	-3.292734
C	2.159420	-3.106062	-4.324874
C	-1.336970	1.250469	-4.352943
C	-2.630474	2.669861	-0.158192
C	-4.627057	-0.055148	-0.120611
C	-0.769123	-4.322003	1.084233
C	-3.724311	-3.719304	0.483398
C	-2.310388	-2.353515	2.875727
C	1.551414	-0.707676	0.586687
C	-0.358821	0.468732	1.793713
C	0.866971	1.622856	-0.052424
O	-2.502501	1.814090	-1.322680
O	-3.358224	-0.170119	0.580621
O	2.571782	-1.171645	0.934573
O	-0.547833	0.776198	2.909922
O	1.461729	2.635317	-0.090867
H	-0.562979	2.364753	-2.689235
H	1.689661	1.478377	-2.618593
H	1.333896	1.953211	-4.282735
H	1.040151	-0.333712	-4.998584
H	2.517189	-0.286961	-4.052665
H	0.086320	-2.751423	-0.900962

H	0.733931	-3.359560	-2.682103
H	1.624153	-3.718297	-5.070780
H	2.903974	-3.773742	-3.861916
H	2.693319	-2.312609	-4.861109
H	-1.064393	2.004380	-5.105831
H	-2.383625	1.417694	-4.064925
H	-1.269532	0.258424	-4.822026
H	-3.288484	2.228837	0.600915
H	-3.057920	3.605222	-0.534573
H	-1.636896	2.850577	0.275267
H	-4.645616	0.827304	-0.773558
H	-5.385894	0.039885	0.662859
H	-4.815484	-0.960383	-0.715879
H	0.216101	-3.929404	1.375096
H	-0.675922	-4.799685	0.097899
H	-1.039199	-5.108436	1.806037
H	-3.993742	-4.598540	1.089120
H	-3.636043	-4.044640	-0.563616
H	-4.552596	-3.000280	0.552219
H	-2.672796	-3.174765	3.513483
H	-3.035199	-1.530538	2.925687
H	-1.356746	-1.998519	3.289887

ACOYIA[6]

(η^6-8-(3-cyanoprop-2-yl)-3,4-dimethoxy-5-methyl-2-trimethylsilyl-5,6,7,8-tetrahydronaphthyl)-tricarbonyl-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	0.027854	0.012307	0.010525
C	1.736216	-1.683255	-2.556308
C	2.046249	-0.521581	-3.509564
C	0.829193	-0.161385	-4.365214
C	-0.398916	0.272726	-3.531139
C	-1.660117	-0.277140	-1.392387
C	-1.953325	-1.057239	-0.250101
C	-0.984004	-2.019249	0.157322
C	0.239666	-2.171609	-0.562891
C	0.479546	-1.402593	-1.752518
C	-0.492960	-0.459008	-2.189373
C	-0.597864	1.821159	-3.462562
C	0.693669	2.565241	-3.036189
C	0.493093	4.000748	-2.876879
C	-1.128229	2.356052	-4.799560

C	1.598845	-3.026256	-3.308744
C	1.708268	-3.130617	1.112170
C	-1.620318	-4.159735	0.926755
C	-3.254651	-0.907164	0.489724
C	-0.422111	1.774487	0.140685
C	0.058795	0.017329	1.832579
C	1.791030	0.485826	0.045021
N	0.332114	5.147820	-2.764616
O	1.171183	-3.119363	-0.236252
O	-1.246505	-2.794354	1.262030
O	-0.718986	2.903490	0.261694
O	0.074398	0.036143	3.005620
O	2.922418	0.798823	0.076055
H	2.567206	-1.793033	-1.844259
H	2.381785	0.347926	-2.924667
H	2.887950	-0.806043	-4.158727
H	1.088784	0.630404	-5.082818
H	0.553923	-1.031363	-4.979059
H	-1.294163	-0.076356	-4.074605
H	-2.395408	0.467323	-1.698668
H	1.065362	2.168079	-2.078343
H	1.489629	2.429135	-3.784831
H	-1.356805	2.030187	-2.693741
H	-1.305774	3.439213	-4.747629
H	-2.079580	1.870228	-5.058083
H	-0.418876	2.172515	-5.620396
H	1.439751	-3.856103	-2.609363
H	2.520585	-3.226395	-3.873935
H	0.759535	-3.013189	-4.018214
H	2.048362	-2.119997	1.378962
H	2.557525	-3.820993	1.074640
H	0.966229	-3.476036	1.841467
H	-2.527572	-4.167140	0.305482
H	-1.821272	-4.653099	1.883355
H	-0.802596	-4.673295	0.401857
H	-3.688960	0.082839	0.305749
H	-3.122772	-1.047160	1.568414
H	-3.976030	-1.663204	0.141310

ACTPCR[7]

Acetophenone tricarbonyl chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	1.232503	2.160003	2.399706
C	1.059723	-0.060538	2.049337
C	2.728736	2.154605	3.458208
C	0.243937	2.494509	3.913488
C	2.152442	0.448171	1.298204
C	-0.429897	1.610982	1.005189
C	-0.209738	0.533594	1.917482
C	0.679121	2.097670	0.256082
C	1.957200	1.499183	0.374144
C	1.469362	3.970262	2.221753
C	-1.797757	2.219923	0.923185
C	-2.004110	3.427251	0.041325
O	-2.728264	1.710807	1.548793
O	1.623159	5.124258	2.116712
O	3.682248	2.160787	4.134467
O	-0.374106	2.713994	4.879254
H	1.216452	-0.860266	2.770665
H	3.147265	0.028291	1.437335
H	-1.047872	0.191593	2.522423
H	0.554339	2.944534	-0.415770
H	2.797748	1.897092	-0.190967
H	-1.307465	4.238037	0.298631
H	-3.034682	3.780607	0.151181
H	-1.822562	3.163172	-1.012247

ACUDOR[8]

(R)-Tricarbonyl-(η^6-1-(methoxymethoxy)-2-(hydroxy(diphenyl)methyl)benzene)-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	1.430001	3.270966	-3.532281
C	1.873588	1.117889	-2.852953
C	1.612038	1.923756	-1.690204
C	0.397166	2.651972	-1.663952
H	0.186261	3.277674	-0.799043
C	-0.544362	2.598265	-2.723392
H	-1.459287	3.184406	-2.671728
C	-0.236726	1.844652	-3.871650
H	-0.919479	1.828751	-4.719184
C	0.967846	1.095633	-3.939178
H	1.180740	0.502077	-4.823501
O	3.032913	0.392834	-2.832218
C	3.477951	-0.270931	-4.060570
H	3.396257	0.433618	-4.898285

H	4.527154	-0.513512	-3.836817
O	2.729274	-1.395300	-4.377053
C	2.959250	-2.512039	-3.488051
H	2.404416	-3.357857	-3.907543
H	2.589424	-2.291271	-2.476324
H	4.033451	-2.752958	-3.447237
C	2.578750	1.892322	-0.477680
O	3.930937	2.117825	-0.916366
H	4.100491	1.447318	-1.611234
C	1.321432	-0.269833	0.188406
H	0.448477	0.060058	-0.376455
C	1.265454	-1.490483	0.871188
H	0.356079	-2.092113	0.825606
C	2.366837	-1.937398	1.604268
H	2.325077	-2.890076	2.134693
C	3.524717	-1.153384	1.651446
H	4.391642	-1.491144	2.222184
C	3.579004	0.064402	0.970476
H	4.484671	0.670159	1.005480
C	2.478968	0.519577	0.227485
C	1.397607	2.855806	1.593245
H	0.928520	1.886198	1.763470
C	1.122859	3.911952	2.467758
H	0.440207	3.754719	3.304490
C	1.726975	5.157564	2.277793
H	1.518657	5.980196	2.963795
C	2.603720	5.339350	1.204053
H	3.082470	6.307164	1.045975
C	2.872055	4.286291	0.325735
H	3.557484	4.431928	-0.507341
C	2.273489	3.031022	0.512143
C	3.219078	3.510545	-3.840408
O	4.356815	3.679638	-4.062518
C	1.347090	5.010436	-2.976126
O	1.284837	6.134299	-2.651597
C	1.131240	3.892835	-5.223666
O	0.941516	4.302891	-6.305153

ACUDUX[8]

(R)-Tricarbonyl-(η^6-1-(methoxymethoxy)-2-(bis(4-methoxyphenyl)hydroxymethyl)benzene)-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	-0.920450	3.682783	10.804530
C	-2.944505	2.598131	11.016520
C	-2.656441	3.303296	12.238085
C	-2.381289	4.687994	12.140211
H	-2.158945	5.236111	13.053788
C	-2.378840	5.376392	10.897838
H	-2.144211	6.438082	10.862705
C	-2.599281	4.650447	9.713747
H	-2.543317	5.144960	8.745680
C	-2.877463	3.256645	9.767491
H	-3.005501	2.695709	8.845645
O	-3.266393	1.274518	11.140400
C	-3.911628	0.599486	10.012362
H	-4.371920	-0.278936	10.488560
H	-4.667007	1.273371	9.588529
O	-3.039654	0.250561	8.991089
C	-2.176577	-0.862951	9.314684
H	-1.644503	-1.116678	8.391990
H	-2.775486	-1.725280	9.648616
H	-1.452085	-0.587716	10.093717
C	-2.787202	2.594334	13.611803
O	-2.072834	1.340925	13.589403
H	-2.438889	0.834643	12.834131
C	-4.280033	2.342499	13.911019
C	-5.307708	3.144651	13.405982
H	-5.078934	3.983096	12.746711
C	-6.651299	2.907303	13.725695
H	-7.420020	3.555245	13.307483
C	-6.983712	1.841726	14.571975
C	-5.959984	1.030400	15.092243
H	-6.224753	0.203663	15.753626
C	-4.632844	1.283180	14.765654
H	-3.849239	0.644014	15.173125
O	-8.260130	1.511241	14.946557
C	-9.329355	2.328490	14.440091
H	-10.248035	1.903354	14.858058
H	-9.371404	2.290152	13.340542
H	-9.221654	3.372924	14.771143
C	-2.126287	3.411651	14.731637
C	-2.854172	4.262466	15.568803
H	-3.934678	4.349152	15.449353
C	-2.232230	5.011468	16.575802
H	-2.837672	5.659486	17.207360
C	-0.847233	4.906679	16.760950
C	-0.102821	4.053110	15.927909

H	0.974932	3.974494	16.078822
C	-0.735818	3.323321	14.928401
H	-0.146929	2.663099	14.293674
O	-0.135385	5.582138	17.717090
C	-0.868302	6.460103	18.589280
H	-1.361927	7.263103	18.020795
H	-0.123158	6.892223	19.265340
H	-1.617733	5.903785	19.172920
C	-0.042431	2.111181	11.136635
O	0.545969	1.114708	11.319486
C	0.439725	4.564445	11.645132
O	1.322553	5.138742	12.159563
C	0.055221	3.797590	9.264326
O	0.687590	3.869238	8.279904

ADOPAL01[9]

Dioxo-(N,N'-bis(2,6-diisopropylphenyl)pent-2-en-2-amido-4-imido)-chromium(V)

Charge = 0
Spin Multiplicity = 2

Cr	7.114810	14.318872	3.400250
O	8.094435	15.421208	4.043569
O	5.802292	14.806406	2.609655
N	6.633568	12.977258	4.727556
N	8.135092	13.086309	2.293910
C	6.420544	10.707557	5.699868
H	5.861469	11.207837	6.495773
H	7.280360	10.185735	6.143534
H	5.780580	9.938803	5.243761
C	6.899871	11.664432	4.633187
C	7.626908	11.102968	3.573046
H	7.769947	10.023979	3.612959
C	8.224980	11.760830	2.488243
C	9.003710	10.897629	1.523436
H	9.444836	11.473108	0.704562
H	8.342851	10.126900	1.101839
H	9.805812	10.372055	2.060843
C	5.912841	13.534857	5.850259
C	4.500500	13.649595	5.785595
C	3.835862	14.224556	6.877836
H	2.748795	14.318316	6.850344
C	4.532362	14.673937	7.997942
H	3.993354	15.117869	8.836745
C	5.920202	14.553290	8.043111

H	6.459806	14.904502	8.924487
C	6.639235	13.989196	6.980795
C	3.682770	13.147339	4.600887
H	4.383056	12.824889	3.818812
C	2.818153	11.933478	4.996895
H	2.276400	11.550958	4.118910
H	2.073001	12.209866	5.758264
H	3.426572	11.114095	5.404790
C	2.805435	14.259440	3.997728
H	2.271190	13.878985	3.114484
H	3.417069	15.115031	3.682359
H	2.051251	14.613134	4.716740
C	8.154273	13.865030	7.093280
H	8.534762	13.494353	6.131828
C	8.822289	15.227119	7.355042
H	8.574317	15.943669	6.560965
H	9.915913	15.110529	7.380799
H	8.509609	15.650470	8.321384
C	8.550333	12.849523	8.183935
H	8.105418	11.860967	8.002479
H	8.221358	13.188628	9.177971
H	9.643842	12.731093	8.213652
C	8.783630	13.747302	1.183782
C	8.081108	13.910066	-0.037690
C	8.726012	14.586212	-1.082699
H	8.204830	14.719007	-2.032426
C	10.017230	15.089004	-0.935454
H	10.499143	15.612353	-1.763118
C	10.691098	14.920715	0.273066
H	11.703045	15.315098	0.381356
C	10.097136	14.255325	1.353725
C	6.678793	13.356899	-0.265867
H	6.313339	12.956572	0.689211
C	5.693652	14.455014	-0.706638
H	5.650814	15.264751	0.033649
H	4.682569	14.033480	-0.808292
H	5.975575	14.883319	-1.680244
C	6.695377	12.204861	-1.290774
H	7.372530	11.395125	-0.984785
H	7.022068	12.560448	-2.279795
H	5.685936	11.781297	-1.401687
C	10.887143	14.083234	2.646010
H	10.215387	13.642534	3.395061
C	12.074991	13.120298	2.448463
H	11.747832	12.139118	2.076598
H	12.600918	12.965353	3.402453

H	12.798953	13.528842	1.727123
C	11.373461	15.432510	3.205468
H	10.528501	16.111159	3.381289
H	12.081533	15.922284	2.520296
H	11.891390	15.276847	4.163497

AESCRI[10]

Charge = 1
Spin Multiplicity = 4

Cr	-2.409531	2.727813	2.658123
C	-0.397717	4.878465	2.637696
C	-3.708724	2.569703	-0.014917
C	-3.405773	1.133363	0.389468
C	-1.444238	0.197525	1.405316
C	-0.392979	0.047824	2.370449
C	0.508872	-1.033390	2.197012
C	1.533987	-1.274798	3.094811
C	1.674528	-0.426105	4.211177
C	0.807859	0.638019	4.415498
C	-0.246908	0.914666	3.508236
C	-1.625301	5.503579	3.285797
C	-3.144613	4.563070	4.886785
C	-4.037685	3.602514	5.467004
C	-4.638548	3.931256	6.709348
C	-5.530835	3.076501	7.332438
C	-5.850753	1.854009	6.708325
C	-5.284025	1.500714	5.492019
C	-4.361317	2.353410	4.834123
N	-2.325939	1.155479	1.388105
N	-0.867731	3.828212	1.681339
N	-2.484291	4.413156	3.774366
N	-3.860340	3.374299	1.234343
O	-1.041904	1.936303	3.764362
O	-3.865443	1.967380	3.674095
H	0.212405	5.638004	2.129618
H	0.216576	4.377636	3.395589
H	-4.612045	2.621173	-0.638789
H	-2.870842	2.990124	-0.587232
H	-3.135378	0.522334	-0.484574
H	-4.297501	0.683963	0.857767
H	0.373364	-1.683617	1.329470
H	2.218217	-2.109680	2.944809
H	2.474964	-0.607125	4.931237
H	0.915893	1.288910	5.284448

H	-2.187281	6.089051	2.537828
H	-1.339652	6.186475	4.099721
H	-4.378857	4.886831	7.171153
H	-5.980646	3.344083	8.288396
H	-6.554553	1.170233	7.186993
H	-5.533225	0.552999	5.012284
H	-1.503060	-0.575886	0.626033
H	-3.019252	5.505043	5.439880
H	-4.766258	3.165238	1.669339
H	-3.885658	4.372990	1.008333
H	-1.170924	4.273585	0.808657
H	-0.080739	3.226018	1.419747

AFEHIC[11]

Dichloro-oxo-(η^5-pentamethylcyclopentadienyl)-chromium(V)

Charge = 0
Spin Multiplicity = 2

Cr	-0.013803	0.003998	0.026226
Cl	-1.296500	1.755267	-0.551104
Cl	-1.523469	-1.542129	-0.591184
O	-0.028755	-0.010732	1.606125
C	2.219319	-0.097109	0.163887
C	1.755107	-1.250032	-0.546543
C	1.243138	-0.810028	-1.836391
C	1.309995	0.594425	-1.876103
C	1.868394	1.053647	-0.613202
C	2.923267	-0.094899	1.480272
H	4.009266	-0.186181	1.320314
H	2.606999	-0.934872	2.111177
H	2.744684	0.834465	2.034913
C	1.911729	-2.675754	-0.129399
H	2.808334	-3.106109	-0.605039
H	1.050475	-3.281209	-0.439416
H	2.031826	-2.772154	0.956343
C	0.797632	-1.721123	-2.929489
H	1.679335	-2.120449	-3.457216
H	0.172292	-1.201799	-3.665325
H	0.230917	-2.574989	-2.537340
C	0.941961	1.482317	-3.016879
H	1.851862	1.778458	-3.564244
H	0.450441	2.400307	-2.670232
H	0.272974	0.980192	-3.725928
C	2.176644	2.477394	-0.284808

H	3.108049	2.779649	-0.791366
H	2.319029	2.627900	0.791993
H	1.379831	3.149258	-0.628091

AFUCAG[12]

Chloro-(N,N'-bis(3,5-di-*t*-butylsalicylidene)-1,2-phenylenediamine-N,N',O,O')-(oxetane-O)-chromium(III) dichloromethane *n*-pentane solvate

Charge = 0
Spin Multiplicity = 4

Cr	10.720540	7.989247	3.383225
Cl	11.164126	9.854588	2.084401
O	8.952621	8.615305	3.896127
O	11.636196	8.723121	4.928198
O	10.370516	6.220985	4.478990
N	9.951712	7.001044	1.802273
N	12.415155	7.095252	2.752437
C	7.669460	7.878095	1.994629
C	7.821979	8.600012	3.232872
C	6.671801	9.298384	3.751872
C	5.485235	9.227925	3.029603
H	4.621113	9.759996	3.426355
C	5.309753	8.520048	1.811524
C	6.415970	7.858453	1.319919
H	6.361166	7.292256	0.388916
C	6.760319	10.118099	5.054564
C	7.170907	9.210199	6.238463
H	8.161612	8.771297	6.076651
H	6.439632	8.399240	6.379250
H	7.201854	9.802579	7.165889
C	7.795424	11.254529	4.878891
H	7.878214	11.831002	5.813238
H	7.479415	11.943728	4.081009
H	8.784756	10.857067	4.626383
C	5.414422	10.770082	5.425997
H	5.542601	11.340007	6.357960
H	4.624294	10.023909	5.600106
H	5.065393	11.473168	4.654929
C	3.938469	8.519566	1.118054
C	3.528473	9.971847	0.779222
H	4.254134	10.434207	0.093718
H	3.465681	10.599088	1.679829
H	2.540707	9.984029	0.293242
C	3.952725	7.705738	-0.187638

H	2.954314	7.733119	-0.648283
H	4.208445	6.650630	-0.008877
H	4.667891	8.115474	-0.916380
C	2.882678	7.900212	2.063811
H	1.891729	7.907507	1.584275
H	2.802222	8.459032	3.007155
H	3.138245	6.858149	2.307507
C	8.711925	7.121326	1.383474
H	8.417825	6.593465	0.469076
C	10.898305	6.194773	1.126906
C	12.222030	6.243955	1.637937
C	13.224899	5.468515	1.032037
H	14.243857	5.482417	1.416916
C	12.928967	4.661183	-0.063224
H	13.717477	4.062498	-0.520476
C	11.622489	4.611887	-0.567323
H	11.386208	3.974216	-1.419894
C	10.615736	5.370074	0.024669
H	9.604000	5.305888	-0.373834
C	13.602576	7.311229	3.269069
H	14.468600	6.821106	2.809697
C	13.912018	8.140339	4.389324
C	12.920383	8.831375	5.177693
C	13.378320	9.633974	6.278880
C	14.749593	9.681307	6.534420
H	15.082396	10.292164	7.370341
C	15.738236	9.000795	5.785298
C	15.288039	8.241913	4.719378
H	15.993931	7.692600	4.091485
C	12.386464	10.445138	7.136341
C	11.364728	9.503911	7.817785
H	11.877700	8.778526	8.468148
H	10.772652	8.958031	7.074888
H	10.676950	10.093193	8.443809
C	11.646898	11.465458	6.238277
H	10.919346	12.033114	6.838744
H	11.111955	10.965386	5.423194
H	12.360125	12.181502	5.802161
C	13.092168	11.238844	8.252757
H	13.812703	11.967762	7.852485
H	13.618700	10.582561	8.962261
H	12.335678	11.800473	8.820378
C	17.240971	9.084552	6.110986
C	18.001504	9.653237	4.890293
H	17.868018	9.021714	4.000398
H	19.079974	9.709490	5.105039

H	17.647743	10.665463	4.643902
C	17.528524	9.990627	7.321410
H	17.198673	11.025613	7.147086
H	18.611949	10.014765	7.509710
H	17.040669	9.621626	8.235911
C	17.778374	7.669372	6.427675
H	17.263447	7.240021	7.300149
H	18.855619	7.711560	6.651728
H	17.637423	6.984587	5.579176
C	9.081440	5.651815	4.948082
H	8.636603	5.024056	4.166988
H	8.396576	6.457982	5.237654
C	9.798176	4.944271	6.110876
H	9.399101	5.149520	7.109304
H	9.907813	3.864242	5.966770
C	11.047519	5.749553	5.714374
H	11.284842	6.601933	6.362297
H	11.954806	5.188941	5.460060

AGOFIM[13]

Trichloro-(1,1-bis(diphenylphosphoryl-O)ethanamine-N)-chromium(III) acetonitrile solvate monohydrate

Charge = 0
Spin Multiplicity = 4

Cr	16.099124	19.633703	12.150577
N	15.821593	17.649121	12.983019
H	16.425855	17.531931	13.807802
H	14.857895	17.524209	13.321385
Cl	17.280336	20.278782	14.027448
Cl	16.514961	21.525812	10.917944
Cl	14.104076	20.372729	13.065370
P	17.922522	17.195526	11.505071
P	14.966459	17.214127	10.549435
O	17.795682	18.719344	11.373455
O	15.046288	18.745148	10.593935
C	16.157893	16.638694	11.920824
C	15.982855	15.191244	12.367898
H	16.544571	15.006960	13.292981
H	16.329798	14.480436	11.605166
H	14.924970	14.978876	12.574592
C	18.992450	16.726654	12.898393
C	19.653714	17.781421	13.550914
H	19.455276	18.810114	13.252184

C	20.542124	17.507198	14.593599
H	21.049707	18.331230	15.096187
C	20.773738	16.188888	14.991967
H	21.466322	15.978183	15.808051
C	20.115876	15.136107	14.346322
H	20.292166	14.105472	14.655903
C	19.230160	15.398403	13.301311
H	18.733886	14.559311	12.816125
C	18.604117	16.492723	9.986480
C	19.042200	15.161875	9.880609
H	18.939293	14.464133	10.710513
C	19.632070	14.719494	8.696770
H	19.970300	13.685892	8.617069
C	19.799259	15.600568	7.623247
H	20.270291	15.252657	6.702893
C	19.370265	16.926126	7.729790
H	19.505779	17.616866	6.897016
C	18.770520	17.376738	8.906849
H	18.444405	18.412416	9.000826
C	15.334895	16.575632	8.901110
C	15.623838	15.229358	8.622821
H	15.737233	14.498168	9.423084
C	15.781024	14.815012	7.299752
H	16.011821	13.771009	7.086280
C	15.645015	15.734104	6.254447
H	15.764309	15.403782	5.221726
C	15.362797	17.074607	6.530551
H	15.263378	17.794756	5.717701
C	15.208867	17.501022	7.850558
H	14.996043	18.547278	8.070927
C	13.320990	16.606429	11.020063
C	12.490964	17.458995	11.768858
H	12.834821	18.461609	12.038112
C	11.218918	17.025252	12.151660
H	10.575103	17.691240	12.727493
C	10.771817	15.750658	11.793915
H	9.776746	15.417569	12.092331
C	11.594371	14.903862	11.042638
H	11.243586	13.913066	10.751701
C	12.864548	15.327816	10.651726
H	13.483529	14.664487	10.047806

AHEZAO[14]

(Acetonitrile)-(carbonylbis(1-methylimidazole))-*mer*-trichloro-chromium(III) acetonitrile solvate

Charge = 0
Spin Multiplicity = 4

Cr	4.868161	10.955844	0.955377
Cl	6.035113	11.693169	-0.921236
Cl	3.542589	9.510777	-0.326872
Cl	6.062473	12.371108	2.378951
N	3.813178	10.293411	2.618888
C	3.877568	9.075953	3.197505
N	2.914705	8.981724	4.174749
C	2.246633	10.171819	4.207779
C	2.809382	10.978658	3.239430
C	2.625416	7.857591	5.072603
C	4.838704	8.006135	2.914960
O	4.716679	6.887685	3.441339
N	6.191676	9.422921	1.314125
C	5.987633	8.313348	2.059548
N	7.076136	7.481794	1.943708
C	7.975208	8.094008	1.118585
C	7.418705	9.295841	0.729892
C	7.307245	6.179511	2.578790
N	3.508162	12.432619	0.607000
C	2.757983	13.265524	0.317157
C	1.825083	14.302793	-0.060051
H	1.439994	10.354746	4.908590
H	2.547356	11.993516	2.969831
H	3.519556	7.592618	5.645280
H	2.299015	6.987822	4.494597
H	1.829594	8.179635	5.751594
H	8.928388	7.639251	0.875566
H	7.809025	10.055686	0.063774
H	7.215260	6.268448	3.665846
H	8.321530	5.863803	2.314291
H	6.578491	5.448033	2.215614
H	2.066197	14.659515	-1.070503
H	1.893333	15.141040	0.646253
H	0.802692	13.900864	-0.052670

ALUGOE[15]

tris(2,2,3,4,4-Pentamethylpentan-3-olato)-chromium chloro-tris(2,2,3,4,4-pentamethylpentan-3-olato)-chromium

Charge = 0
Spin Multiplicity = 3

Cr	11.69761103924882	3.44045763727553	2.74816749437065
Cl	11.69671551571495	3.48482115780187	0.54029067586364
O	13.37859917275884	3.34210574822351	3.30207894413313
O	10.92597628795134	4.93098888074125	3.31306441125502
O	10.77816381516626	2.01798093148350	3.26386797053749
C	10.12057005634344	7.14683775727209	2.58088975546938
C	14.66903063043635	4.02141979848245	3.19660347203815
C	14.50198740473240	5.24457831524466	2.28339090529509
H	14.34909274446168	4.93978161538644	1.24201111348198
H	15.37922271825846	5.90241835267368	2.32580827246467
H	13.62956325781727	5.83113968580952	2.59044777787561
C	10.72510455144011	0.56497073605433	3.12013309293741
C	9.04261573548642	5.67430839776226	4.64923101875658
C	10.90024094108045	8.02849558033011	3.57594933460458
H	11.75956778840890	7.49446658800867	4.00226973162615
H	10.27213523411387	8.39345895427958	4.39899455776666
H	11.28371091598526	8.91218651272356	3.04302218788983
C	8.90323021198741	7.95711325804878	2.07244730217832
H	9.27695811477927	8.89181024511244	1.62679118962129
H	8.19873949323297	8.23325569755566	2.86399500354864
H	8.34983277314075	7.42426144401831	1.28771316800123
C	14.98823110539522	4.50435482635623	4.70167131295980
C	9.02317467377740	1.12478627891497	1.26198443307467
H	8.07338969089070	0.81625246170877	0.80016074140617
H	9.80408582997691	1.05821344348311	0.49457378714972
H	8.93277819740874	2.17670701187647	1.55201320563410
C	14.07672200251584	5.70300191823810	5.05529132947858
H	13.02179301505245	5.48061303998951	4.84871598976360
H	14.35641884354372	6.61590860205976	4.51181778720237
H	14.17262466453539	5.91915733699338	6.12968455957508
C	9.69971240002499	5.71418673742556	3.17826287985806
C	15.69039722212140	2.99004372794756	2.50285422324216
C	11.04718109325034	0.00541407757935	4.59800757746363
C	11.83005590660441	0.12055201898519	2.14949456829185
H	11.60453082732353	0.42338330041679	1.12086420689886
H	11.95781314963100	-0.96936261625941	2.17108905161924
H	12.78648967361067	0.57291154737005	2.43180121577428
C	16.08007886790237	1.80198029688030	3.40242066017573
H	15.19602064524003	1.28576539535864	3.79876180450389
H	16.71818272633551	2.10121672895737	4.24412002340361
H	16.65152537570365	1.07585157294528	2.80421220437902
C	10.31400819390878	0.78452470450352	5.71311757510876
H	10.64393333154771	0.39162708741090	6.68686567712173
H	9.22513227393074	0.68406842226713	5.67163566019339
H	10.56221720448335	1.85255359743307	5.67973171233512
C	11.03973164668183	6.95462905404797	1.35299583262142

H	11.29347467988186	7.94651948368983	0.94993502457683
H	10.56564715571615	6.38116393089903	0.54653052541100
H	11.97488685939197	6.44956983719328	1.61432232708100
C	14.68982839139935	3.42105225733429	5.76262870165946
H	15.29807166932023	2.51905586387009	5.64408793728122
H	13.63326929497992	3.12716296473047	5.74521014576417
H	14.90585414066718	3.83901428180298	6.75781801903200
C	8.76934309826666	5.01636511097574	2.17512362013398
H	9.15831994594545	5.09108712007944	1.15374271751193
H	7.76267757958851	5.45351665780863	2.19671620096646
H	8.67797492855493	3.95363696894433	2.42059435714043
C	8.40928966774623	4.28368082928174	4.89655895254923
H	8.10748186642086	4.21667533693279	5.95257156785122
H	9.11925456069100	3.46872069205345	4.69910007292927
H	7.50881766086266	4.12179313783235	4.28886941770917
C	9.29567204433842	0.21054553969932	2.47697226186372
C	12.55710369071566	0.17588288192439	4.89127601199132
H	12.74128876221045	-0.06002959411520	5.94988523338166
H	12.89007546290292	1.20672138646974	4.71233046309754
H	13.18035572441145	-0.50210991115787	4.29243874862254
C	9.23924864780170	-1.23925512472216	1.93428492714459
H	9.41195802591243	-2.00080999150263	2.70119094039799
H	9.95729328425475	-1.40126516996672	1.11917224132222
H	8.23389023844921	-1.41226994741781	1.52032038245851
C	15.04659121343396	2.38946268949943	1.23294311813060
H	15.77029995985773	1.70533975948264	0.76473949490056
H	14.78612855779293	3.15270760696273	0.48848276195595
H	14.13992174169892	1.81812216419853	1.45930637066597
C	16.44263168782759	4.97906129642540	4.89672341406779
H	16.52311723262704	5.44721821587416	5.89006553004538
H	16.74118167628251	5.73428725426531	4.15651763547647
H	17.16691677549971	4.15508875615767	4.86672816648309
C	16.99243637786798	3.67973091401181	2.02774559274880
H	17.60708711301431	2.92904132593295	1.50739255412035
H	17.59556286988181	4.08253243555857	2.84756978368979
H	16.79531580310666	4.48904880222450	1.31227226916636
C	10.08134708947933	5.86836999570840	5.77682476588469
H	10.60543208667341	6.82748782803067	5.72799296554618
H	10.83097325687675	5.06807300902363	5.76119864908854
H	9.55871479485303	5.82271149811091	6.74442547798674
C	8.11715811371098	0.40831805523755	3.44962609866920
H	8.12357063454286	1.41271732361280	3.89384894600876
H	8.11262051587982	-0.33282725382246	4.25955567498971
H	7.17371826765370	0.29288075926878	2.89442696079327
C	10.72988053092901	-1.49402731852589	4.76398005070045
H	11.22151412160223	-2.11192226063427	3.99862081950955

H	9.65282637356315	-1.70517946423704	4.74447338318557
H	11.10922033551956	-1.82398706004890	5.74380467893916
C	7.91782545033629	6.71117979572309	4.84055482461572
H	7.41664038211942	6.51064561453068	5.80056493477764
H	7.15225361929806	6.64838285499220	4.05472515431101
H	8.29266107369940	7.74158199261884	4.87867172671487

ALUHAR[15]

Oxo-tris(2,2,3,4,4-pentamethylpentan-3-olato)-chromium(V)

Charge = 0
Spin Multiplicity = 2

Cr	0.008880	-0.011230	-0.049465
O	-0.006149	-0.019052	1.550846
O	-1.279336	-1.104876	-0.583951
O	-0.242919	1.541951	-0.876855
O	1.558961	-0.710847	-0.588763
C	-3.191772	3.735473	-1.874481
H	-3.015125	4.733711	-1.459796
H	-3.933379	3.227816	-1.243202
H	-3.646215	3.867053	-2.868369
C	-2.337519	1.523691	-2.594313
H	-2.972846	1.685430	-3.478106
H	-2.917383	0.936957	-1.870676
H	-1.473806	0.921052	-2.898993
C	-0.962832	5.239734	-0.042747
H	-1.892140	5.184444	0.541363
H	-1.198374	5.634844	-1.039002
H	-0.310337	5.975818	0.452127
C	1.065686	4.105831	-0.937972
H	1.766610	4.730689	-0.364792
H	0.875393	4.616266	-1.887190
H	1.563823	3.155377	-1.157615
C	3.112533	-1.326531	1.946914
H	2.015746	-1.307082	1.993351
H	3.494502	-0.414630	2.425246
H	3.466114	-2.179855	2.544731
C	-1.757173	-4.454547	-2.360055
H	-2.580053	-4.967356	-1.849589
H	-0.812130	-4.898688	-2.019982
H	-1.850656	-4.671231	-3.435244
C	-3.029440	-2.372432	-2.893049
H	-2.927964	-2.579041	-3.969916
H	-3.126297	-1.286133	-2.771034

H	-3.959655	-2.849951	-2.559138
C	3.238631	-2.925426	0.066975
H	3.569290	-3.624573	0.850258
H	3.708294	-3.241422	-0.869371
H	2.153692	-3.026722	-0.037133
C	0.241217	3.575873	1.345546
H	0.969452	4.337227	1.660907
H	0.726774	2.595042	1.423197
H	-0.591403	3.603997	2.060710
C	-1.040407	3.546624	-3.141884
H	-1.583911	3.477495	-4.096932
H	-0.081415	3.026562	-3.266083
H	-0.845016	4.610898	-2.958651
C	-0.561614	-2.352703	-2.925221
H	-0.560405	-2.755479	-3.949237
H	0.394072	-2.622821	-2.457283
H	-0.604214	-1.258384	-2.990861
C	-3.741789	-3.926657	0.182001
H	-3.082818	-4.777676	0.405338
H	-4.199185	-4.090295	-0.802327
H	-4.554751	-3.940903	0.924725
C	5.163650	-1.413594	0.547918
H	5.520924	-2.133546	1.300830
H	5.526901	-0.421140	0.850201
H	5.636346	-1.681604	-0.405783
C	-4.026321	-1.454654	-0.043724
H	-4.831674	-1.481429	0.706021
H	-4.492255	-1.562541	-1.027856
H	-3.552370	-0.467055	0.009717
C	3.760452	-1.516397	-2.673700
H	3.978358	-1.297283	-3.730585
H	2.870379	-2.158387	-2.643929
H	4.615361	-2.079323	-2.277875
C	-1.784492	-2.918816	-2.167484
C	-2.622683	-2.372073	1.769158
H	-3.541982	-2.282035	2.367037
H	-2.031404	-1.457514	1.912838
H	-2.053388	-3.220212	2.172444
C	-0.575696	-3.340195	0.043787
H	0.285268	-3.445225	-0.623687
H	-0.935249	-4.346362	0.294824
H	-0.232274	-2.858609	0.965829
C	4.843315	0.627184	-1.977462
H	5.184875	0.676672	-3.022817
H	5.650542	0.177012	-1.389241
H	4.702636	1.660465	-1.632736

C	2.497727	0.596870	-2.782464
H	2.207508	1.552592	-2.328572
H	1.583934	0.013135	-2.945906
H	2.944795	0.817111	-3.763693
C	3.623929	-1.492044	0.492398
C	-2.158377	2.306317	0.439210
H	-2.878152	1.573775	0.055256
H	-2.722725	3.183639	0.779223
H	-1.660047	1.864889	1.308605
C	-3.011427	-2.572378	0.281970
C	3.075087	1.000508	0.292535
H	2.771119	1.825912	-0.358692
H	4.103091	1.195287	0.623353
H	2.431097	1.013526	1.178643
C	-1.899929	2.898487	-2.039484
C	-0.214967	3.890850	-0.101076
C	-1.681675	-2.502301	-0.618744
C	3.526724	-0.185009	-1.933654
C	-1.131455	2.688231	-0.641479
C	2.967214	-0.350519	-0.431290

ALUHUL[15]

tris(2,2,3,4,4-Pentamethylpentan-3-olato)-(trimethylsilanolato)-chromium(IV) diethyl ether solvate

Charge = 0
Spin Multiplicity = 3

Cr	4.36389845450448	4.95620201057431	9.56137486741036
Si	2.45537725020859	7.72915036659703	8.75821680016842
O	4.23943675086221	4.57620343287698	11.30913308347971
O	6.09839268631799	5.22941160939128	9.18520292457852
O	3.82975316487532	3.51074090833225	8.64387477265038
O	3.38291270606094	6.39607359813418	9.13731774555526
C	1.51944178406482	3.39704888062213	9.41059596791532
H	1.70118434547372	3.20257596688309	10.47337580807216
H	0.51582695205080	3.02683636962252	9.16517699465850
H	1.52749757436577	4.48271268872938	9.26412220927461
C	1.63632171940937	0.49843971396307	9.50093199590822
H	0.96836084410149	0.33962955089850	8.64738445461925
H	1.06488532453342	0.99716696764125	10.29519445581018
H	1.92463337894995	-0.49375083801346	9.88090914694167
C	3.22358463799965	5.42598958178069	13.36305290720831
C	6.86443327442233	5.55209925149011	7.98944940442156
C	5.88447602545774	5.75547992287984	6.81986599959931

H	5.47061182749543	4.79621074878134	6.48852829243407
H	6.36573668707980	6.23358619299413	5.95696644033581
H	5.04682481894209	6.38627440024504	7.13591161304823
C	2.60166933992606	2.73739493702093	8.53691599323133
C	4.60281244389360	5.23245051405221	12.55525953662670
C	5.73876761596804	4.32052605781175	13.24261907554558
C	5.20731620704764	3.02892634505735	13.89446553229951
H	6.06480167449975	2.40618478770424	14.19421228802792
H	4.60160285102403	2.44336135288840	13.19069485349244
H	4.61425154429615	3.21873308711810	14.79830322014090
C	3.42957027861233	5.87277363821811	14.82520650227898
H	2.44483635697706	6.09709063388056	15.26440570911391
H	4.03509355071710	6.78754727400590	14.90105780466551
H	3.89231654038779	5.09597322431292	15.44729286400069
C	3.76065544124936	0.38036073237039	8.19361736539416
H	4.04822169870196	-0.52992759240647	8.74296328689402
H	4.68442260526528	0.88302764612088	7.87771677586929
H	3.20551948015125	0.05896967046550	7.30244664893582
C	3.74773068238284	1.41742640983312	10.42622269527821
H	3.86480850998193	0.42259664611992	10.88259819305148
H	3.27522007288230	2.07528528737660	11.16594748653495
H	4.74669482537317	1.81896451078128	10.21757334958573
C	7.60352207787444	6.94428665008382	8.31388311919414
C	2.67267693510184	8.16219911660500	6.93513685974621
H	3.69569736449763	8.49848646906193	6.71317740742008
H	1.98622671628036	8.98141118614694	6.66817663040298
H	2.44416324546526	7.30578459737353	6.28451630524825
C	7.79609890004091	4.27805362637611	7.67332080675004
C	3.33065208336802	2.59010208805120	6.00818754840386
H	3.71350720746563	1.56521032075532	6.02439419265931
H	4.16456420763789	3.27169101584102	6.21442696204659
H	2.97598054341840	2.79426783737013	4.98621356887220
C	6.97437965164296	2.98458183289241	7.86224074636337
H	7.57526027380785	2.13048737647492	7.51394055403381
H	6.03350957825157	2.98603051903648	7.29885727824275
H	6.72661016102525	2.82280644866979	8.91836944012054
C	2.33400232500886	4.16305224033985	13.36382316339682
H	1.35689597288690	4.42166598896733	13.79996739397444
H	2.74405400592759	3.33631391009949	13.95111236746822
H	2.16192175010827	3.80726923312591	12.34085498031484
C	2.92295139425346	1.27479582417749	9.12875306143422
C	8.61453080005576	7.36504203590830	7.22729657261988
H	8.16683640751020	7.39290636543052	6.22370382114330
H	9.49727682026505	6.71396280996942	7.19579129968549
H	8.97000844992653	8.38261273996262	7.45416364524045
C	6.75068146984088	3.86326800690246	12.16878761511391

H	7.57557051999841	3.32827155081657	12.66408175397129
H	7.18410035287768	4.69897135419737	11.60602293963988
H	6.28541758158791	3.18322124418142	11.44511452392324
C	2.98249631671612	9.20647430673886	9.80394254509596
H	2.77377166426576	9.04885901756989	10.87168342141314
H	2.42389550456363	10.09989749629684	9.48212260668614
H	4.05466963284887	9.42083490155327	9.68912138020317
C	1.01968900341846	1.86777546960927	6.61881183335881
H	0.69094033564392	2.09623474017761	5.59288993730118
H	0.14363061669921	1.98054950844544	7.27332764714516
H	1.33189570341250	0.81589172209305	6.63090553120156
C	1.66033409797689	4.26397550880046	6.69743124930809
H	2.40010397684715	5.01578226091975	7.00294069824105
H	0.70906100321664	4.48393873659450	7.20071560922831
H	1.49179430255541	4.37133237170402	5.61530175251301
C	2.16489327011939	2.83236109784466	6.99135500236024
C	8.34260727404139	6.94974185594203	9.67142743967726
H	9.28133682888594	6.38668243797447	9.65667684323871
H	7.71348208770335	6.54274376420597	10.47127904944249
H	8.59036520275837	7.98943218974106	9.93427267589380
C	6.54959496176134	5.09679718233444	14.30829289424683
H	5.93205406001206	5.48940610769793	15.12384458158253
H	7.11032353295943	5.93376238441099	13.87105274415538
H	7.28538847592430	4.40979071792969	14.75410393653137
C	9.01795053293588	4.13448739985766	8.60061529942308
H	8.72990519248483	4.18504524938329	9.65878546224202
H	9.79281318512603	4.88649208422105	8.40520895634833
H	9.47759081315403	3.14829024019798	8.42858454748611
C	8.30084052392219	4.27182473014629	6.21034873690446
H	8.89633289747329	5.15491114701967	5.95319378655550
H	7.47537971742662	4.19378506591439	5.49023046703704
H	8.94240563068075	3.38857735976646	6.06727646945968
C	6.54171093034447	8.06562229023013	8.39898520070882
H	7.02350332828729	8.99098230222947	8.74854114099515
H	5.74518872950574	7.80825787243537	9.10882564944191
H	6.08441140319810	8.28238098639936	7.42428348078109
C	5.20259144849109	6.61309639338929	12.23542873756929
H	6.20085375610634	6.51304091587277	11.79610521764138
H	5.28728075782748	7.23774102925215	13.13388790947734
H	4.57473794697229	7.14350631474254	11.51060642367651
C	2.38522054367937	6.52634895544536	12.67265959849456
H	2.24738239094094	6.30695092630251	11.60628298926317
H	2.84027523598901	7.52081934925714	12.76940130769061
H	1.39159853603156	6.57153948368683	13.14264188786089
C	0.63527207091912	7.35653054965064	9.08191023470551
H	0.26514170176953	6.55166571955037	8.43062214186109

H	0.03324027402160	8.25615580095087	8.87673236344158
H	0.45592987774324	7.06348617954152	10.12635798962358

AMAYAP[16]

Pentacarbonyl-(3-chloro-3a,4,5,6,6a-pentamethyl-2-phenyl-3,3a,4,6a-tetrahydro-2H-cyclopenta[d][1,3]oxaphosphole)-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	6.103195	-6.375037	2.062530
Cl	2.886146	-5.052704	0.835655
P	3.720620	-6.504852	2.095513
O	1.373732	-6.526445	3.271470
O	9.097606	-5.983589	2.176923
O	5.965713	-3.468451	2.990533
O	6.260531	-7.515723	4.888937
O	6.753440	-9.105190	0.875623
O	6.100019	-5.377646	-0.823235
C	2.694098	-6.223912	3.671724
H	3.100825	-6.990427	4.363782
C	1.291629	-7.761255	2.450925
C	2.683196	-8.059354	1.758794
C	2.762663	-4.879689	4.340312
C	3.640577	-4.686355	5.417731
H	4.257192	-5.515473	5.770629
C	3.720253	-3.446641	6.055960
H	4.407279	-3.312000	6.892752
C	2.910579	-2.388562	5.632975
H	2.965432	-1.421499	6.135382
C	2.019777	-2.579849	4.571514
H	1.375832	-1.761691	4.244536
C	1.944828	-3.816508	3.926638
H	1.241587	-3.966942	3.108786
C	0.361321	-7.477681	1.288699
C	0.945910	-7.722087	0.100517
C	2.361220	-8.246502	0.236586
H	3.039742	-7.624947	-0.375560
C	0.768569	-8.855695	3.385530
H	1.449899	-9.028735	4.229818
H	0.626805	-9.804217	2.849380
H	-0.202823	-8.545784	3.792972
C	-1.028142	-6.983314	1.550020
H	-1.540142	-6.694363	0.623682

H	-1.009501	-6.109732	2.219490
H	-1.645074	-7.751080	2.044577
C	0.348881	-7.543886	-1.260984
H	-0.642486	-7.075506	-1.223320
H	0.243801	-8.507464	-1.785113
H	1.001937	-6.915395	-1.888519
C	2.494886	-9.689526	-0.286772
H	1.824368	-10.381217	0.243001
H	3.523782	-10.063142	-0.196656
H	2.231472	-9.718812	-1.353049
C	3.460126	-9.219805	2.398922
H	2.851692	-10.133229	2.394096
H	3.731509	-9.020775	3.445374
H	4.381081	-9.439200	1.850487
C	7.947120	-6.136903	2.128238
C	5.959149	-4.579740	2.669392
C	6.164795	-7.074333	3.820706
C	6.441950	-8.090713	1.344233
C	6.070500	-5.747766	0.272466

AMOWEF[17]

bis(μ^2-chloro)-(bis(2,5-di-*t*-butyl-1H-pyrrol-1-yl))-bis(tetrahydrofuran)-di-chromium

Charge = 0
Spin Multiplicity = 5

Cr	12.697529	0.267095	1.514740
Cl	10.435893	0.295439	0.732343
N	12.190133	0.706831	3.406770
C	12.175618	1.978166	3.987873
C	12.069654	1.833998	5.369762
H	12.023886	2.639880	6.095948
C	12.011057	0.445528	5.651572
H	11.915556	-0.009215	6.633288
C	12.086234	-0.229994	4.435201
C	12.119395	3.292591	3.211731
C	10.662081	3.581933	2.781478
H	10.281911	2.793405	2.119124
H	10.594600	4.541008	2.244271
H	10.003721	3.635967	3.659404
C	12.598271	4.449089	4.111820
H	13.628771	4.288760	4.457128
H	11.958288	4.570025	4.995850
H	12.568044	5.396338	3.553600
C	13.010209	3.282335	1.956955

H	12.669355	2.526675	1.222868
H	14.059549	3.072417	2.199556
H	12.962049	4.248335	1.433432
C	11.965043	-1.744285	4.254484
C	10.475990	-2.150793	4.385258
H	10.080152	-1.857105	5.366333
H	10.353968	-3.239745	4.274580
H	9.865197	-1.660238	3.614300
C	12.770481	-2.462775	5.359095
H	12.421710	-2.178260	6.359304
H	13.840390	-2.219406	5.294158
H	12.662271	-3.553715	5.263150
C	12.479242	-2.251367	2.899421
H	13.540090	-2.014031	2.738009
H	11.872811	-1.872829	2.057070
H	12.391147	-3.347433	2.846002
O	14.735970	0.304977	2.025771
C	15.856690	0.321818	1.053101
H	15.747156	1.232301	0.449817
H	15.749740	-0.559066	0.413036
C	17.123429	0.328205	1.898223
H	17.944053	0.842487	1.384526
H	17.446478	-0.699316	2.115590
C	16.676547	1.032280	3.186176
H	17.328702	0.816520	4.040815
H	16.643963	2.122030	3.045619
C	15.280511	0.475979	3.396601
H	15.301894	-0.517692	3.865730
H	14.585760	1.125856	3.937099
Cr	10.942631	-0.293454	-1.546078
Cl	13.205788	-0.329007	-0.772223
N	11.443481	-0.707730	-3.424478
C	11.479421	-1.970522	-4.019578
C	11.618846	-1.811716	-5.397117
H	11.684318	-2.609706	-6.130832
C	11.679028	-0.418616	-5.661269
H	11.794467	0.048610	-6.635019
C	11.572571	0.240825	-4.438087
C	11.515849	-3.283005	-3.243246
C	12.971031	-3.604487	-2.828629
H	13.377498	-2.821626	-2.175502
H	13.022915	-4.562502	-2.287835
H	13.616464	-3.677786	-3.714598
C	10.997678	-4.432110	-4.131028
H	9.965631	-4.250414	-4.460655
H	11.621091	-4.565322	-5.025201

H	11.017557	-5.379970	-3.573252
C	10.640181	-3.240970	-1.979774
H	10.985526	-2.465167	-1.260995
H	9.586740	-3.042280	-2.211216
H	10.701159	-4.189195	-1.425743
C	11.682854	1.747353	-4.212452
C	13.174589	2.161150	-4.258358
H	13.616794	1.900368	-5.228942
H	13.287718	3.246168	-4.106995
H	13.749952	1.646470	-3.476043
C	10.926332	2.498962	-5.328110
H	11.322938	2.245263	-6.318969
H	9.855447	2.251140	-5.320900
H	11.026619	3.586626	-5.194617
C	11.100597	2.198967	-2.865370
H	10.034194	1.959945	-2.767833
H	11.670954	1.784542	-2.008393
H	11.188694	3.290447	-2.750172
O	8.916787	-0.337996	-2.050087
C	7.791947	-0.315465	-1.080499
H	7.888303	-1.213132	-0.456485
H	7.911090	0.578295	-0.460830
C	6.526885	-0.322419	-1.927803
H	5.698457	-0.814565	-1.405020
H	6.217907	0.704477	-2.167429
C	6.966037	-1.058824	-3.200241
H	6.318058	-0.851511	-4.060168
H	6.983538	-2.145864	-3.037680
C	8.369037	-0.525202	-3.419133
H	8.361729	0.460958	-3.904681
H	9.057082	-1.191006	-3.948417

AROWUZ[18]

Aqua-(2,2'-diamino-4,4'-bi-(1,3)thiazole-N,N')-(iminodiacetato-N,O,O')-chromium(III) chloride monohydrate

Charge = 1
Spin Multiplicity = 4

Cr	5.031705	2.318537	1.817073
S	5.731160	6.614932	3.438617
S	6.884974	3.687195	-2.217571
O	4.313108	1.780383	3.541168
O	4.789609	0.864885	5.542010

O	4.850077	0.519420	1.089003
O	5.821544	-1.500262	0.875396
O	3.092342	2.783214	1.270032
N	5.394594	4.275649	2.389026
N	4.429503	4.500605	4.545044
N	5.832361	3.091798	0.070819
N	5.613923	1.379387	-1.555970
N	6.806523	1.549676	2.593552
C	5.105880	4.978287	3.490888
C	6.370662	6.323617	1.848732
H	6.882532	7.115003	1.312059
C	6.091482	5.050941	1.450376
C	6.343604	4.395946	0.178628
C	6.951753	4.869501	-0.944053
H	7.413147	5.835279	-1.119756
C	6.025840	2.588326	-1.156457
C	5.145440	1.289873	4.449866
C	6.621231	1.380911	4.068416
H	7.028382	2.267992	4.573939
H	7.171060	0.505598	4.437194
C	7.103935	0.269207	1.881407
H	7.587715	-0.452869	2.551570
H	7.802626	0.481757	1.059949
C	5.850021	-0.335651	1.254828
H	7.588482	2.191673	2.440444
H	4.144566	5.114780	5.299503
H	3.978056	3.588708	4.460469
H	5.082084	0.797230	-0.906816
H	5.754067	1.062167	-2.508092
H	2.452945	2.088163	1.524824
H	2.915565	2.974291	0.328814

ATUREN[19]

Dichloro-(2,6-bis(2,6-diethylphenyliminomethyl)phenyl)-tetrahydrofuran-chromium(III)

Charge = 0
Spin Multiplicity = 4

C	0.483602	-0.051390	5.313801
C	-0.810560	0.442433	5.109307
C	-1.915053	-0.246422	5.646511
H	-2.932592	0.121730	5.496521
C	-1.697849	-1.417279	6.387756
H	-2.550777	-1.951306	6.807616
C	-0.402726	-1.913052	6.598326

H	-0.257008	-2.827979	7.177189
C	0.695703	-1.222196	6.051260
C	2.091667	-1.605716	6.104874
H	2.409684	-2.541887	6.580645
C	-0.823147	1.691926	4.375698
H	-1.755255	2.241725	4.194613
C	0.337203	3.522103	3.444398
C	0.030827	4.613684	4.299265
C	0.162449	5.913763	3.783636
H	-0.046612	6.759109	4.443305
C	0.556541	6.144949	2.468813
H	0.660615	7.165378	2.096050
C	0.808611	5.058515	1.631193
H	1.091634	5.225649	0.589373
C	0.705231	3.740662	2.093448
C	-0.441782	4.475013	5.732909
H	-0.221390	3.473458	6.119918
H	0.144533	5.170579	6.354138
C	-1.936188	4.800246	5.911432
H	-2.166336	5.822250	5.577056
H	-2.222867	4.717949	6.970021
H	-2.572561	4.113468	5.333719
C	0.893736	2.607162	1.115519
H	1.364021	1.746354	1.608628
H	1.575701	2.942435	0.318864
C	-0.432579	2.150310	0.478717
H	-1.132250	1.776661	1.240371
H	-0.253860	1.337167	-0.239968
H	-0.924695	2.977023	-0.054935
C	4.310235	-1.339062	5.381004
C	4.537641	-2.503666	4.596580
C	5.862059	-2.945600	4.448834
H	6.056152	-3.837123	3.850868
C	6.930893	-2.278361	5.042294
H	7.950167	-2.643947	4.905924
C	6.685509	-1.147470	5.818853
H	7.513744	-0.626875	6.305190
C	5.385177	-0.662144	6.006897
C	3.425651	-3.298863	3.932453
H	3.222905	-4.196140	4.543306
H	2.501477	-2.709073	3.925314
C	3.719184	-3.734217	2.489311
H	3.903790	-2.858498	1.851214
H	2.854065	-4.275143	2.079350
H	4.588252	-4.402794	2.418090
C	5.173518	0.499328	6.946796

H	6.075521	1.130783	6.930220
H	4.330700	1.119706	6.614753
C	4.906264	0.045757	8.394269
H	3.993330	-0.563926	8.456614
H	4.773598	0.916975	9.052117
H	5.741742	-0.554697	8.783934
C	4.799512	1.475908	2.926816
H	4.414898	0.589042	2.413041
H	5.596865	1.183813	3.630169
C	5.234207	2.617235	2.011285
H	6.298216	2.541381	1.752808
H	4.654956	2.595570	1.078966
C	4.083234	3.398721	4.028156
H	4.676890	3.370759	4.954420
H	3.161933	3.960643	4.211277
Cl	2.140587	2.209980	6.491569
Cl	1.930140	-0.386341	2.638873
Cr	2.013202	0.911779	4.568632
N	2.971493	-0.829776	5.527957
N	0.317385	2.180193	3.966487
O	3.688370	2.033063	3.690559
C	4.908363	3.897414	2.827778
H	4.335554	4.611544	2.223600
H	5.818389	4.403528	3.174505

AVIZIP[20]

cis-(η^4-butadiene-)-(*t*-butyl[(*t*-butylimino)phosphanyl]amido)-trimethylphosphine-chromium(III)

Charge = 0
Spin Multiplicity = 4

Cr	12.564074	12.546191	0.585830
P	11.849362	12.547734	3.272281
P	10.381608	12.549055	-0.510245
N	12.152193	13.768743	2.217594
C	12.108261	15.196841	2.597135
C	11.214406	15.948469	1.593522
H	10.177873	15.585899	1.653568
H	11.214899	17.027932	1.807396
H	11.579261	15.793962	0.569292
C	13.539698	15.769533	2.532895
H	14.195240	15.241410	3.240319
H	13.958058	15.656896	1.524133
H	13.538839	16.839779	2.790065

C	11.552770	15.415201	4.017862
H	12.182868	14.928156	4.777515
H	11.523718	16.491212	4.243651
H	10.530502	15.018585	4.112791
C	8.902398	12.550947	0.593228
C	10.018815	13.972801	-1.625496
H	9.018969	13.872087	-2.072243
H	10.070438	14.909420	-1.056556
H	10.771822	14.010501	-2.423104
C	13.499350	13.937748	-0.830072
H	13.269869	13.600537	-1.845620
H	13.420102	15.018717	-0.694563
C	14.506872	13.248393	-0.078517
H	15.156932	13.775328	0.623903
N	12.148320	11.325456	2.217981
C	12.099938	9.897601	2.598006
C	11.204682	9.148163	1.594011
H	10.169211	9.513923	1.652934
H	11.201735	8.068829	1.808457
H	11.570916	9.300977	0.570019
C	13.529782	9.320795	2.535001
H	14.186253	9.847226	3.242835
H	13.949242	9.432043	1.526543
H	13.525714	8.250622	2.792436
C	11.542774	9.681379	4.018395
H	12.173724	10.166876	4.778334
H	11.510449	8.605533	4.244497
H	10.521597	10.081014	4.112439
C	10.015581	11.126323	-1.625674
H	9.015781	11.228593	-2.072150
H	10.066026	10.189473	-1.056999
H	10.768270	11.087522	-2.423544
C	13.495027	11.151361	-0.829759
H	13.266679	11.488987	-1.845435
H	13.412425	10.070677	-0.693920
C	14.504674	11.837745	-0.078319
H	15.153078	11.308956	0.624238
H	8.926993	11.662224	1.237062
H	7.971440	12.553602	0.008401
H	8.929476	13.440332	1.236330

AVUDAW[21]

(η^5-Cyclopentadienyl)-(N,N'-bis(2,6-di-isopropylphenyl)pentane-2,4-di-iminato-N,N')-methyl-chromium(III)

Charge = 0
Spin Multiplicity = 4

Cr	8.398803	3.635301	-1.727878
N	7.599890	2.701837	-0.078795
N	7.518157	2.304549	-3.022422
C	7.437548	3.435978	1.155555
C	6.208293	4.113203	1.390164
C	6.068432	4.872861	2.559128
C	7.104084	4.975969	3.487108
C	8.293479	4.289999	3.259834
C	8.483958	3.505527	2.111317
C	5.027016	3.989169	0.431846
C	4.240915	5.298827	0.250033
C	4.065307	2.870121	0.883640
C	9.788202	2.724878	1.979606
C	11.020748	3.646628	1.929344
C	9.954656	1.711395	3.131090
C	6.997377	0.634455	1.168453
C	7.297709	1.397035	-0.107987
C	7.242064	0.629405	-1.288582
C	7.247913	1.049719	-2.631902
C	6.936502	-0.027769	-3.652666
C	7.268478	2.672775	-4.397678
C	6.007058	3.238838	-4.735077
C	5.778011	3.634635	-6.059867
C	6.754666	3.486032	-7.043488
C	7.979048	2.916794	-6.706661
C	8.259294	2.494786	-5.397857
C	4.887292	3.381942	-3.707955
C	3.972340	2.139395	-3.695294
C	4.027898	4.641916	-3.910127
C	9.609986	1.840454	-5.126801
C	10.776661	2.822238	-5.346897
C	9.821609	0.583290	-5.994586
C	10.144955	2.525018	-1.616139
C	9.763283	5.383717	-2.232787
C	9.185043	5.648357	-0.957962
C	7.782027	5.823935	-1.142931
C	7.489370	5.654930	-2.515432
C	8.715810	5.372176	-3.193776
H	5.129137	5.394704	2.748778
H	6.978182	5.578936	4.388351
H	9.095882	4.353085	3.997922
H	5.435504	3.699573	-0.548112
H	3.711275	5.589166	1.169505

H	3.480268	5.170813	-0.533814
H	4.889250	6.136573	-0.043018
H	3.644019	3.099374	1.874740
H	4.570038	1.897593	0.947391
H	3.229529	2.772924	0.174264
H	9.747827	2.165588	1.035675
H	10.967824	4.352100	1.089676
H	11.937644	3.049682	1.810944
H	11.119717	4.230318	2.857163
H	9.090735	1.038087	3.213432
H	10.072088	2.225323	4.097225
H	10.852988	1.096918	2.968350
H	6.229195	-0.128732	0.991646
H	6.673116	1.289208	1.983960
H	7.906231	0.109997	1.502916
H	7.023852	-0.427332	-1.137890
H	6.431378	0.368791	-4.540379
H	6.318168	-0.817052	-3.208674
H	7.874901	-0.493519	-3.992530
H	4.814037	4.068472	-6.329305
H	6.557398	3.805806	-8.068427
H	8.739132	2.786891	-7.479949
H	5.365631	3.448936	-2.718816
H	3.173661	2.261056	-2.947886
H	4.525583	1.223983	-3.450718
H	3.497747	1.999163	-4.678880
H	4.635915	5.553682	-3.999149
H	3.345848	4.769583	-3.057136
H	3.404116	4.569442	-4.813543
H	9.624242	1.532409	-4.073185
H	11.735491	2.335959	-5.111501
H	10.682960	3.712389	-4.710552
H	10.819431	3.157609	-6.394394
H	8.999939	-0.137149	-5.879106
H	10.758710	0.080929	-5.710967
H	9.892209	0.841527	-7.062021
H	9.872007	1.472607	-1.435137
H	10.783434	2.878904	-0.792501
H	10.728350	2.589008	-2.546529
H	10.815380	5.200584	-2.429206
H	9.714459	5.712301	-0.012303
H	7.065575	6.019511	-0.351479
H	6.507536	5.713194	-2.974080
H	8.822435	5.177327	-4.256830

AWAVAV[22]

trans-Tricarbonyl-(η^6-7-(1-methoxycarbonyl)cyclohexyl-1,3,5-cycloheptatriene)-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	-3.708548	10.741082	11.698674
O	-4.615452	14.557671	14.687408
O	-6.594560	13.463051	14.648492
O	-2.278933	8.383642	12.913692
O	-4.926417	8.931633	9.632366
O	-1.573552	10.986961	9.600557
C	-5.408349	13.487320	14.941984
C	-4.652404	12.330833	15.606222
C	-4.067524	11.349939	14.500222
C	-2.961864	11.883009	13.618109
C	-3.067216	12.723364	12.515656
C	-4.189734	12.917297	11.648418
C	-5.397343	12.198190	11.651900
C	-5.758067	11.121512	12.522601
C	-5.066731	10.630636	13.624058
C	-3.475394	12.818742	16.485616
C	-3.933567	13.583285	17.736561
C	-4.912436	12.754199	18.578034
C	-6.102526	12.285838	17.731024
C	-5.642972	11.522926	16.479917
C	-5.273467	15.675267	14.033331
C	-2.833411	9.297018	12.441925
C	-4.486698	9.641010	10.454001
C	-2.390311	10.917004	10.437360
H	-3.598548	10.564912	15.113540
H	-1.946629	11.746360	13.993984
H	-2.141326	13.189697	12.172790
H	-4.040943	13.607571	10.817517
H	-6.080473	12.396842	10.825587
H	-6.610917	10.529564	12.184396
H	-5.429435	9.673818	14.002787
H	-2.784855	13.433746	15.892902
H	-2.914446	11.922043	16.802640
H	-3.050979	13.858948	18.334718
H	-4.415408	14.529378	17.436892
H	-5.265057	13.340328	19.441110
H	-4.385846	11.873264	18.986006
H	-6.706607	13.157953	17.429102
H	-6.766036	11.638292	18.325312
H	-5.127977	10.597843	16.791356

H	-6.511656	11.225648	15.876521
H	-4.498680	16.439238	13.919326
H	-6.097303	16.047756	14.654697
H	-5.663053	15.367980	13.054749

BABFOZ[23]

Dicarbonyl-(1-3a(7a)-η^5-indenyl)-nitrosyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	-1.679754	1.444322	2.902117
O	-1.625062	-0.955108	4.465427
O	1.323998	1.531618	2.604066
O	-2.100582	-0.044111	0.307856
N	-1.634366	0.027554	3.806395
C	-3.660734	2.404678	2.974647
C	-3.033384	2.474893	4.255420
C	-1.837662	3.247619	4.154773
C	-0.859263	4.653113	2.165522
C	-1.099322	5.014357	0.857129
C	-2.215666	4.499069	0.135942
C	-3.102205	3.617247	0.716031
C	-2.904544	3.244313	2.075828
C	-1.770310	3.768465	2.809033
C	0.165050	1.503922	2.699373
C	-1.927943	0.541185	1.298078
H	-4.587880	1.890200	2.740250
H	-3.383354	1.973749	5.154188
H	-1.152739	3.480617	4.964648
H	-0.007126	5.057622	2.713544
H	-0.424513	5.710991	0.357535
H	-2.367862	4.814020	-0.897456
H	-3.958747	3.232790	0.160522

BARKAG[24]

(μ_2-t-Butyldisulfonyl)-(μ_2-t-butylthiolato)-bis(η^5-cyclopentadienyl)-dinitrosyl-di-chromium

Charge = 0
Spin Multiplicity = 1

Cr	1.011945	3.760673	8.807490
Cr	-1.096994	5.342473	9.968604
S	0.946506	6.028212	9.174866

S	-0.952412	3.073327	9.753799
S	-2.361850	2.299703	8.361434
O	0.295960	3.346377	6.080459
O	-2.899492	5.946571	7.841187
N	0.528012	3.620857	7.223130
N	-2.065757	5.663890	8.657630
C	0.983683	7.240898	7.703971
C	2.475754	7.501515	7.456916
C	0.290179	8.513784	8.201338
C	0.316629	6.706339	6.442552
C	-2.875957	0.663683	9.132067
C	-3.893429	0.125400	8.113265
C	-3.538506	0.890327	10.493078
C	-1.674775	-0.277885	9.247588
C	2.255401	1.928316	8.780119
C	3.050687	3.037019	8.346548
C	3.165742	3.943929	9.433662
C	2.444224	3.407358	10.543836
C	1.893147	2.159699	10.135784
C	-0.687052	5.225308	12.206289
C	-2.045000	4.855050	11.940372
C	-2.702260	5.967380	11.355082
C	-1.752804	7.033509	11.247055
C	-0.519323	6.572193	11.787162
H	2.586025	8.243168	6.649342
H	2.994402	6.583830	7.145438
H	2.971180	7.897273	8.354795
H	0.387463	9.301085	7.436538
H	0.745514	8.885246	9.130699
H	-0.779067	8.339398	8.380305
H	0.326469	7.499655	5.676300
H	-0.725790	6.419336	6.618254
H	0.855295	5.842229	6.038337
H	-3.434650	-0.025851	7.125603
H	-4.752516	0.802705	8.003254
H	-4.270488	-0.847539	8.465961
H	-4.405777	1.558965	10.406480
H	-2.829615	1.326442	11.210744
H	-3.881489	-0.074184	10.901670
H	-1.202866	-0.441739	8.269352
H	-2.005835	-1.251982	9.643077
H	-0.919896	0.125632	9.936668
H	1.967916	1.073573	8.174972
H	3.473984	3.168578	7.354816
H	3.696681	4.890008	9.420145
H	2.343677	3.865428	11.522842

H	1.283991	1.504649	10.750900
H	0.070842	4.592864	12.658224
H	-2.492687	3.888058	12.145858
H	-3.735083	5.996259	11.019599
H	-1.942570	8.017200	10.828285
H	0.404047	7.140418	11.833679

BARKEK[24]

(η^5-Cyclopentadienyl)-nitrito-dinitrosyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	-0.001162	0.046167	0.005492
O	2.736313	-0.755604	0.319855
O	-0.483321	0.096709	2.834317
O	-0.917720	-1.608037	-0.604840
O	-0.007566	-2.872358	0.924371
N	1.593787	-0.534809	0.175747
N	-0.331143	-0.021933	1.677643
N	-0.760284	-2.800869	-0.032787
C	-1.148338	0.873445	-1.766455
C	0.242535	1.083774	-1.961308
C	0.712455	1.926111	-0.895056
C	-0.388751	2.213892	-0.047831
C	-1.546542	1.551597	-0.583577
H	-1.781789	0.232603	-2.372262
H	0.847160	0.677458	-2.767185
H	1.733880	2.268142	-0.754915
H	-0.359197	2.814211	0.857016
H	-2.544688	1.563472	-0.155116

BEFJEC[25]

(3,3'-(Pyridine-2,6-diyl)bis(1-isopropylimidazol-2-ylidene))-trichloro-chromium(III) dichloromethane solvate

Charge = 0
Spin Multiplicity = 4

Cr	2.984214	0.929079	2.244748
Cl	3.109988	-1.042224	0.959170
Cl	2.744441	2.988161	3.367078
Cl	4.091514	-0.053716	4.034258
N	0.112291	0.997285	1.640628

N	2.006950	1.774729	0.648747
C	-1.205295	0.029378	3.100476
H	-2.026944	-0.380331	3.675206
N	0.127800	-0.074449	3.508613
C	0.958423	0.513294	2.625610
N	4.081117	2.400986	-0.046880
C	2.090657	2.977526	-1.421999
H	2.669503	3.483184	-2.191849
C	-0.037432	2.225518	-0.517014
H	-1.120362	2.143879	-0.580199
C	0.669474	1.683797	0.554092
C	0.576650	-0.734526	4.761291
H	1.671195	-0.639554	4.732266
C	0.699956	2.877257	-1.508530
H	0.182587	3.313317	-2.362808
C	-1.220155	0.704910	1.921411
H	-2.044806	0.992228	1.281221
C	2.705613	2.403358	-0.311772
C	0.034016	0.015759	5.979429
H	0.329669	1.073288	5.953843
H	0.443823	-0.435282	6.893374
H	-1.063199	-0.043269	6.036238
C	0.193922	-2.215286	4.751163
H	-0.897383	-2.353649	4.771687
H	0.610941	-2.700490	5.644126
H	0.597207	-2.721491	3.863710
N	5.869108	1.970247	1.073503
C	5.127817	2.967379	-0.770299
H	4.992264	3.502591	-1.701777
C	4.535928	1.777053	1.104034
C	6.253168	2.693393	-0.059506
H	7.284351	2.951914	-0.267221
C	6.804399	1.496914	2.126185
H	6.157860	0.954222	2.829991
C	7.833850	0.534146	1.532304
H	7.341836	-0.307697	1.026727
H	8.459495	0.133065	2.341268
H	8.496782	1.039070	0.813930
C	7.442595	2.690353	2.840266
H	6.674196	3.356893	3.254643
H	8.086726	3.271190	2.163260
H	8.065890	2.325101	3.667840

BEKGOP[26]

Chloro-methyl-(η^5-1-(2,6-diisopropylphenyl)-2-(2-(4,7-dimethylindenyl)ethyl)imidazol-2-ylidene)-chromium(III) tetrahydrofuran solvate

Charge = 0
Spin Multiplicity = 4

Cr	18.705478	1.726347	15.542114
Cl	17.665738	3.786931	15.389333
C	17.293558	0.444893	16.323651
N	16.056387	0.620283	16.899570
N	17.495234	-0.910279	16.398373
C	15.519721	-0.593682	17.315832
H	14.552023	-0.659067	17.797253
C	18.682743	-1.613595	15.896773
H	18.722404	-1.480659	14.808198
H	18.529758	-2.679975	16.103954
C	19.987961	-1.128974	16.549094
H	19.917182	-1.289003	17.635470
H	20.791439	-1.786715	16.188398
C	16.427530	-1.556061	16.999449
H	16.402844	-2.629811	17.142871
C	20.313519	0.318270	16.287700
C	20.906363	0.935400	15.115389
C	21.413334	0.417096	13.879703
C	20.972151	2.364713	15.373991
C	21.909270	2.739917	13.206902
H	22.300974	3.402991	12.431994
C	20.481673	2.597683	16.708293
H	20.394478	3.564344	17.194526
C	21.454655	3.282801	14.396075
C	21.900403	1.340753	12.968487
H	22.304711	0.973691	12.021820
C	20.142727	1.351382	17.268580
H	19.748780	1.187944	18.269270
C	15.344346	1.862695	17.122554
C	15.544886	2.543809	18.339751
C	16.531524	2.069887	19.398727
H	17.097639	1.225268	18.980680
C	13.669766	3.444129	16.440944
H	12.940314	3.803920	15.713625
C	14.179983	1.542684	14.849534
H	14.974289	0.789784	14.746379
C	14.412732	2.290533	16.155511
C	17.547038	3.168369	19.761347
H	18.063407	3.538259	18.864710
H	18.299134	2.774536	20.461058

H	17.057081	4.024456	20.248491
C	14.777926	3.694250	18.571408
H	14.909378	4.246642	19.503358
C	14.274381	2.475463	13.629251
H	13.457744	3.212769	13.619224
H	14.202351	1.889321	12.701118
H	15.229392	3.018909	13.626820
C	12.829072	0.800162	14.869706
H	12.767509	0.092087	15.708795
H	12.689599	0.235472	13.935706
H	11.992692	1.509292	14.964788
C	18.190153	1.185930	13.609943
H	18.347935	0.121916	13.370972
H	18.836762	1.788103	12.948382
H	17.139694	1.445336	13.414827
C	13.848014	4.141166	17.634721
H	13.259162	5.037896	17.835965
C	15.798849	1.559869	20.655121
H	15.221655	2.367204	21.130617
H	16.522678	1.182422	21.392814
H	15.101894	0.744769	20.412339
C	21.469807	-1.055528	13.566989
H	21.933484	-1.217520	12.584842
H	20.469567	-1.514817	13.538420
H	22.060700	-1.611619	14.310757
C	21.471255	4.759324	14.674751
H	21.868349	5.318169	13.817157
H	22.090192	4.996007	15.555174
H	20.454308	5.124938	14.889660

BEQLIU00[27]

(N,N'-Bis(2,6-diisopropylphenyl)pentane-2,4-diiminato)-(η^2-1,2-diphenylacetylene)-chromium

Charge = 0
Spin Multiplicity = 4

Cr	9.450172	4.676400	14.147827
N	10.829668	3.253832	14.297409
C	5.476028	4.674349	12.130391
H	5.011650	4.672939	13.117565
C	4.679085	4.674012	10.985433
H	3.591480	4.672318	11.081240
C	5.269973	4.675891	9.715431
H	4.645632	4.675692	8.820192
C	6.664354	4.677998	9.601503

H	7.131297	4.679613	8.614782
C	7.459802	4.678187	10.748136
H	8.547663	4.679713	10.662245
C	6.885640	4.676469	12.034618
C	7.729043	4.676737	13.227634
C	7.528185	4.676849	14.548045
C	6.423115	4.677950	15.492372
C	5.877715	3.467960	15.974849
H	6.295760	2.521338	15.628513
C	4.813709	3.472818	16.878437
H	4.405873	2.523554	17.232119
C	4.271265	4.680382	17.332731
H	3.440556	4.681309	18.040165
C	10.284592	1.935751	14.516814
C	9.858439	1.153929	13.410875
C	9.342730	-0.125028	13.662044
H	9.019574	-0.744600	12.824246
C	9.227849	-0.622904	14.959093
H	8.821699	-1.621743	15.129278
C	9.626541	0.165436	16.036132
H	9.521997	-0.221905	17.051625
C	10.160512	1.446770	15.843284
C	10.558113	2.270706	17.063789
H	11.033376	3.194943	16.705440
C	9.315813	2.674789	17.879784
H	8.600910	3.241778	17.267249
H	9.606793	3.300380	18.736854
H	8.796742	1.786813	18.271645
C	11.573147	1.538818	17.961964
H	11.889526	2.193895	18.787403
H	12.471622	1.238033	17.404250
H	11.136315	0.632305	18.407058
C	9.960857	1.652291	11.972369
H	10.043603	2.749994	12.013575
C	11.221092	1.113692	11.265389
H	12.144370	1.417694	11.776215
H	11.268765	1.491119	10.232535
H	11.203603	0.013575	11.222803
C	8.711145	1.312073	11.143396
H	7.794287	1.662525	11.635978
H	8.618907	0.229389	10.970309
H	8.772380	1.796066	10.158003
C	13.086448	2.220049	14.378868
H	12.665558	1.323287	13.910097
H	13.262562	1.976051	15.438114
H	14.060105	2.444358	13.926592

C	12.165887	3.414563	14.266829
C	12.778433	4.676202	14.187777
H	13.866382	4.676139	14.139412
N	10.829750	6.098699	14.298041
C	10.284942	7.416975	14.517182
C	9.860842	8.199607	13.411022
C	9.345634	9.478788	13.662050
H	9.024117	10.098948	12.824046
C	9.229218	9.976150	14.959144
H	8.823699	10.975268	15.129193
C	9.625617	9.186944	16.036394
H	9.519746	9.573804	17.051937
C	10.158935	7.905315	15.843718
C	10.553913	7.080474	17.064470
H	11.027291	6.155186	16.706308
C	9.310204	6.679232	17.879736
H	8.594261	6.114092	17.266699
H	9.599221	6.052772	18.736834
H	8.793059	7.568361	18.271551
C	11.569996	7.810137	17.963262
H	11.883818	7.154726	18.789417
H	12.469869	8.108206	17.406339
H	11.135046	8.718071	18.407324
C	9.964463	7.701987	11.972352
H	10.050443	6.604528	12.013134
C	11.222687	8.244655	11.264928
H	12.147162	7.943432	11.775231
H	11.271036	7.867568	10.231975
H	11.201778	9.344716	11.222543
C	8.713256	8.038843	11.144174
H	7.797796	7.684930	11.636876
H	8.617420	9.121395	10.972234
H	8.775623	7.555988	10.158283
C	13.086617	7.132247	14.380045
H	12.666596	8.028708	13.909917
H	13.260953	7.377157	15.439377
H	14.060945	6.907450	13.929487
C	12.166005	5.937849	14.267388
C	5.872880	5.889283	15.966033
H	6.287107	6.835001	15.612689
C	4.809054	5.886771	16.869828
H	4.397512	6.836948	17.216703

BEXPID[28]

Tricarbonyl-(η^6-fulvene)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	3.913676	3.166893	22.757626
C	6.014345	2.970868	23.271815
C	5.320851	2.253957	24.264843
C	4.572501	1.195129	23.634318
C	4.795934	1.249321	22.245831
C	5.659358	2.396490	21.975685
C	5.378857	3.244347	20.888527
C	2.570822	3.368548	24.013462
O	1.709917	3.512788	24.788582
C	2.553701	2.959117	21.533854
O	1.694870	2.800033	20.758156
C	3.996243	5.007159	22.757670
O	4.067942	6.172906	22.776931
H	6.646282	3.841518	23.419878
H	5.336034	2.460330	25.331274
H	3.937676	0.482313	24.152943
H	4.354964	0.604717	21.491205
H	4.922882	2.841744	19.984808
H	5.887123	4.203633	20.798722

BILDIJ[29]

Tris(2-((Dimethylamino)-methyl)-phenyl-C^1,N)-chromium(III)

Charge = 0
Spin Multiplicity = 4

Cr	0.001756	-0.000104	-0.048598
N	1.458003	-1.504125	1.185162
C	-0.147791	-1.747919	-1.132228
C	-0.623764	-1.919536	-2.447913
C	-0.664214	-3.170783	-3.077275
C	-0.213522	-4.310431	-2.402215
C	0.271640	-4.178784	-1.097228
C	0.294285	-2.922317	-0.474734
C	0.755663	-2.798605	0.955271
C	1.661931	-1.334626	2.640594
C	2.796065	-1.588990	0.548576
H	-0.989070	-1.050143	-3.001037
H	-1.045625	-3.257059	-4.098435
H	-0.231997	-5.288497	-2.887575
H	0.635905	-5.060289	-0.560248

H	1.412637	-3.641399	1.247667
H	-0.109410	-2.822870	1.638273
H	2.257256	-0.433254	2.831960
H	0.697336	-1.244543	3.153162
H	2.206400	-2.198618	3.066209
H	3.334277	-0.643933	0.680979
H	3.382822	-2.408162	1.006016
H	2.681480	-1.776130	-0.523617
N	0.573894	2.014335	1.190860
N	-2.029274	-0.510447	1.189068
C	1.589553	0.748417	-1.129034
C	-1.438509	1.001283	-1.130550
C	2.045534	2.057672	0.958533
C	0.327505	2.106647	2.646620
C	-0.026468	3.213203	0.554472
C	-2.801388	0.743019	0.955725
C	-1.986315	-0.768364	2.645099
C	-2.768841	-1.629730	0.554376
C	1.976095	0.423384	-2.445101
C	2.382792	1.720870	-0.471837
C	-1.348756	1.498080	-2.446678
C	-2.678164	1.201846	-0.475093
H	2.444364	3.049391	1.249855
H	2.502295	1.322410	1.641342
H	-0.750793	2.165308	2.840105
H	0.738311	1.229536	3.159665
H	0.798964	3.013648	3.069969
H	-1.113922	3.202786	0.687710
H	0.386648	4.132592	1.011325
H	0.192067	3.207951	-0.517890
H	-3.859579	0.593954	1.248025
H	-2.391601	1.506589	1.637330
H	-1.499714	-1.732151	2.839522
H	-1.430623	0.025658	3.157007
H	-3.007557	-0.811177	3.068596
H	-2.219456	-2.567408	0.693226
H	-3.773201	-1.726949	1.008748
H	-2.869650	-1.441710	-0.519024
C	3.077396	1.017644	-3.075299
H	1.407617	-0.329292	-2.997874
C	3.479508	2.333386	-1.095437
C	-2.413682	2.153326	-3.078810
H	-0.411769	1.382769	-2.997963
C	-3.756721	1.843897	-1.100598
C	3.836091	1.980521	-2.400819
H	3.342996	0.731392	-4.096681

H	4.058602	3.091708	-0.559077
C	-3.628073	2.328164	-2.406241
H	-2.297450	2.525823	-4.100305
H	-4.703756	1.966016	-0.565526
H	4.690231	2.456594	-2.886961
H	-4.467260	2.828528	-2.894017

BIPMAO[30]

N-(1,3-Diphenylpropylidene)-aniline-dicarbonyl-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	6.358665	-0.392089	1.048372
O	7.687638	1.925157	-0.320378
O	5.853058	-1.483572	-1.696343
N	4.539237	0.651647	1.265939
C	6.189414	-0.766742	3.240901
C	5.815730	-1.957512	2.543224
C	6.690920	-2.521022	1.586813
C	7.942642	-1.917468	1.304043
C	8.296203	-0.722574	1.976126
C	7.448145	-0.182641	2.989290
C	5.216777	-0.069649	4.154009
C	4.840270	1.322082	3.602647
C	4.066380	1.293286	2.306002
C	2.777666	2.047715	2.312204
C	2.531857	3.106557	1.420280
C	1.345990	3.839772	1.497678
C	0.379535	3.521773	2.456646
C	0.615730	2.474880	3.353675
C	1.810776	1.756368	3.293296
C	3.686873	0.567535	0.100733
C	3.948270	1.342554	-1.035816
C	3.129545	1.228137	-2.160430
C	2.051479	0.336071	-2.166109
C	1.797280	-0.441154	-1.032163
C	2.607658	-0.325175	0.100050
C	7.135180	1.034640	0.223366
C	5.977808	-1.021111	-0.617693
H	4.833397	-2.397342	2.710178
H	6.379124	-3.403032	1.028140
H	8.591984	-2.332621	0.535506
H	9.233261	-0.223085	1.734506
H	7.742349	0.728844	3.509183

H	5.664327	0.060995	5.151466
H	4.313418	-0.682111	4.282886
H	5.765271	1.900068	3.431028
H	4.261087	1.874686	4.352340
H	3.280206	3.370406	0.674144
H	1.179286	4.666909	0.805667
H	-0.549610	4.091245	2.510171
H	-0.130082	2.220024	4.108432
H	1.985903	0.947452	4.005061
H	4.794354	2.029931	-1.036019
H	3.338208	1.841288	-3.038893
H	1.417841	0.244820	-3.049518
H	0.962002	-1.143800	-1.024680
H	2.413087	-0.933647	0.984225

BOLMEU[31]

(η^4,η^2-6,6-bis(Methylthio)fulvene)-tricarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	4.721398	0.440446	10.697406
S	5.041603	-2.352370	13.768036
S	2.264173	-1.664356	12.660448
O	2.311632	-0.335956	9.073804
O	5.535572	2.098726	8.336962
O	6.509567	-1.716423	9.604948
C	3.551324	1.206941	12.375180
C	4.405864	2.251289	11.964666
C	5.766995	1.815663	12.113990
C	5.764661	0.497866	12.617255
C	4.378829	0.092096	12.814853
C	3.931594	-1.236212	13.018617
C	4.585840	-3.990377	13.109232
C	1.653506	-2.410870	14.218025
C	3.249877	-0.045448	9.713796
C	5.219591	1.454227	9.265636
C	5.802507	-0.883652	10.030353
H	2.466878	1.226014	12.394678
H	4.088094	3.220375	11.591449
H	6.649973	2.398792	11.869419
H	6.637207	-0.112455	12.825313
H	3.708936	-4.407850	13.613689
H	4.421169	-3.921214	12.028787
H	5.459090	-4.621909	13.314923

H	2.108413	-3.386146	14.418795
H	1.813188	-1.722133	15.054286
H	0.577620	-2.543525	14.046834

BOLMIY[31]

(η^4,η^2-6,6-Dicyclopropylfulvene)-tricarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	1.451341	7.495526	4.950353
C	0.901429	7.373444	3.205651
O	0.543905	7.282149	2.092535
C	0.947870	9.248009	5.143408
O	0.628138	10.367680	5.282627
C	-0.250015	7.031350	5.423110
O	-1.348319	6.740981	5.719469
C	3.080598	7.685927	6.378271
C	2.300367	6.599006	6.815818
C	2.298752	5.594181	5.789113
C	3.076200	6.054708	4.709604
C	3.599979	7.378658	5.043580
C	4.033922	8.333544	4.093781
C	4.468479	9.701646	4.483043
C	5.034152	10.102434	5.825877
C	5.959656	10.030184	4.642734
C	4.178626	7.942976	2.681276
C	4.135448	8.961478	1.541300
C	5.430910	8.290190	1.853673
H	3.241712	8.602570	6.930952
H	1.776830	6.535061	7.765368
H	1.779581	4.641456	5.836204
H	3.264812	5.503739	3.794496
H	3.920321	10.491518	3.965583
H	5.172686	9.338054	6.587520
H	4.748698	11.082160	6.208376
H	6.662477	9.197646	4.622939
H	6.317062	10.949557	4.180108
H	3.743765	6.980078	2.424601
H	3.581466	8.655314	0.655116
H	4.028670	10.010957	1.811460
H	5.787441	7.498076	1.195704
H	6.205021	8.877014	2.341841

BOLMOE[31]

(η^4,η^2-6,6-Ethylenedithiofulvene)-tricarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	7.313322	6.859645	0.972137
S	3.411456	6.831954	-0.633373
S	5.308763	8.462220	-2.189515
O	9.019979	6.780825	-1.497573
O	6.527925	3.969872	0.721835
O	9.700120	5.996906	2.562796
C	6.732258	8.945759	0.656252
C	7.217829	8.845277	1.978334
C	6.388390	7.922152	2.701285
C	5.386730	7.440691	1.830499
C	5.554328	8.099938	0.543901
C	4.861138	7.790147	-0.645910
C	3.285190	6.678081	-2.457056
C	3.759678	7.988528	-3.055287
C	8.355073	6.805923	-0.529374
C	6.838378	5.098904	0.816534
C	8.761363	6.335830	1.939704
H	7.135639	9.577451	-0.129636
H	8.079331	9.371648	2.378361
H	6.518089	7.631459	3.739546
H	4.606368	6.728843	2.082296
H	2.230776	6.480838	-2.690154
H	3.899964	5.825571	-2.772748
H	4.007546	7.884113	-4.119329
H	3.030158	8.796913	-2.920254

BOZYIY[32]

Nitrido-(5,10,15,20-tetra-*p*-tolylporphinato)-chromium(V) benzene solvate

Charge = 0
Spin Multiplicity = 2

Cr	4.44583277928436	1.83050637458661	1.81920965894958
N	4.48238615059093	0.29216069920470	1.85423528204368
N	2.43060393329304	2.23784415119873	1.91783183099024
C	1.53829154532119	2.23185592179676	0.85771854007575
C	0.20125753793991	2.46416171582054	1.33835343398307
C	0.27908204739663	2.59339878310166	2.69420940359598
C	1.66217074257428	2.42341295133842	3.05715801283703

C	2.13137437704294	2.42475433158945	4.37865177175592
C	1.13673311024099	2.53927713016985	5.48685509313790
C	1.12738099772563	3.66381177573937	6.33127128435966
C	0.19784182133298	3.77437891072883	7.36511628389590
C	-0.75233507568036	2.76651686948077	7.60133505279245
C	-0.73785404297781	1.64530372247572	6.75901050976632
C	0.18686611642762	1.53190870303887	5.71725263449180
C	-1.75016317834664	2.89210036991259	8.72526619048732
N	4.54983915757505	2.31386918149154	3.81914498018144
C	3.48941711053835	2.32123693864168	4.71250403077075
C	3.98061432477121	2.20714343892605	6.06095466781548
C	5.34155922609033	2.13842217538657	5.98894641487001
C	5.69629844290579	2.22764612968805	4.59684904872646
C	7.01300840540038	2.28044052673032	4.11986734694513
C	8.13851885865348	2.23815152123350	5.10046816770481
C	9.03603086700078	1.15542490072229	5.10439655280088
C	10.09372892642166	1.10629173254699	6.01203426253331
C	10.30282483239611	2.13748360135979	6.94330841145967
C	9.40724461876967	3.21670773601875	6.93445479900570
C	8.34107976549902	3.26808423944752	6.03208663942113
C	11.45876624979640	2.08367383729097	7.91047938899504
N	6.44013587511036	2.32549813484668	1.70046888014264
C	7.33084230737269	2.40328968052265	2.75874040956129
C	8.65728521551991	2.67135266465225	2.26719247000014
C	8.57509107788724	2.73880110989584	0.90709133663979
C	7.20075184730116	2.49462389595206	0.55341464385823
C	6.73302439951139	2.41720261380402	-0.76613247883556
C	7.72226368098765	2.53104433901904	-1.87963369905237
C	8.71031805425817	1.55041382346058	-2.07684809288259
C	9.62840950863074	1.66055166141607	-3.12140038750880
C	9.60087104787732	2.75387421498689	-4.00371704787461
C	8.61648860006996	3.73177552466169	-3.80042267676911
C	7.68975050456404	3.62347165892103	-2.76029432769177
C	10.59454976295974	2.86515874647161	-5.13279937360676
N	4.32191722311954	2.21881567268396	-0.19993360603832
C	5.38184264601623	2.23645048813002	-1.09392096231229
C	4.89772342706007	2.04307733752540	-2.43582714964662
C	3.54124135517203	1.91592630962339	-2.35952113502978
C	3.18138372132933	2.04874095857828	-0.97210831279030
C	1.86282502204656	2.06546358418034	-0.49719560570702
C	0.74305281597196	1.94249989292491	-1.47764381748002
C	-0.11830471052696	0.83151832286550	-1.44219949202260
C	-1.16635386202602	0.70965590021557	-2.35442821341705
C	-1.40117701797243	1.69331971027462	-3.32985635524333
C	-0.54269626327900	2.80205833344292	-3.35886555829434
C	0.51329602363088	2.92636280801202	-2.45201075843350

C	-2.54338357464624	1.55912370310010	-4.30553878700790
H	-0.68034819762883	2.54647022937105	0.71133839531433
H	-0.52694112550994	2.80020404398989	3.39028186988206
H	1.84942878835727	4.46558215704600	6.16592722112678
H	0.20859011741957	4.66429389502683	7.99911740489283
H	-1.46057385943357	0.84216183965431	6.92109106510352
H	0.17897588001544	0.64401635607217	5.08235065795553
H	-2.43037230794632	2.03087573070083	8.75241746979428
H	-2.35650806626913	3.80430256465111	8.61736796203312
H	-1.24346931568762	2.95699309450565	9.70046819905871
H	3.36000968008102	2.17451057174704	6.95021348934564
H	6.04550498129614	2.03970720487600	6.80847324238329
H	8.89387876429405	0.33839055592196	4.39467374080911
H	10.76921149014180	0.24751961379812	5.99833008854717
H	9.54640277231438	4.03656303438682	7.64299567689476
H	7.66653698343666	4.12626832393532	6.04228575328951
H	11.42431294213751	2.91979931357850	8.62116555234042
H	12.42188818079890	2.13061795841983	7.37867660223996
H	11.45468259386212	1.14468924679181	8.48411982428126
H	9.53414536941304	2.81700045051103	2.88939597189955
H	9.37239714560765	2.94876464071863	0.20191010765817
H	8.75064641448951	0.68667650950923	-1.41054889671142
H	10.37948440652865	0.87828859014552	-3.25518712540553
H	8.57483768733537	4.59796249692508	-4.46483405911772
H	6.93937250805191	4.40411627942079	-2.62233021919194
H	10.47611642778049	3.81238961134368	-5.67534738349438
H	10.46828181518418	2.04308580550135	-5.85440276679078
H	11.62868522221637	2.80958236482706	-4.76073719246690
H	5.51991490193877	2.00118288927224	-3.32359315519027
H	2.84284450980206	1.75144884108233	-3.17321848578504
H	0.04524824807176	0.04901236429712	-0.69891616349208
H	-1.81288212853988	-0.17011244348548	-2.30933487254692
H	-0.70350392685032	3.58655514952847	-4.10211729390035
H	1.15952576254383	3.80508914998591	-2.49336324478198
H	-2.53933248283443	2.37674650970804	-5.03806673185439
H	-3.51332432236604	1.57466373851103	-3.78457441704312
H	-2.48866619598261	0.60638185789041	-4.85345788402699

CALWER[33]

N,N'-Ethylene-bis(salicylideneaminato)-oxo-chromium(V) hexafluorophosphate acetonitrile solvate

Charge = 1
Spin Multiplicity = 2

Cr	0.005227	0.052981	-0.099640
O	0.012735	0.243265	1.453965
O	-1.308464	-1.150898	-0.565218
C	-2.635947	-1.027008	-0.598936
C	-3.418682	-2.192957	-0.533246
C	-4.803924	-2.098727	-0.599732
C	-5.449454	-0.853440	-0.745225
C	-4.693713	0.299937	-0.827179
C	-3.276872	0.240968	-0.747823
C	-2.521599	1.428258	-0.882231
N	-1.207686	1.509519	-0.765329
C	-0.552578	2.721118	-0.980154
O	1.209914	-1.260830	-0.562908
N	1.341223	1.397855	-0.764298
C	0.794665	2.662056	-0.979594
C	2.543174	-1.253033	-0.593325
C	2.643261	1.202407	-0.879582
C	3.221334	-2.482514	-0.523346
C	3.292256	-0.045820	-0.742618
C	4.609663	-2.509233	-0.586275
C	4.709046	-0.110505	-0.818841
C	5.361380	-1.325083	-0.732552
H	-2.919431	-3.156009	-0.429493
H	-5.399913	-3.010631	-0.541748
H	-6.536575	-0.804489	-0.797484
H	-5.170867	1.273476	-0.950554
H	-3.056303	2.354579	-1.122259
H	-1.134031	3.627545	-1.144619
H	1.453292	3.514218	-1.143141
H	3.256815	2.078407	-1.119965
H	2.639971	-3.398288	-0.419157
H	5.123951	-3.469374	-0.524811
H	5.269417	0.817547	-0.942844
H	6.448764	-1.370975	-0.782096

CAMWOC[34]

($\sigma^1(C_2)$,$\eta^3(C_{4-6})$-3-t-Butyl-1-methyl-1-oxo-5-phenyl-1-thiacyclohexene)-dicarbonyl-nitrosyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	-0.019455	0.000783	0.010678
S	-0.935642	-1.561874	-2.213125
C	1.002267	1.552234	-0.031475

C	-1.583471	0.996344	-0.068245
C	-2.637313	-0.944371	-2.189603
H	-3.017718	-0.924090	-1.166284
H	-3.197091	-1.647394	-2.814572
H	-2.643648	0.056978	-2.633055
C	-0.549899	-2.022846	-0.582700
C	0.849159	-2.017749	-0.200764
C	1.783179	-1.136215	-0.778342
C	1.624747	-0.522973	-2.156656
C	0.126400	-0.178283	-2.216318
H	-1.246705	-2.712507	-0.108459
H	2.776016	-1.128584	-0.327314
H	2.091206	0.475111	-2.122552
H	-0.190319	0.556434	-2.961734
C	2.167899	-2.445192	1.922367
C	2.564997	-3.291401	2.957598
C	2.050849	-4.590123	3.045595
C	1.135074	-5.033673	2.088540
C	0.733772	-4.185265	1.052772
C	1.246195	-2.880241	0.953442
H	2.560717	-1.428569	1.878970
H	3.273003	-2.931281	3.705691
H	2.361399	-5.249940	3.857053
H	0.731395	-6.045931	2.142632
H	0.034585	-4.552293	0.299909
C	2.401915	-1.247499	-3.330988
C	2.356926	-2.782418	-3.246935
H	1.333818	-3.170051	-3.322606
H	2.797143	-3.144293	-2.305745
H	2.944696	-3.212189	-4.072811
C	1.837648	-0.773060	-4.680663
H	0.807803	-1.124965	-4.834281
H	2.453594	-1.163239	-5.505311
H	1.841361	0.326086	-4.752404
C	3.876912	-0.803066	-3.225575
H	4.478891	-1.285524	-4.010206
H	4.315400	-1.079927	-2.254597
H	3.974593	0.287158	-3.345534
N	-0.108200	-0.025272	1.706027
O	-0.217152	0.026118	2.884963
O	1.651725	2.518791	-0.024996
O	-2.536340	1.668100	-0.075941
O	-0.892922	-2.595633	-3.278557

CATLAL[35]

Bis(tetraphenylarsonium) tetrakis(isothiocyanato)-nitrido-chromium(V) toluene solvate

Charge = -2
Spin Multiplicity = -2

Cr	-6.53107212420862	-6.01886971133909	8.12282014516321
N	-5.23576930235402	-6.01808217432631	8.95008777151962
N	-7.95811689050525	-6.01672242487658	9.47986109391392
C	-8.82468364615304	-6.01360536344337	10.28828566977702
S	-10.01306917223059	-6.01591891823557	11.39926510279766
N	-6.93653522949726	-7.92896645055461	7.86617350269650
C	-7.19872801495927	-9.07370315280932	7.70660326109988
S	-7.55597887754637	-10.64421110788401	7.47820702172095
N	-5.90730513998644	-6.02107789894941	6.25478045094779
C	-5.56531884243664	-6.01139429193185	5.12009286459707
S	-5.09389356409310	-5.99986043168000	3.56295189646495
N	-6.93562242019305	-4.10934863138342	7.86089724604955
C	-7.19628071199404	-2.96451525629430	7.69961926819579
S	-7.55252406384236	-1.39367418629213	7.47188270505608

CATYOM[36]

((*Z*)-(η^2-Allylamino)(ferrocenyl)methylidene)-cis-tetracarbonyl-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	5.120341	1.465554	2.535847
Fe	6.457685	1.807009	6.958902
O	7.429824	-0.320600	3.261954
O	5.481405	0.521569	-0.317545
O	3.380672	-0.951836	3.172037
O	7.302649	3.545730	2.115955
N	4.087273	3.504267	4.372910
H	3.776892	3.972792	5.227050
C	6.524869	0.385600	3.026674
C	5.327622	0.895571	0.781710
C	4.020276	-0.007705	2.934489
C	6.441194	2.778138	2.280654
C	4.667501	2.309865	4.409301
C	4.797681	1.750771	5.752460
C	4.518256	2.412356	7.021099
H	4.183143	3.436606	7.167200
C	4.767309	1.484068	8.078301
H	4.666304	1.689120	9.140806
C	5.221558	0.254754	7.496961

H	5.524722	-0.634738	8.042468
C	5.254451	0.414634	6.078973
H	5.567281	-0.335933	5.362127
C	7.962336	2.865162	6.026514
H	7.880299	3.345104	5.055399
C	7.636624	3.462692	7.287284
H	7.274926	4.475811	7.440550
C	7.845600	2.476239	8.309138
H	7.665541	2.609702	9.372420
C	8.299508	1.270374	7.675244
H	8.521764	0.331543	8.175295
C	8.368320	1.509978	6.262233
H	8.651701	0.786703	5.503254
C	3.923174	4.253213	3.127866
H	4.762698	4.957078	3.009431
H	3.003302	4.855354	3.206637
C	3.856670	3.297603	1.961487
H	4.222323	3.680098	1.008444
C	3.003499	2.202775	1.974304
H	2.352713	2.031844	2.832471
H	2.710742	1.719189	1.044495

CECVUB[37]

Triphenyl-tris(tetrahydrofuran)-chromium(III)

Charge = 0
Spin Multiplicity = 4

Cr	0.019094	-0.023986	0.053069
O	0.349867	2.247628	-0.086378
C	-0.732805	3.228296	-0.230591
C	-0.039972	4.574260	-0.392657
C	1.197354	4.405959	0.501401
C	1.592326	2.954012	0.245348
O	2.303742	-0.048699	0.090181
C	3.084229	-0.410474	1.282905
C	4.496739	-0.703489	0.785307
C	4.604327	0.185407	-0.462315
C	3.205773	0.068719	-1.055134
O	0.358259	0.074438	-2.223590
C	0.316610	1.295602	-3.028617
C	0.679751	0.867374	-4.444790
C	0.065876	-0.538051	-4.519160
C	0.330712	-1.090509	-3.121672
C	-2.016965	0.296995	-0.122399

C	-2.852052	0.714171	0.939561
C	-4.224479	0.946897	0.776579
C	-4.828937	0.767710	-0.472182
C	-4.037928	0.348382	-1.547047
C	-2.667320	0.119651	-1.365945
C	-0.142045	-2.079472	-0.083031
C	0.998876	-2.881754	-0.316779
C	0.942581	-4.280560	-0.390955
C	-0.277918	-4.943993	-0.230157
C	-1.430036	-4.185011	0.005231
C	-1.355761	-2.787863	0.075156
C	0.018408	-0.032331	2.125919
C	0.038910	1.183755	2.849480
C	0.067300	1.238398	4.249747
C	0.075073	0.057854	4.999282
C	0.050330	-1.165985	4.322011
C	0.023327	-1.201845	2.921267
H	-1.356627	3.192931	0.675518
H	-1.344269	2.922534	-1.086983
H	0.256611	4.736580	-1.439755
H	-0.685875	5.406055	-0.082933
H	2.011045	5.099592	0.253018
H	0.929134	4.553270	1.557970
H	2.044088	2.459043	1.113184
H	2.272551	2.866386	-0.616597
H	3.053890	0.445756	1.973400
H	2.591241	-1.264832	1.760137
H	4.598505	-1.763687	0.510134
H	5.252681	-0.472351	1.546808
H	5.376811	-0.149108	-1.166900
H	4.818923	1.226746	-0.179790
H	3.103968	-0.833474	-1.679804
H	2.895814	0.942559	-1.640309
H	1.016715	2.012916	-2.584403
H	-0.703219	1.710174	-2.979727
H	1.772018	0.821157	-4.567861
H	0.274979	1.556751	-5.197141
H	-1.015029	-0.474186	-4.712968
H	0.517572	-1.166863	-5.297242
H	-0.438735	-1.779532	-2.755311
H	1.309884	-1.588341	-3.054005
H	-2.420561	0.859231	1.932287
H	-4.826281	1.266662	1.632198
H	-5.898472	0.945510	-0.604393
H	-4.490720	0.194749	-2.530783
H	-2.093316	-0.221547	-2.230489

H	1.974938	-2.408009	-0.447540
H	1.855974	-4.853774	-0.573921
H	-0.330408	-6.033583	-0.284980
H	-2.394002	-4.684931	0.136384
H	-2.275482	-2.230709	0.264439
H	0.016099	2.133105	2.309670
H	0.079587	2.207653	4.756437
H	0.094730	0.091091	6.090817
H	0.049041	-2.101793	4.888278
H	-0.000074	-2.178255	2.433567

CEDRYL10[38]

Cedryl chromate

Charge = 0
Spin Multiplicity = 1

Cr	0.314443	-0.060275	0.182945
C	0.643130	2.886394	0.314780
C	1.437790	-2.272639	-1.437295
C	1.932011	3.045549	1.166151
C	2.907034	-2.763367	-1.602489
C	1.916392	4.469668	1.763441
C	2.873565	-4.023593	-2.488047
C	-0.628510	2.963052	1.174863
C	0.850349	-1.789631	-2.770478
C	1.918368	7.952314	0.670352
C	1.736383	-7.615767	-1.370069
C	4.414687	2.725600	1.446610
C	5.171154	-3.259090	-0.636174
C	3.486818	2.025050	-0.727949
C	3.459185	-2.527383	0.979884
C	0.595765	3.918930	-0.831205
C	0.556860	-3.357544	-0.783937
C	0.997330	5.339289	-0.377108
C	0.799999	-4.769287	-1.358685
C	2.245032	5.331744	0.528966
C	2.300856	-5.077532	-1.515832
C	2.838478	6.743791	0.855331
C	2.662811	-6.529607	-1.936629
C	4.136106	6.808101	0.021994
C	4.106272	-6.685610	-1.403835
C	4.675702	5.371525	0.080533
C	4.095063	-5.967383	-0.039783
C	3.409997	4.521778	-0.145900

C	3.097371	-4.787372	-0.191151
C	3.318640	3.049713	0.406733
C	3.656912	-3.312927	-0.327977
H	1.279535	3.584158	-1.622859
H	0.778157	-3.369852	0.292449
H	3.237089	4.490256	-1.234490
H	2.412114	-4.799029	0.669466
H	1.916505	2.258984	1.937821
H	3.475876	-1.935702	-2.054040
H	0.969615	4.746461	2.246562
H	2.268892	-3.923727	-3.399265
H	2.703768	4.568972	2.524761
H	3.891720	-4.284028	-2.807950
H	-0.548084	2.316757	2.059517
H	0.655701	-2.627160	-3.451776
H	-0.821838	3.989451	1.509854
H	-0.108097	-1.285926	-2.583337
H	-1.489054	2.639074	0.573512
H	1.532501	-1.085530	-3.267015
H	2.439529	8.876015	0.965031
H	2.101303	-8.612017	-1.662128
H	1.605138	8.070762	-0.377824
H	1.691727	-7.587749	-0.270407
H	1.010546	7.875645	1.287603
H	0.708704	-7.516452	-1.747628
H	-0.413094	3.927227	-1.270933
H	-0.502087	-3.077786	-0.885915
H	4.391139	3.386175	2.323995
H	5.759160	-3.629249	0.215646
H	4.292534	1.691687	1.803741
H	5.458059	-3.846469	-1.519109
H	5.415007	2.805626	0.996467
H	5.475081	-2.216259	-0.813592
H	2.771774	2.172568	-1.546726
H	3.797876	-1.486354	0.877081
H	4.501055	2.116191	-1.148776
H	2.414882	-2.504843	1.315354
H	3.369523	0.993127	-0.367211
H	4.057163	-2.997533	1.777069
H	1.176141	5.944830	-1.280032
H	0.320419	-5.491606	-0.681107
H	0.159070	5.814215	0.158402
H	0.301949	-4.875983	-2.337385
H	3.141272	6.719374	1.917653
H	2.646049	-6.610280	-3.036883
H	3.896244	7.081815	-1.020881

H	4.412716	-7.739931	-1.328783
H	4.846078	7.558508	0.402588
H	4.817143	-6.194273	-2.086573
H	5.463557	5.171799	-0.660810
H	3.726042	-6.654190	0.736780
H	5.107834	5.187941	1.076414
H	5.099020	-5.655001	0.276504
O	0.625870	1.571824	-0.339926
O	1.494096	-1.099695	-0.561092
O	0.457815	-0.165520	1.769493
O	-1.158795	-0.493347	-0.257148

CIQQAU[39]

Dichloro-oxo-(spiro(adamantane-2,2'-homoadamantan-3-on-4-olato))-chromium(V) dichloromethane solvate

Charge = 0
Spin Multiplicity = 2

Cr	0.034431	-0.039285	-0.049095
Cl	1.925181	-0.695782	-1.004930
Cl	-1.008045	-1.954961	-0.533443
O	0.097534	-0.069880	1.515280
O	0.831699	1.839399	-0.201134
O	-1.313635	0.868914	-0.801555
C	-1.390153	2.298622	-0.706222
C	-2.111687	2.777205	-1.984859
H	-1.443652	2.654948	-2.850598
H	-2.944728	2.071211	-2.124249
C	-2.664866	4.208446	-1.901537
H	-3.275020	4.369980	-2.804451
C	-3.543760	4.365772	-0.651851
H	-3.968697	5.381758	-0.621348
H	-4.388327	3.658413	-0.679091
C	-2.681597	4.115134	0.594779
H	-3.296447	4.237947	1.500614
C	-2.191754	2.662541	0.577816
H	-3.053389	1.977165	0.578677
H	-1.590982	2.427442	1.470071
C	-1.528978	5.133891	0.660175
H	-0.906877	4.940139	1.547906
H	-1.971879	6.131191	0.814435
C	-0.652572	5.208852	-0.617740
H	-0.166869	6.187437	-0.577276
C	-1.551450	5.262140	-1.876011

H	-2.026506	6.257299	-1.891582
H	-0.951201	5.201075	-2.794673
C	0.048274	2.768286	-0.511472
C	0.551124	4.190306	-0.646636
C	1.619495	4.570640	0.472453
H	1.138297	4.485371	1.458248
C	2.107196	6.026260	0.262319
H	1.300266	6.763373	0.375576
H	2.834014	6.250603	1.059975
C	2.793212	6.163800	-1.112800
H	3.092014	7.212490	-1.269874
C	4.034395	5.252776	-1.150462
H	4.754612	5.561455	-0.374593
H	4.543369	5.345162	-2.124672
C	3.592470	3.796482	-0.914928
H	4.470532	3.131538	-0.930441
C	2.613017	3.373766	-2.025748
H	2.347862	2.312987	-1.920207
H	3.096295	3.477914	-3.011400
C	1.361968	4.276130	-2.022991
H	0.703969	3.977083	-2.851430
C	1.823444	5.738410	-2.233114
H	2.337203	5.786264	-3.207402
H	0.971271	6.429279	-2.298733
C	2.891653	3.689884	0.451893
H	3.563487	4.062705	1.243146
H	2.669399	2.645394	0.692895

COZYAR[40]

Carbonyl-(η^5-cyclopentadienyl)-(diphenylcarbene)-nitrosyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	0.013888	-0.053759	0.013078
O	2.779927	-1.252975	-0.163877
O	0.048328	-0.175472	2.870064
N	0.088734	-0.035077	1.684662
C	1.712521	-0.790236	-0.121592
C	-2.202034	-0.173812	-0.197118
C	-1.673381	0.344285	-1.418182
C	-0.839362	-0.650499	-1.994133
C	-0.847882	-1.789724	-1.123186
C	-1.702794	-1.502818	-0.027783
C	0.823832	1.650876	-0.375966

C	1.283145	2.598604	0.659532
C	2.551036	3.217885	0.544693
C	3.021392	4.086152	1.529547
C	2.217026	4.404290	2.629653
C	0.944894	3.832238	2.741702
C	0.491453	2.928402	1.780711
C	1.064081	2.133526	-1.753472
C	1.668322	1.340901	-2.752669
C	1.866430	1.832239	-4.044461
C	1.437935	3.119190	-4.384555
C	0.832878	3.921873	-3.410393
C	0.670654	3.446632	-2.109610
H	-2.866893	0.348817	0.485055
H	-1.867646	1.331729	-1.825509
H	-0.294879	-0.567868	-2.928744
H	-0.304140	-2.716503	-1.283544
H	-1.901406	-2.154918	0.818230
H	3.180533	2.987142	-0.316054
H	4.015853	4.525654	1.432437
H	2.576931	5.097871	3.391455
H	0.302860	4.088227	3.586405
H	-0.500799	2.487761	1.873005
H	2.018361	0.340387	-2.500362
H	2.359514	1.204434	-4.788863
H	1.582623	3.497657	-5.397740
H	0.496558	4.929266	-3.662665
H	0.209878	4.086493	-1.355490

CPNOCC10[41]

Isocyanato-cyclopentadienyl-dinitrosyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	0.028353	0.000097	0.015953
C	-0.024804	-0.000407	3.165829
C	-2.228464	0.000249	0.290118
C	-1.839364	-1.153777	-0.440980
C	-1.215134	-0.709919	-1.656269
H	-2.680372	0.000416	1.276755
H	-1.977503	-2.185789	-0.131665
H	-0.802795	-1.348809	-2.431707
N	0.029733	0.000013	1.975519
N	1.145833	-1.250149	-0.304556
O	-0.076184	-0.000743	4.374538

O	1.856421	-2.084294	-0.723208
C	-1.839286	1.153947	-0.441433
C	-1.215060	0.709564	-1.656540
N	1.145644	1.250541	-0.304358
H	-1.977276	2.186078	-0.132456
H	-0.802661	1.348100	-2.432232
O	1.856117	2.084881	-0.722886

CRCAAZ[42]

Chromium tricarbonyl-1-ethoxy-3-oxo-3a-phenyl-3,3a-dihydroazulene

Charge = 0
Spin Multiplicity = 1

Cr	3.536627	-2.565917	-1.132413
C	6.723472	-4.731323	-1.906419
C	6.364028	-3.302491	-1.356343
C	7.685863	-2.623819	-0.972079
C	8.421285	-1.929114	-1.944999
C	9.659672	-1.363042	-1.631605
C	10.184171	-1.484277	-0.340973
C	9.460251	-2.179071	0.632204
C	8.221968	-2.746910	0.317450
C	4.921799	-7.059923	1.222957
C	4.132476	-7.416834	2.461820
C	2.252615	-1.676537	-2.094431
C	6.258720	-5.714482	-0.956550
C	2.130861	-2.972936	-0.015579
C	3.189838	-4.109966	-2.085787
C	5.503003	-5.089040	0.011513
C	5.447322	-3.640785	-0.198621
C	4.844372	-2.738851	0.675256
C	4.606578	-1.353075	0.414203
C	4.703154	-0.687421	-0.825200
C	5.035002	-1.247288	-2.102434
C	5.537092	-2.521289	-2.353484
O	7.300196	-4.915345	-2.979324
O	4.844854	-5.605309	1.045433
O	1.397255	-1.136590	-2.681051
O	1.199897	-3.217347	0.646697
O	2.965311	-5.082923	-2.687533
H	8.025372	-1.826572	-2.956155
H	10.215837	-0.824080	-2.400575
H	11.149239	-1.038558	-0.094811
H	9.858130	-2.280145	1.643436

H	7.671775	-3.285445	1.090802
H	5.983129	-7.333453	1.317783
H	4.507849	-7.532765	0.320149
H	4.551140	-6.928337	3.352062
H	4.177498	-8.504463	2.612560
H	3.078407	-7.127091	2.356685
H	6.429982	-6.781482	-1.068333
H	4.446745	-3.129133	1.613303
H	4.166921	-0.779712	1.230512
H	4.328467	0.336585	-0.838925
H	4.743427	-0.643544	-2.963771
H	5.567649	-2.848718	-3.394228

DERNOE[43]

bis(1,1'-Methylene-3,3'-bis(2,6-di-isopropylphenyl)-2,3-dihydroimidazole-2,2'-diylidene)-triphenyl-chromium(III) tetrahydrofuran solvate

Charge = 0
Spin Multiplicity = 4

Cr	-0.077709	0.030689	0.024393
N	2.280317	-2.333332	-0.876075
N	0.683326	-2.989970	0.388556
N	-3.121239	-1.465065	-0.601409
N	-1.688581	-2.613719	0.499449
C	1.288481	-0.187453	2.716396
H	2.202549	-0.282084	2.125784
C	1.381815	-0.261981	4.111977
H	2.355560	-0.414573	4.585279
C	0.233405	-0.139105	4.903014
H	0.301004	-0.197241	5.991306
C	-1.002383	0.064537	4.277673
H	-1.907851	0.169461	4.881466
C	-1.082475	0.137847	2.881083
H	-2.060107	0.302449	2.421598
C	0.055720	0.006096	2.053017
C	-1.429328	2.759530	0.778007
H	-1.089960	2.600512	1.805238
C	-2.064679	3.969676	0.471526
H	-2.218087	4.718257	1.254821
C	-2.501932	4.227535	-0.832372
H	-2.998231	5.169581	-1.076943
C	-2.290247	3.258212	-1.818606
H	-2.627569	3.437032	-2.843162
C	-1.651232	2.056783	-1.491831

H	-1.499640	1.332541	-2.301482
C	-1.199670	1.758143	-0.188333
C	1.834984	1.444352	-1.759406
H	1.383965	0.775946	-2.503132
C	2.749367	2.396747	-2.224376
H	2.995549	2.444782	-3.288565
C	3.353921	3.281326	-1.325106
H	4.068683	4.028746	-1.677304
C	3.025904	3.193130	0.032604
H	3.486645	3.879948	0.749118
C	2.108088	2.233347	0.477046
H	1.864310	2.205912	1.542799
C	1.479489	1.324022	-0.398859
C	3.096676	-1.582982	-3.076706
C	4.113732	-0.982126	-3.831316
H	4.020217	-0.936105	-4.916921
C	5.246316	-0.448365	-3.220458
H	6.024740	0.017348	-3.827609
C	5.390155	-0.517648	-1.837048
H	6.287010	-0.108559	-1.370137
C	4.407342	-1.110897	-1.032981
C	3.257280	-1.616135	-1.675611
C	1.908617	-2.227993	-3.780720
H	1.103523	-2.349863	-3.040648
C	2.282554	-3.630929	-4.304462
H	1.410875	-4.107932	-4.777212
H	2.633429	-4.288317	-3.497031
H	3.082923	-3.561697	-5.056832
C	1.359262	-1.368439	-4.930353
H	0.462977	-1.842216	-5.354686
H	2.088355	-1.265300	-5.746982
H	1.085421	-0.359974	-4.590507
C	4.641530	-1.251737	0.465838
H	3.679334	-1.507095	0.932802
C	5.138148	0.050636	1.114576
H	4.460470	0.886075	0.893213
H	6.146030	0.318711	0.763871
H	5.195432	-0.074711	2.206134
C	5.626221	-2.404476	0.755185
H	5.271567	-3.360160	0.344085
H	5.758876	-2.528857	1.840450
H	6.612335	-2.192395	0.314496
C	1.147151	-1.859979	-0.242204
C	2.485163	-3.691054	-0.631689
H	3.328552	-4.228247	-1.046685
C	1.472327	-4.107851	0.169137

H	1.252009	-5.078326	0.598445
C	-0.497366	-3.001773	1.235748
H	-0.348270	-2.301360	2.066105
H	-0.640070	-4.016304	1.620288
C	-4.789720	0.331745	-0.467487
C	-5.632720	1.236160	-1.127624
H	-6.311644	1.857982	-0.542609
C	-5.624777	1.348890	-2.515378
H	-6.290626	2.058862	-3.009380
C	-4.772899	0.549990	-3.274860
H	-4.786086	0.638856	-4.361571
C	-3.904251	-0.367944	-2.668413
C	-3.918227	-0.445291	-1.260032
C	-4.891359	0.173804	1.044595
H	-4.012031	-0.392689	1.383612
C	-4.883679	1.522636	1.782803
H	-4.008617	2.123223	1.500387
H	-4.857294	1.353089	2.869594
H	-5.790080	2.107317	1.565449
C	-6.148671	-0.637133	1.422780
H	-6.157402	-1.627106	0.945267
H	-7.061214	-0.104708	1.113816
H	-6.193856	-0.783929	2.512404
C	-3.038391	-1.279398	-3.530371
H	-2.217432	-1.656396	-2.901678
C	-2.412353	-0.548214	-4.728795
H	-1.742413	-1.228158	-5.272883
H	-1.827897	0.327054	-4.412580
H	-3.176088	-0.206621	-5.442242
C	-3.851162	-2.495997	-4.022344
H	-3.213035	-3.169208	-4.614309
H	-4.686218	-2.169277	-4.660654
H	-4.270222	-3.072911	-3.186447
C	-1.846001	-1.375796	-0.077041
C	-2.793055	-3.437028	0.347282
H	-2.837403	-4.443636	0.746601
C	-3.701383	-2.708272	-0.349259
H	-4.702065	-2.952990	-0.682256

DERPAS[43]

Dichloro-bis(1,1'-methylene-3,3'-bis(2,6-di-isopropylphenyl)-2,3-dihydroimidazole-2,2'-diylidene)-(tetrahydrofuran)-(p-tolyl)-chromium(III) dichloromethane solvate

Charge = 0
Spin Multiplicity = 4

Cr	0.036195	0.018007	-0.008295
N	0.420481	3.250259	0.685052
N	-1.353124	2.730132	-0.406002
N	-2.864173	0.863414	-0.412892
N	-3.000728	-0.982368	0.679790
O	2.239081	0.089043	-0.204803
Cl	0.193737	-0.010729	2.371777
Cl	0.305230	-2.330743	-0.108490
C	-0.218948	2.165181	0.117092
C	-1.429480	4.097098	-0.190342
H	-2.259064	4.701226	-0.538159
C	-0.304565	4.425825	0.492049
H	0.048848	5.383005	0.852540
C	2.855323	3.589541	0.586365
C	4.084202	3.687721	1.255389
H	4.990556	3.887789	0.682580
C	4.163104	3.552988	2.638945
H	5.129512	3.626001	3.141156
C	3.002924	3.356538	3.386032
H	3.072607	3.294096	4.472083
C	1.745691	3.250249	2.773289
C	1.706510	3.313878	1.361050
C	2.791149	3.893634	-0.905447
H	1.820940	3.540521	-1.281481
C	2.852314	5.418830	-1.137379
H	3.813698	5.826154	-0.789348
H	2.049777	5.946387	-0.603324
H	2.754653	5.645095	-2.209699
C	3.889316	3.192416	-1.719269
H	4.890794	3.563411	-1.456431
H	3.741231	3.382933	-2.792179
H	3.873153	2.107064	-1.558244
C	0.488617	3.177352	3.632761
H	-0.295527	2.695159	3.032800
C	0.022020	4.598372	4.019950
H	0.783524	5.102951	4.634501
H	-0.906130	4.542755	4.608662
H	-0.173397	5.228954	3.142262
C	0.668279	2.334459	4.904426
H	1.025321	1.326684	4.659018
H	-0.299190	2.235715	5.417788
H	1.366548	2.803668	5.613958
C	-2.343927	1.988900	-1.167846
H	-3.173900	2.661537	-1.403776
H	-1.878186	1.617663	-2.089455

C	-2.075888	-0.122234	0.121502
C	-4.217323	0.641853	-0.213955
H	-4.982434	1.319357	-0.573932
C	-4.301203	-0.526045	0.470311
H	-5.162654	-1.075583	0.826200
C	-2.749058	-2.234982	2.794059
C	-2.629722	-3.474887	3.439375
H	-2.564996	-3.505616	4.527251
C	-2.607194	-4.668285	2.720974
H	-2.510688	-5.620226	3.246707
C	-2.734327	-4.647416	1.334166
H	-2.749665	-5.588358	0.782910
C	-2.849220	-3.439079	0.633568
C	-2.809279	-2.243108	1.383140
C	-2.909916	-0.964739	3.622651
H	-2.581082	-0.119036	3.002874
C	-2.047431	-0.954019	4.894100
H	-2.381589	-1.706805	5.624047
H	-2.125185	0.028802	5.381510
H	-0.991512	-1.129693	4.653914
C	-4.392081	-0.757389	4.005221
H	-5.046705	-0.702143	3.125012
H	-4.509806	0.178417	4.572682
H	-4.748188	-1.584827	4.638305
C	-3.104295	-3.464347	-0.868935
H	-2.877755	-2.463824	-1.263586
C	-2.214988	-4.467567	-1.621006
H	-1.153770	-4.272215	-1.419276
H	-2.387551	-4.377967	-2.704038
H	-2.444558	-5.506399	-1.340684
C	-4.592708	-3.760605	-1.153920
H	-4.865379	-4.762297	-0.787852
H	-4.786631	-3.730354	-2.236820
H	-5.258360	-3.032793	-0.669171
C	0.552996	1.177024	-2.846515
H	1.117602	1.951284	-2.320867
C	0.503555	1.247768	-4.245960
H	1.021101	2.060581	-4.765448
C	-0.198184	0.293714	-4.995454
C	-0.832642	-0.737291	-4.282172
H	-1.380668	-1.509261	-4.832269
C	-0.767164	-0.801495	-2.886105
H	-1.252443	-1.641788	-2.385448
C	-0.077731	0.154672	-2.106394
C	-0.276543	0.370190	-6.501317
H	-0.015657	-0.592044	-6.967806

H	0.404693	1.136133	-6.897302
H	-1.294761	0.622989	-6.838809
C	3.083895	-0.099688	0.983745
H	2.691659	-0.952704	1.555469
H	2.994065	0.810169	1.585463
C	4.473087	-0.374944	0.434457
H	4.967284	0.561528	0.135724
H	5.109155	-0.882815	1.171919
C	4.156526	-1.246304	-0.789443
H	3.973784	-2.284694	-0.476899
H	4.957645	-1.247839	-1.540425
C	2.872033	-0.624923	-1.336186
H	3.063138	0.125555	-2.114725
H	2.154941	-1.364853	-1.706261

DIJSEU[44]
(η^5-Cyclopentadienyl)-(formaldoxime-N)-dinitroso-chromium hexafluorophosphate

Charge = 1
Spin Multiplicity = 1

Cr	-0.046286	-0.003165	-0.028455
N	-0.107447	-2.044991	-0.136499
O	-0.651008	-2.627304	-1.290722
C	0.327700	-2.911037	0.700837
N	-0.116739	0.131867	1.672484
O	-0.154483	0.350038	2.815987
N	-1.713498	0.294135	-0.278328
O	-2.816011	0.640356	-0.427586
C	1.678664	-0.210232	-1.464143
C	2.124835	0.416621	-0.267745
C	1.397949	1.647710	-0.121646
C	0.499175	1.760179	-1.214966
C	0.668587	0.601442	-2.049844
H	2.017920	-1.170776	-1.841761
H	2.885195	0.039570	0.410241
H	1.507926	2.359276	0.691721
H	-0.198933	2.574032	-1.388206
H	0.134765	0.399359	-2.974364
H	0.234177	-3.979353	0.494887
H	0.791659	-2.547086	1.613862
H	-1.078277	-1.885961	-1.768254

DOGKUF[45]
(7,7'-Dimethyl-N,N'-ethylene-bis(salicylideneiminato))-oxo-chromium(V) trifluoromethanesulfonate

Charge = 1
Spin Multiplicity = 2

Cr	0.051885	-0.028438	-0.397837
O	-0.023846	0.169042	1.155582
O	-0.330811	1.500153	-1.325229
O	1.793183	0.329989	-0.897894
N	-1.811824	-0.621763	-0.830611
N	0.466900	-1.954000	-0.736457
C	-2.760376	1.537773	-1.370734
C	2.851125	-1.778149	-0.363672
C	-1.481093	2.151636	-1.514665
C	2.873195	-0.363003	-0.531309
C	-1.374905	3.501291	-1.899943
C	4.076467	0.350616	-0.364864
C	-2.516990	4.260497	-2.109122
C	5.230466	-0.313466	0.024577
C	-3.788475	3.686556	-1.945361
C	5.217831	-1.703463	0.239547
C	-3.901502	2.352625	-1.590810
C	4.052934	-2.420944	0.027966
C	-2.876597	0.120015	-1.078866
C	1.653035	-2.533409	-0.668581
C	-1.948397	-2.064908	-0.568075
C	-0.714750	-2.754669	-1.110070
C	-4.227505	-0.543356	-1.074595
C	1.760669	-4.005914	-0.957124
H	-0.378385	3.927371	-2.014552
H	4.067128	1.427736	-0.531545
H	-2.421494	5.308688	-2.396026
H	6.152122	0.252191	0.168765
H	-4.686204	4.284928	-2.097626
H	6.122767	-2.217425	0.562777
H	-4.899083	1.936039	-1.475817
H	4.059116	-3.496608	0.196046
H	-2.838943	-2.491045	-1.041165
H	-2.027116	-2.211779	0.521172
H	-0.653655	-3.769758	-0.700494
H	-0.762388	-2.823378	-2.208398
H	-4.370739	-1.114935	-0.147904
H	-4.302283	-1.247274	-1.917554
H	-5.046897	0.169354	-1.166884
H	1.279508	-4.595268	-0.161233
H	2.799616	-4.326341	-1.051559
H	1.245441	-4.242447	-1.898470

DOGLAM[45]
(5,5'-Dichloro-8,8,8',8'-tetramethyl-N,N'-ethylene-bis(salicylideneiminato))-oxo-(pyridine N-oxide)-chromium(V) trifluoromethanesulfonate

Charge = 1
Spin Multiplicity = 2

Cr	-0.047773	-0.014889	0.087779
Cl	-5.754003	-4.317530	1.036528
Cl	4.091745	5.225862	-2.828142
O	-0.073855	0.023039	1.662637
O	-1.883133	-0.076338	-0.281210
O	0.009146	1.826601	-0.287909
O	0.094708	-0.136134	-2.228727
N	0.110286	-2.020502	-0.063031
N	1.923575	-0.208539	-0.251574
N	-0.947322	-0.019329	-3.040468
C	-2.284003	-2.399225	0.256508
C	2.257617	2.045424	-1.139958
C	-2.717139	-1.058065	0.037901
C	0.952391	2.550663	-0.864923
C	-4.095609	-0.765443	0.122890
C	0.660318	3.891402	-1.200319
C	-5.013618	-1.757116	0.434538
C	1.615762	4.700541	-1.798346
C	-4.577033	-3.075570	0.650956
C	2.895584	4.190186	-2.071460
C	-3.237378	-3.401934	0.553835
C	3.220940	2.886068	-1.743754
C	-0.913274	-2.802073	0.111652
C	2.667715	0.720042	-0.774403
C	1.477678	-2.616568	-0.296912
C	2.507404	-1.524410	0.187044
C	1.613778	-2.903746	-1.805167
C	3.902672	-1.771157	-0.401599
C	1.659364	-3.931555	0.478414
C	2.634349	-1.482156	1.725137
C	-1.170702	-0.993653	-3.970775
C	-2.221809	-0.888712	-4.865730
C	-3.072054	0.219097	-4.818495
C	-2.829584	1.202118	-3.858209
C	-1.766919	1.069910	-2.977358
H	-4.424838	0.258821	-0.051084
H	-0.332490	4.282339	-0.977166
H	-6.073816	-1.515237	0.508828

H	1.373993	5.731968	-2.054745
H	-2.903841	-4.428607	0.706873
H	4.219087	2.496716	-1.946114
H	-0.739061	-3.883181	0.141860
H	3.726556	0.498687	-0.942567
H	0.780159	-3.544048	-2.125562
H	1.592617	-1.982348	-2.397256
H	2.545990	-3.447983	-2.001786
H	4.644066	-1.107075	0.062770
H	4.213337	-2.798777	-0.175035
H	3.937072	-1.635786	-1.489775
H	1.099833	-4.749024	0.005150
H	2.716774	-4.224524	0.456235
H	1.344843	-3.847136	1.525928
H	3.205589	-0.591231	2.018368
H	1.662173	-1.450581	2.229646
H	3.182859	-2.365147	2.075931
H	-0.464592	-1.819040	-3.948138
H	-2.363697	-1.684102	-5.596214
H	-3.901952	0.314700	-5.517398
H	-3.459542	2.087325	-3.780141
H	-1.515074	1.792660	-2.207858

DOJXUV[46]
Tricarbonyl-(η^6-4,6-diethyl-bis(α-methyl)-3,5-divinyl-o-quinodimethane)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	0.421766	3.086090	3.610330
O	1.559120	5.785555	4.310987
O	-2.299053	3.594462	4.768604
O	0.932250	2.310267	6.466230
C	0.197120	3.046196	1.425377
C	-0.389868	1.833996	2.023596
C	0.509153	0.996338	2.737196
C	1.870786	1.460089	2.983461
C	2.375627	2.568158	2.243140
C	1.619555	2.932969	1.015962
C	1.112010	4.739303	4.045584
C	-1.246156	3.415204	4.283128
C	0.766080	2.582778	5.337987
C	-0.462385	4.260095	1.574950
C	0.038228	5.590516	1.109674
C	-1.828324	1.451911	1.761205
C	-1.976367	0.692724	0.429614

C	-0.000731	-0.281669	3.308626
C	0.418519	-1.495298	2.934237
C	2.755271	0.708080	3.963316
C	3.799874	-0.180160	3.266210
C	3.644271	3.205892	2.601266
C	4.206837	4.271336	2.000668
C	2.034090	3.078406	-0.256641
C	3.405372	2.870026	-0.820956
H	-1.518592	4.227662	1.848164
H	1.126961	5.609782	0.983936
H	-0.420893	5.832432	0.135563
H	-0.264604	6.385197	1.805218
H	-2.451863	2.356574	1.730014
H	-2.210910	0.833056	2.584528
H	-1.630963	1.305778	-0.415157
H	-1.391565	-0.238027	0.438045
H	-3.030307	0.433834	0.254729
H	-0.803388	-0.205521	4.047964
H	-0.016677	-2.395974	3.369927
H	1.195765	-1.633815	2.180364
H	2.123518	0.089434	4.612975
H	3.269922	1.418322	4.624342
H	3.323219	-0.939119	2.630671
H	4.472180	0.414090	2.631181
H	4.412575	-0.701857	4.015264
H	4.154301	2.791940	3.473314
H	5.143111	4.684631	2.376459
H	3.751338	4.767338	1.143552
H	1.257190	3.334961	-0.985906
H	3.834094	3.814037	-1.198438
H	4.103970	2.449032	-0.089696
H	3.348190	2.190500	-1.686546

DPBPCR[47]
cis-Diphenyl-bis(2,2'-bipyridyl) chromium(III) iodide

Charge = 1
Spin Multiplicity = 4

Cr	-0.945954	1.021823	3.933474
C	-2.960350	-1.297503	4.619140
C	1.281789	1.668681	5.920863
C	-2.121350	2.405026	4.959703
C	-3.480537	2.160816	5.257112
C	-4.268356	3.066392	5.981076
C	-3.710270	4.258012	6.452469

C	-2.363189	4.528098	6.187382
C	-1.592169	3.616206	5.456475
C	-3.501778	-2.335990	5.371254
C	-2.914661	-2.647725	6.598645
C	-1.810725	-1.913922	7.024081
C	-1.317721	-0.880931	6.216716
C	-0.153950	-0.052711	6.577359
C	0.526245	-0.178899	7.793273
C	1.613017	0.647552	8.065973
C	1.997872	1.588625	7.110967
H	-3.391368	-1.024082	3.655932
H	1.545018	2.388513	5.147769
H	-3.960351	1.236744	4.920538
H	-5.317485	2.835590	6.181960
H	-4.315949	4.966403	7.020787
H	-1.911018	5.454357	6.550595
H	-0.547097	3.870341	5.263000
H	-4.365391	-2.883830	4.996698
H	-3.309241	-3.454226	7.216663
H	-1.337262	-2.146500	7.975898
H	0.205067	-0.915306	8.527173
H	2.147263	0.558673	9.011826
H	2.839337	2.259873	7.277007
N	-1.896165	-0.578401	5.024225
N	0.228247	0.870045	5.644535
C	0.229625	2.405112	2.907562
N	0.004139	-0.578568	2.842852
N	-2.120123	0.870189	2.222361
C	1.589881	2.162591	2.613660
C	-0.300215	3.614898	2.408103
C	1.068223	-1.297793	3.247957
C	-0.574370	-0.881108	1.650395
C	-3.173278	1.669220	1.945695
C	-1.738018	-0.052739	1.289655
C	2.377960	3.068389	1.890256
H	2.070413	1.239846	2.952816
C	0.471050	4.526908	1.677600
H	-1.346082	3.867751	2.598948
C	1.609557	-2.336363	2.495898
H	1.499275	-1.024396	4.211157
C	-0.081436	-1.914148	0.843049
C	-3.889181	1.589272	0.755471
H	-3.436295	2.389360	2.718563
C	-2.418043	-0.178828	0.073636
C	1.819126	4.258492	1.415915
H	3.427914	2.838951	1.692134

H	0.018289	5.451966	1.312067
C	1.022424	-2.648054	1.268503
H	2.473106	-2.884282	2.870486
H	-0.554890	-2.146672	-0.108785
C	-3.504503	0.647941	-0.199342
H	-4.730332	2.260852	0.589175
H	-2.096924	-0.915344	-0.660179
H	2.425043	4.967017	0.848018
H	1.416942	-3.454585	0.650477
H	-4.038478	0.559110	-1.145353

DUNCUK[48]

(η^6-Fulvenylbenzoato)-tricarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	6.174108	1.914290	1.885767
C	5.198894	3.721835	2.568178
C	5.701423	4.026598	1.288430
C	5.098239	3.136426	0.331088
C	4.210251	2.274385	1.005339
C	4.273899	2.602344	2.423585
C	4.224418	1.623545	3.428979
C	3.364061	-0.393550	4.298307
C	2.447435	-1.511003	3.991880
C	2.287717	-2.509389	4.970010
C	1.431537	-3.583130	4.736879
C	0.728511	-3.668897	3.529144
C	0.884271	-2.678041	2.553464
C	1.740174	-1.600675	2.779140
C	6.092234	0.103827	1.570221
C	7.261446	1.843920	3.370030
C	7.728341	1.892894	0.896198
O	3.441210	0.517216	3.235725
O	3.992844	-0.235637	5.326395
O	6.021029	-1.042828	1.356896
O	7.956597	1.830880	4.309223
O	8.719750	1.868441	0.277852
H	5.460783	4.205146	3.504396
H	6.427601	4.800589	1.058171
H	5.302435	3.129681	-0.735643
H	3.620139	1.477599	0.565093
H	4.519448	1.823134	4.458262
H	2.840879	-2.430361	5.905962

H	1.310576	-4.355942	5.496868
H	0.058153	-4.510550	3.348378
H	0.336314	-2.746091	1.612941
H	1.859372	-0.830516	2.019153

FANJEJ[49]

Tetracarbonyl-(η^2-5-methoxycarbene-5-methyl-bicyclo(2.2.1)hept-2-ene)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	-0.001226	4.801910	3.091805
O	-2.824847	5.358480	2.082902
O	1.233626	6.712604	1.073704
O	2.610622	4.595514	4.648376
O	-0.488455	7.281696	4.721187
O	-1.065834	3.213643	5.505038
C	-1.744943	5.103977	2.437080
C	0.757240	5.961307	1.828987
C	1.626262	4.655726	4.030544
C	-0.316078	6.280971	4.135527
C	-0.603305	3.266587	4.276097
C	-1.320387	4.421874	6.277930
C	-0.560603	1.862469	3.698361
C	-1.767705	1.872019	2.671458
C	-1.041774	2.000683	1.322892
C	-0.154990	3.261158	1.265345
C	0.967654	3.013273	2.058542
C	0.682884	1.678072	2.742978
C	0.061610	0.921072	1.537652
C	-0.673041	0.722705	4.716327
H	-2.047289	5.049639	5.753054
H	-0.380844	4.960032	6.439007
H	-1.728654	4.066078	7.228855
H	-2.301745	0.912545	2.733144
H	-2.491739	2.672214	2.866251
H	-1.695586	1.887200	0.450024
H	-0.169880	3.914839	0.396547
H	1.977240	3.347164	1.828777
H	1.539178	1.214917	3.245871
H	-0.340045	-0.075420	1.777182
H	0.761575	0.840832	0.694896
H	-1.632020	0.750337	5.250443
H	-0.604073	-0.243289	4.195789
H	0.134392	0.769442	5.460867

FAWBOU[50]

bis((μ^2-Chloro)-(η^5-cyclopentadienyl)-methyl-chromium(III))

Charge = 0
Spin Multiplicity = 3

Cr	14.351145	5.857004	0.862175
Cl	14.721557	5.114113	-1.348440
C	12.459448	4.730467	1.236545
C	13.521938	3.845990	1.619903
C	14.232080	4.450373	2.678244
C	13.618450	5.715078	2.963916
C	12.501358	5.867582	2.092794
C	13.817505	7.756897	0.253920
H	11.745724	4.560908	0.434635
H	13.768952	2.905036	1.135718
H	15.125751	4.058931	3.156735
H	13.945840	6.428388	3.715445
H	11.829162	6.719118	2.057930
H	12.840594	7.748416	-0.254922
H	13.766700	8.445188	1.112301
H	14.583337	8.118753	-0.449566
Cl	16.594374	6.458139	1.280407
Cr	16.959652	5.619722	-0.897585
C	18.889932	6.647256	-1.255838
C	17.853605	7.539666	-1.685672
C	17.148416	6.913365	-2.740507
C	17.740284	5.627672	-2.972634
C	18.831284	5.478947	-2.068331
C	17.474021	3.755852	-0.182086
H	19.588094	6.824413	-0.442089
H	17.619574	8.502370	-1.239645
H	16.273458	7.308722	-3.249236
H	17.409780	4.894363	-3.703231
H	19.479352	4.612231	-1.986923
H	18.434173	3.767398	0.357477
H	17.536123	3.019596	-0.999495
H	16.682328	3.444038	0.518056

FENFUB[51]

(η^5-Pentamethylcyclopentadienyl)-tricarbonyl-trifluoromethyl-chromium

Charge = 0

Spin Multiplicity = 1

Cr	2.373410	2.634718	7.065043
F	0.552530	2.933127	9.455600
F	1.964043	1.289422	9.732420
F	2.630990	3.355229	9.978688
O	1.524321	5.473447	7.643076
O	4.885847	1.524987	8.315440
O	4.550931	4.269011	5.794224
C	0.404704	2.326262	6.028193
C	0.643653	1.154191	6.817223
C	1.872825	0.559129	6.381547
C	2.378758	1.342489	5.283249
C	1.469737	2.436834	5.065178
C	-0.838460	3.161714	6.067746
H	-1.622641	2.690754	5.452771
H	-0.668085	4.169468	5.668790
H	-1.230662	3.258064	7.087972
C	-0.330870	0.536458	7.769320
H	-0.991094	-0.141968	7.203286
H	-0.964105	1.286001	8.256816
H	0.167259	-0.055222	8.545456
C	2.415522	-0.755113	6.853233
H	1.914278	-1.578433	6.318695
H	2.242679	-0.902732	7.926705
H	3.492270	-0.845448	6.663180
C	3.547566	0.977121	4.419522
H	3.222040	0.281482	3.629110
H	4.339644	0.477797	4.992322
H	3.985095	1.854315	3.926466
C	1.519047	3.417175	3.932655
H	0.935842	3.030179	3.081308
H	2.543731	3.587417	3.579139
H	1.089724	4.387711	4.212853
C	1.854926	2.550831	9.158074
C	1.846332	4.372856	7.453318
C	3.905352	1.959177	7.866859
C	3.704412	3.634492	6.286093

FEWMEA[52]

(Pentane-2,4-bis(2,6-dimethylphenyliminato))-(diethyl ether-O)-(trimethylsilylmethyl)-chromium(III) tetrakis(3,5-bis(trifluoromethylphenyl))borate

Charge = 0
Spin Multiplicity = 2

Cr	0.391642	15.166412	13.050285
Si	-0.475323	17.853073	10.910268
N	2.296197	14.814479	12.872941
N	0.016654	13.264743	13.090302
O	-0.936299	16.126599	14.403841
C	4.449451	13.606790	12.763751
H	4.846101	13.977804	13.721010
H	4.867257	14.248441	11.976597
H	4.810983	12.583819	12.614886
C	2.942933	13.637250	12.776249
C	2.251470	12.420264	12.730774
H	2.850668	11.520580	12.609873
C	0.871442	12.239634	12.876613
C	0.332997	10.832517	12.819831
H	-0.250410	10.590050	13.719297
H	1.153257	10.113318	12.724773
H	-0.341393	10.708148	11.959822
C	3.038130	16.048179	12.899005
C	3.362869	16.637308	14.145195
C	4.021606	17.875432	14.143845
H	4.267190	18.344684	15.098532
C	4.380145	18.497066	12.948859
H	4.891315	19.460674	12.966703
C	4.099712	17.877891	11.729019
H	4.406136	18.352838	10.795103
C	3.430415	16.649537	11.676394
C	3.103947	15.933651	15.453183
H	3.014229	16.654042	16.276100
H	3.941820	15.261791	15.700821
H	2.203070	15.305626	15.431905
C	3.202656	15.967518	10.353072
H	2.170482	15.613374	10.239443
H	3.852357	15.085096	10.242220
H	3.434734	16.647219	9.524176
C	-1.380888	12.979459	13.308964
C	-2.273146	12.864079	12.218491
C	-3.631976	12.645014	12.497184
H	-4.333461	12.563551	11.664205
C	-4.089827	12.512730	13.805716
H	-5.149742	12.340997	13.999371
C	-3.186761	12.581225	14.869547
H	-3.539813	12.449053	15.894107
C	-1.825640	12.812761	14.645434
C	-1.821183	12.903110	10.780302
H	-2.418089	13.620093	10.198599

H	-1.968616	11.916420	10.313828
H	-0.765231	13.172028	10.676356
C	-0.861269	12.840928	15.801763
H	-1.396708	12.724841	16.752218
H	-0.296628	13.783296	15.840352
H	-0.118861	12.031200	15.730785
C	-0.408702	16.000660	11.382618
H	0.038841	15.443699	10.541393
H	-1.458788	15.659489	11.449479
C	-2.288747	18.341366	10.651026
H	-2.353868	19.391460	10.325835
H	-2.889083	18.239889	11.567053
H	-2.755463	17.718180	9.873216
C	0.279362	19.027826	12.188029
H	0.307580	20.045717	11.768544
H	1.310916	18.748976	12.449726
H	-0.312719	19.075487	13.112883
C	0.417057	18.119791	9.263550
H	0.239392	19.147863	8.911275
H	0.045713	17.428994	8.491894
H	1.502902	17.980489	9.351435
C	-3.264116	16.386548	15.318970
H	-4.301543	16.463247	14.961306
H	-3.074590	17.258317	15.958264
H	-3.176772	15.468664	15.913886
C	-2.364202	16.350957	14.100143
H	-2.633052	15.514088	13.445158
H	-2.432892	17.288692	13.529767
C	-0.343667	17.164186	15.274224
H	0.657286	17.365216	14.864869
H	-0.937703	18.080235	15.150490
C	-0.257561	16.737842	16.726789
H	0.246200	17.536242	17.291909
H	0.333033	15.819983	16.844328
H	-1.246192	16.577472	17.171318

FIHPUI[53]

tris(bis(1-Phenylethyl)amido)-chromium(III)

Charge = 0
Spin Multiplicity = 4

C	7.13668386669397	10.02339714574990	8.75057214129595
H	7.63182967738823	9.37779013222879	9.50348237146787
C	8.22067879254011	10.87121305131870	8.08430900124300

H	7.79607728330983	11.50511996804940	7.29186027422380
H	8.97554447654395	10.22139526724683	7.61920031821774
H	8.72253812569064	11.52290067063880	8.81080307476285
C	6.54286561549157	9.06420966869229	7.71121091793554
C	6.77620096460498	7.68463210558864	7.80631350197726
H	7.34010752621697	7.29854735127438	8.65888421534184
C	6.30149513812593	6.80089700212611	6.83069236186273
H	6.49525270205804	5.73072373737266	6.92681467387099
C	5.57937571097717	7.28760514883275	5.73733502731219
H	5.20546399733888	6.60219107603155	4.97470144401508
C	5.34261913319979	8.66273319692437	5.62719202311886
H	4.78530450321112	9.05435577563480	4.77413745985829
C	5.82416470372576	9.53813075217654	6.60364513226593
H	5.64385800837087	10.60909028741696	6.49912609530216
C	7.65732083896126	13.51080264839448	11.77642607798853
H	6.91199818382848	12.73120682964542	12.01786736527008
C	7.27657972027727	14.74756536156577	12.60557510623715
H	7.95962636472091	15.59308631430701	12.44239948242058
H	7.28345327571477	14.51096512688985	13.67979734926729
H	6.26648786781647	15.08130704413714	12.33587198581348
C	9.02347386955070	12.92538773609514	12.16540786907471
C	9.95582601342566	13.62086104305248	12.95010241853391
H	9.72407498521923	14.61818166188215	13.32531798839062
C	11.19621208231046	13.05339281799395	13.26981947749530
H	11.90647319627101	13.61731114530820	13.87762242712001
C	11.52195876481275	11.77269291732105	12.81875748763461
H	12.48618928875662	11.32797402793247	13.07100360133569
C	10.59706545821673	11.06360120211047	12.04311187104832
H	10.83587244564744	10.05897989112829	11.68923266016288
C	9.36730734514298	11.63818197264945	11.72052129909152
H	8.65518921348035	11.08466325724511	11.10714765170808
C	8.53834523049115	14.70112691059529	9.78206592076116
H	9.24679553741508	14.89235616379613	10.60535637962550
C	7.91026623086767	16.05445455267694	9.41807830637080
H	7.15873008952246	15.94940022873243	8.62521797918864
H	8.68697082056712	16.75323829777886	9.07223917919662
H	7.41140572826010	16.49347815401985	10.29116991517389
C	9.39808173283897	14.16427219081649	8.63775697556515
C	10.67613714783793	13.65096523403618	8.90973788847753
H	11.02691614831283	13.61363193249825	9.94339225108602
C	11.50319851240759	13.18698889899013	7.88290033880739
H	12.49473682305091	12.79642234595457	8.11995023857238
C	11.06645866904779	13.23107279645045	6.55518178456262
H	11.71156136350186	12.87406590671613	5.75045205551292
C	9.79869811324075	13.74509339982159	6.26757502779500
H	9.44868337014275	13.79143211070063	5.23451029211495

C	8.97817551339835	14.20900494924903	7.30005770839995
H	7.99787431882163	14.61848192973867	7.05226859676532
N	6.13996479785556	10.86154899331612	9.45604617039638
N	7.53748303155930	13.72433542416703	10.30571352835628
Cr	6.14207757870220	12.77819038190909	9.45239431199399
C	5.14090970546516	10.02803328979148	10.16341534099668
H	4.64481018779632	9.38122034406241	9.41217330366232
C	4.05811036283156	10.88042168422467	10.82598045149730
H	4.48334203905110	11.51603011996970	11.61673283019241
H	3.30140225425016	10.23372439795128	11.29242215908457
H	3.55831946388333	11.53054503936666	10.09665273771892
C	5.73087469734804	9.07072031094884	11.20678854876982
C	5.48754110202226	7.69230096683289	11.11999145647778
H	4.91920060007303	7.30526459366105	10.27078836639494
C	5.95770063537489	6.81085098212796	12.09986450750828
H	5.75609421708358	5.74155222735949	12.01033329496306
C	6.68534825706362	7.29864904616477	13.18907785486997
H	7.05583443416304	6.61494108161828	13.95491071430105
C	6.93207412951175	8.67264840385370	13.29090731957794
H	7.49388408923257	9.06519579187917	14.14058040636759
C	6.45489513213121	9.54584678081572	12.31034743273854
H	6.64294139946808	10.61603948015200	12.40827313969629
C	4.63015590037555	13.50920881202584	7.12572366687524
H	5.37448126489569	12.72800230578271	6.88650114872586
C	5.01294781456044	14.74334112182762	6.29357201864210
H	4.33111303842965	15.59026901120919	6.45435772173151
H	5.00621589938770	14.50404250556274	5.21995656674526
H	6.02338333932423	15.07646582690174	6.56275798734689
C	3.26323563919874	12.92494004409591	6.73753734392170
C	2.33213656352959	13.62025382980453	5.95119618260995
H	2.56546018984104	14.61645258714121	5.57400539335585
C	1.09095999832731	13.05407512760988	5.63228504818332
H	0.38176390752747	13.61789819181633	5.02315124920798
C	0.76312602966302	11.77477111173123	6.08573651115525
H	-0.20171903671822	11.33103724110515	5.83410358966763
C	1.68670927364005	11.06576089177423	6.86301332888741
H	1.44624610541663	10.06220398121170	7.21878992079601
C	2.91728334882587	11.63909652948396	7.18491822326351
H	3.62841850106861	11.08567397892165	7.79954527008989
C	3.75025735260750	14.70637212129577	9.11634977154200
H	3.04221879788626	14.89594473690013	8.29231723994978
C	4.38002302290353	16.06001229281084	9.47629467657138
H	5.13020313205795	15.95672544983700	10.27062480636632
H	3.60385819096034	16.76110408195197	9.81868064960548
H	4.88051151642572	16.49537990278744	8.60229595596699
C	2.88963524623958	14.17434129913320	10.26219882390206

C	1.61108166113775	13.66159963945469	9.99150513352085
H	1.26062856794722	13.62106131899321	8.95784459018785
C	0.78309625872372	13.20216697047058	11.01964627159951
H	-0.20880622580035	12.81190078230881	10.78361627356256
C	1.21942894036463	13.25040755858628	12.34735258073689
H	0.57360282665001	12.89701759997368	13.15310269106160
C	2.48771201781237	13.76392507123400	12.63361354175726
H	2.83734030920350	13.81342604400171	13.66667203739040
C	3.30922538282455	14.22331141863233	11.59986573729511
H	4.28971018507770	14.63305359407995	11.84655606296264
N	4.74956143545191	13.72619034183686	8.59602811861103

FIRFIW[54]

(3-(1*R*,2*R*,3*R*,5*S*-(-)-Isopinocamphanylamino)-3-phenylpropa-1,2-dienylidene)-pentacarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	8.810034	4.469566	7.924738
N	3.601775	5.783996	9.036602
H	2.656493	6.150231	8.926782
O	8.164426	2.922960	5.372961
C	8.416311	3.507101	6.341909
C	9.204841	5.996874	6.875492
O	9.446644	6.929005	6.230106
C	9.094761	5.464100	9.511605
O	9.264697	6.072159	10.483871
O	8.065229	2.037289	9.612390
C	8.348846	2.960619	8.971816
C	10.608558	3.931101	7.876934
O	11.723705	3.597176	7.847244
C	6.902298	5.022665	7.968369
C	5.700345	5.355530	8.001369
C	4.365148	5.726376	7.938622
C	3.735923	6.066282	6.639938
C	4.543595	6.506790	5.575777
H	5.620167	6.587648	5.727120
C	3.973339	6.846785	4.350424
H	4.609921	7.196795	3.536924
C	2.590965	6.737294	4.163935
H	2.145972	6.996973	3.202350
C	1.780977	6.283032	5.210163
H	0.705468	6.175607	5.064307
C	2.346363	5.950871	6.440783

H	1.698615	5.561069	7.227952
C	4.015868	5.443586	10.402041
H	4.993379	4.963254	10.271944
C	4.209575	6.735384	11.261300
H	5.275997	7.006380	11.245580
H	3.669393	7.572773	10.791770
C	3.696784	6.575091	12.697699
H	3.943422	7.462565	13.299935
C	4.049652	5.168649	13.305418
C	2.783910	4.665413	12.505749
H	2.210986	3.838549	12.953172
C	3.029242	4.392245	11.009291
H	2.049890	4.539830	10.518842
C	2.216886	6.108535	12.632120
H	1.662742	6.282551	13.560884
H	1.617077	6.478103	11.786407
C	5.440351	4.573580	13.071501
H	5.768235	4.579922	12.026002
H	5.478976	3.531343	13.424318
H	6.188009	5.139967	13.649179
C	3.784061	5.126524	14.820032
H	2.804865	5.536007	15.099668
H	4.554747	5.701090	15.357352
H	3.828999	4.088096	15.184061
C	3.478548	2.959044	10.698184
H	3.609216	2.809820	9.615847
H	2.725322	2.237390	11.046638
H	4.431303	2.717115	11.189287

FIVHOH[55]

(η^6-1,2,3,4,5,6-Benzocyclo-octatetraene)-tricarbonyl-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	6.932992	3.369850	2.103707
O	9.136603	4.408388	0.335330
O	8.089647	0.586600	2.072147
O	5.735151	3.008319	-0.633493
C	8.299622	4.031241	1.059826
C	7.644653	1.664349	2.073077
C	6.156854	3.148937	0.448204
C	7.960495	3.358963	4.227948
C	7.789380	4.642607	3.692493
C	6.600903	5.295928	3.235208

C	5.341333	4.775843	2.872941
C	4.853577	3.430636	2.847979
C	5.354070	2.282567	3.476677
C	5.849290	2.173922	4.873123
C	5.065826	1.511220	5.831776
C	5.521862	1.375408	7.145640
C	6.771630	1.889572	7.505399
C	7.558464	2.537263	6.549271
C	7.095687	2.687452	5.231995
H	9.010427	3.058045	4.285857
H	8.699983	5.204571	3.472339
H	6.756389	6.327151	2.911847
H	4.718127	5.485235	2.324583
H	4.042014	3.281313	2.132678
H	4.901924	1.359888	3.101527
H	4.102017	1.088439	5.540995
H	4.910205	0.851304	7.881610
H	7.142797	1.770075	8.523924
H	8.545422	2.918134	6.820219

FIVZOZ[56]

trans-bis(Acetylacetonato-O,O')-chloromethyl-pyridine-chromium(III)

Charge = 0
Spin Multiplicity = 4

Cr	2.156735	-0.000073	3.817116
Cl	3.753036	0.001821	0.896596
N	0.311148	-0.000052	5.063745
C	3.933793	-0.000325	2.732789
C	-0.909416	-0.000900	4.490766
C	-2.088613	-0.000702	5.233280
C	-2.007358	0.000480	6.627227
C	-0.745376	0.001348	7.224967
C	0.384915	0.001008	6.410037
O	2.907179	1.368439	5.031872
O	1.328932	1.381425	2.683910
C	3.594801	3.456977	5.907409
C	2.873216	2.645752	4.860667
C	2.223602	3.297633	3.797909
C	1.484673	2.654798	2.786420
C	0.800981	3.476542	1.723267
H	-0.923541	-0.001830	3.400201
H	-3.050759	-0.001437	4.721280
H	-2.911662	0.000772	7.237122

H	-0.631327	0.002214	8.308888
H	1.390815	0.001716	6.831419
H	2.274900	4.384713	3.768433
H	4.533889	0.894118	2.949334
O	2.907014	-1.368665	5.031864
O	1.329173	-1.381475	2.683599
H	4.532417	-0.896233	2.947377
C	2.873057	-2.645964	4.860580
C	1.485103	-2.654848	2.785930
C	3.593870	-3.457293	5.907771
C	2.223863	-3.297746	3.797499
C	0.801957	-3.476509	1.722361
H	2.275257	-4.384819	3.767884
H	3.517460	4.534333	5.721907
H	4.656732	3.168722	5.926953
H	3.180436	3.229376	6.900987
H	-0.274007	3.242854	1.709958
H	1.203469	3.200990	0.736722
H	0.936157	4.552728	1.880174
H	3.519318	-4.534514	5.720358
H	3.176294	-3.232305	6.900623
H	4.655065	-3.166663	5.930648
H	-0.272699	-3.241465	1.707172
H	0.935609	-4.552751	1.880204
H	1.206355	-3.202203	0.736235

FOBPOB[57]

Pentacarbonyl-(dichloro-(2,6-di-t-butyl-4-methylphenoxy)phosphine-P)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	1.649721	3.451051	2.050173
P	3.050131	5.028266	3.001923
Cl	4.759395	4.279101	3.957582
Cl	4.078283	6.271687	1.663926
O	-0.172393	1.379260	0.794047
O	0.907743	5.279845	-0.279773
O	3.992284	2.374630	0.411333
O	-0.745032	4.467944	3.649341
O	2.231786	1.385103	4.221520
O	2.356063	6.025632	4.073478
C	0.526305	2.169068	1.271749
C	1.204025	4.615406	0.618203
C	3.117245	2.792969	1.039885

C	0.174325	4.099878	3.054038
C	2.030457	2.190739	3.417707
C	2.982790	7.083682	4.800344
C	3.538088	6.797274	6.071692
C	4.388490	7.781833	6.599836
C	4.621914	9.006114	5.971095
C	3.860678	9.303871	4.839840
C	2.988602	8.383052	4.236808
C	3.164290	5.632664	7.034708
C	2.456241	6.295786	8.249931
C	4.424634	4.897199	7.542157
C	2.178639	4.582201	6.491262
C	5.614015	9.995128	6.529314
C	2.011920	8.966996	3.174734
C	1.005024	7.982481	2.552532
C	2.779982	9.663389	2.029294
C	1.161799	10.034976	3.918990
H	4.870205	7.595080	7.560735
H	3.929067	10.309069	4.421407
H	2.164355	5.518308	8.972087
H	1.546976	6.826886	7.931969
H	3.107588	7.012688	8.766880
H	4.956520	4.401907	6.719222
H	4.129777	4.125988	8.269624
H	5.126988	5.575879	8.044652
H	2.617848	3.963591	5.701023
H	1.254170	5.037561	6.114358
H	1.908152	3.907254	7.316751
H	5.331848	11.028394	6.284690
H	6.617165	9.820308	6.107897
H	5.698814	9.906374	7.621265
H	1.485845	7.248480	1.896578
H	0.302314	8.558125	1.932065
H	0.421114	7.450727	3.314265
H	3.437478	10.462672	2.396997
H	2.061262	10.118944	1.331541
H	3.393096	8.947779	1.465994
H	1.782342	10.836859	4.340112
H	0.589232	9.578220	4.739654
H	0.448797	10.489824	3.214757

FOMBIT[58]

trans-bis(2-Methylquinolin-8-olato)-nitrido-chromium(V)

Charge = 0

Spin Multiplicity = 2

Cr	-0.80224159148642	1.57754126184690	3.22561194120176
C	1.31379332517237	2.60708028823946	1.59460581625140
C	1.66834169589523	2.81662737114895	2.95871715837201
C	2.86879368958824	3.46670190741141	3.23926026212362
C	3.70115140370800	3.90338703006620	2.18215292349865
C	3.37005902693913	3.69808783570899	0.85293462750541
C	2.15827683500720	3.03119730380292	0.53179805873298
C	1.70896437725813	2.73273773952446	-0.77804032748402
C	0.52354282528463	2.05091116811297	-0.95768883086312
C	-0.27141388021996	1.65378526165331	0.14902376375874
C	-1.53444556375372	0.87539912263805	-0.05393919089396
N	-0.80223409821136	0.03234626413857	3.22561858902702
N	0.12264660926158	1.95493245505775	1.39523540338428
O	0.81818392893771	2.37074764836064	3.88889072614411
H	-1.43597999285793	-0.12495491077215	0.39522393751661
H	-1.75100408622737	0.76304032586329	-1.12238896336973
H	-2.37916575438579	1.36863046481729	0.44494384712729
H	3.15886610655151	3.63317023854581	4.27748212844523
H	4.63427405617387	4.41198225712783	2.43069325198897
H	4.02734345168266	4.03447227057027	0.05029908970975
H	2.30900382463279	3.03455569710417	-1.63874233131449
H	0.17481940729662	1.80108535566523	-1.95948926814334
C	-2.91828205076786	2.60708716925329	4.85659758621997
C	-3.27281862447256	2.81659320590828	3.49247212257504
C	-4.47328539544817	3.46664282893008	3.21191024849003
C	-5.30564884264704	3.90335270443974	4.26900164594119
C	-4.97456387164018	3.69809232418332	5.59822884647102
C	-3.76278364915584	3.03120966882677	5.91938915783122
C	-3.31349904927502	2.73274855134432	7.22923672046142
C	-2.12809678300630	2.05089429443200	7.40890912433285
C	-1.33312078767057	1.65376194848408	6.30221371131924
C	-0.07011954930733	0.87532860575654	6.50520880043057
N	-1.72713807430883	1.95493934929359	5.05599163855822
O	-2.42265490151518	2.37072202988124	2.56231309484946
H	-0.16860965187100	-0.12501901870750	6.05603872735230
H	0.14639962448778	0.76295543843048	7.57366445403611
H	0.77464855595741	1.36851343180490	6.00636097492098
H	-4.76335598298444	3.63308062225405	2.17368298357850
H	-6.23877288536693	4.41193710180606	4.02044307359299
H	-5.63185782370932	4.03448909851490	6.40085139675667
H	-3.91355176986210	3.03457432024817	8.08992704950754
H	-1.77940408368365	1.80105196828337	8.41071603005548

FOSVEO[59]

(*t*-Butyl-tris(dimethylphosphinomethyl)silane-P,P',P'')-trimethyl-chromium(III)

Charge = 0
Spin Multiplicity = 4

Cr	18.281524	3.288890	14.591521
P	20.595494	3.286761	15.939035
P	17.415923	1.584745	16.526719
Si	19.825686	3.287693	18.090100
C	16.424927	3.291305	13.618291
C	18.916986	1.722888	13.359285
C	21.771900	1.862048	15.733538
C	18.078343	-0.112509	16.810722
C	15.620943	1.313651	16.877921
C	18.123630	2.606385	17.825214
C	20.792961	3.288140	19.746886
C	19.784631	3.293154	20.908872
C	21.672392	2.023498	19.813779
H	15.826190	4.187925	13.858385
H	16.604540	3.283862	12.529735
H	19.839284	1.223715	13.705173
H	19.093249	2.094484	12.335417
H	18.117810	0.962353	13.310583
H	22.111953	1.846109	14.688177
H	21.259001	0.914700	15.940700
H	22.647512	1.952772	16.389615
H	17.732067	-0.766726	15.998761
H	17.741180	-0.520405	17.773444
H	19.174773	-0.087190	16.787828
H	15.223047	0.636962	16.108706
H	15.067791	2.257366	16.820040
H	15.476156	0.860526	17.867917
H	19.140665	4.184281	20.887961
H	20.333151	3.293859	21.866763
H	22.405043	1.985748	18.993927
H	21.070621	1.103373	19.778382
H	22.237779	2.018018	20.761512
P	17.418586	4.991058	16.521744
C	18.922744	4.851942	13.359207
C	21.771279	4.712278	15.735690
H	15.819622	2.402088	13.869435
C	18.125064	3.972752	17.823685
C	21.679322	4.548239	19.808921
H	19.136235	2.405166	20.891801
C	18.081384	6.688809	16.801144

C	15.623516	5.263728	16.870613
H	19.837152	5.358511	13.715023
H	19.114953	4.475818	12.339867
H	18.119530	5.607089	13.295840
H	22.111323	4.730148	14.690342
H	21.258164	5.659153	15.944535
H	22.646933	4.620738	16.391569
H	22.413054	4.578110	18.989693
H	21.082695	5.471511	19.768774
H	22.243751	4.554818	20.757229
H	17.734982	7.340890	15.987505
H	17.744471	7.099486	17.762774
H	19.177821	6.663343	16.778013
H	15.226010	5.936189	16.097497
H	15.070593	4.319615	16.817586
H	15.478042	5.722069	17.858103

GABQUV[60]

bis(bis(Cyclohexyl)amino)-dioxo-chromium(VI)

Charge = 0
Spin Multiplicity = 1

Cr	0.015483	-0.055452	-0.292288
O	0.068806	-0.281585	1.305270
O	-0.026075	-1.403605	-1.139180
N	-1.506777	0.894300	-0.678413
N	1.522504	0.898522	-0.724770
C	-2.757949	2.125767	1.128588
C	-2.844995	3.463049	1.881535
C	-3.080556	4.637306	0.922594
C	-2.000281	4.687662	-0.165951
C	-1.902327	3.357842	-0.930338
C	-1.672071	2.175405	0.034638
C	-3.301051	-0.873840	-0.790025
C	-4.560735	-1.315283	-1.550975
C	-4.266693	-1.548540	-3.038787
C	-3.629162	-0.307338	-3.677622
C	-2.372255	0.142654	-2.915680
C	-2.675931	0.384266	-1.427083
C	1.507633	0.996108	-3.227190
C	2.371967	0.857394	-4.489492
C	3.028266	-0.526862	-4.576194
C	3.832162	-0.835420	-3.306331
C	2.967404	-0.703191	-2.042506

C	2.320043	0.693110	-1.955920
C	3.428495	1.322658	0.863776
C	3.936985	2.267551	1.964685
C	4.058871	3.711092	1.460006
C	2.729663	4.205252	0.874535
C	2.215626	3.270514	-0.232580
C	2.088396	1.822283	0.286072
H	-3.734926	1.905712	0.666902
H	-2.532972	1.303483	1.824394
H	-1.905452	3.629384	2.437438
H	-3.647745	3.412083	2.633660
H	-4.071190	4.526203	0.447295
H	-3.102734	5.586751	1.480269
H	-2.202704	5.506551	-0.873914
H	-1.025423	4.912722	0.301681
H	-1.084137	3.389731	-1.666241
H	-2.835753	3.195156	-1.494370
H	-0.714463	2.370816	0.548955
H	-2.553943	-1.683881	-0.807481
H	-3.536494	-0.673687	0.266126
H	-5.340314	-0.539194	-1.450319
H	-4.969183	-2.229216	-1.091506
H	-3.577672	-2.405142	-3.142130
H	-5.190990	-1.820047	-3.573001
H	-4.365368	0.516012	-3.686222
H	-3.371587	-0.506243	-4.729903
H	-1.592502	-0.632516	-2.993447
H	-1.961961	1.063001	-3.358471
H	-3.437712	1.182676	-1.378876
H	1.082570	2.008973	-3.157243
H	0.659147	0.294624	-3.279074
H	1.755349	1.048474	-5.381887
H	3.158463	1.632858	-4.480474
H	3.678458	-0.585664	-5.463344
H	2.244677	-1.293831	-4.705919
H	4.256301	-1.850594	-3.356489
H	4.688480	-0.140899	-3.240374
H	3.571503	-0.885404	-1.141210
H	2.169286	-1.462033	-2.056873
H	3.143003	1.427518	-1.911721
H	3.293338	0.305487	1.261202
H	4.180279	1.263348	0.059104
H	3.238016	2.237871	2.818753
H	4.907178	1.906776	2.340454
H	4.840757	3.761060	0.681744
H	4.383901	4.374148	2.277063

H	1.977353	4.264016	1.680601
H	2.839779	5.224751	0.473201
H	2.914449	3.303706	-1.084582
H	1.238887	3.613687	-0.606568
H	1.368625	1.841778	1.119561

GAGVUG[61]

bis(2-Phenyl-2-propoxy)-(bis(trimethylsilyl)amido)-chromium(III)

Charge = 0
Spin Multiplicity = 4

C	0.58850428953742	0.79923024635189	4.94799436625447
C	0.78139890084083	-0.50584654757419	5.74546393693231
H	0.42210106213621	-0.36658129472345	6.77510859762870
H	1.84406684262903	-0.78769275361874	5.77451694182703
H	0.21569984865148	-1.32627258658488	5.28352961666046
C	1.32256017086972	1.94863191105500	5.65052337731524
H	1.19792606732641	2.88899377954386	5.09588272202746
H	2.39580465419198	1.74054578418205	5.76312328413165
H	0.89297162417353	2.08005399098315	6.65253929458102
C	1.05038069256933	0.58108380530076	3.49851454776141
C	2.23953904608081	1.12690849980552	2.99201970795187
H	2.86618282226753	1.75673495550717	3.62363171585746
C	2.64543155730601	0.87439261245210	1.67611315035204
H	3.57312223370627	1.31434107166534	1.30481510313411
C	1.86907197892098	0.06753099644821	0.84138479121357
H	2.18421217670482	-0.12833466937010	-0.18506442473878
C	0.68165355248232	-0.48492180776230	1.33392517694177
H	0.06356032074708	-1.11520214150468	0.69183261440540
C	0.28007756237063	-0.23106374688935	2.64675731065204
H	-0.65218213480494	-0.66313976187659	3.01387422656028
C	-1.54606309964503	6.08023210700972	5.88691891349741
H	-0.54751738994649	5.71745586851131	6.17149029909245
H	-2.00565469990671	6.54085837054930	6.77571158986250
H	-1.41916712237050	6.87012110986387	5.13184030833070
C	-2.85391144837264	3.42642579554885	6.68100756354294
H	-3.56512392405309	2.62452181597155	6.42991888295275
H	-3.24869770482422	3.95351663732546	7.56501644624908
H	-1.89962098970153	2.95610674014225	6.95773954599997
C	-4.34550884771897	5.36551702202228	4.84939241231201
H	-4.30287925281411	6.11478635533868	4.04624745055493
H	-4.77896279893658	5.84907982523637	5.73942979486000
H	-5.03340446049239	4.56705944737400	4.53381074190759
N	-1.90301678240672	3.85954053178352	3.87797862553978

O	-0.82329683062698	1.09754523286651	4.99698912493775
Si	-2.64066178025893	4.66514272476248	5.27170683364909
Cr	-1.90310415685750	2.00005533954943	3.87804712470269
C	-2.25924156471195	6.08074624896394	1.86947052590992
H	-3.25785891035012	5.71832206309192	1.58470574438800
H	-1.79943215945895	6.54148620450336	0.98085076444827
H	-2.38604385340409	6.87046440497931	2.62474014754313
C	-0.95223263164339	3.42669834618752	1.07486132231546
H	-0.24135680075459	2.62444405161726	1.32576513559440
H	-0.55720161809198	3.95377120906028	0.19095238654870
H	-1.90667929789997	2.95680567776720	0.79797100416277
C	0.53996508933446	5.36491404158870	2.90690355131962
H	0.49754762085312	6.11402452738889	3.71020155442414
H	0.97363647282100	5.84852755862043	2.01700351804880
H	1.22756746669917	4.56614764468482	3.22231709412867
Si	-1.16510745011753	4.66518877876562	2.48439835008713
C	-4.39488035466861	0.79917000883073	2.80883810987978
C	-4.58809349035546	-0.50560948147149	2.01096572402514
H	-4.22926650973814	-0.36593489879015	0.98121699933129
H	-5.65076786780041	-0.78747841021949	1.98230589201567
H	-4.02213469313815	-1.32616585372285	2.47234005866576
C	-5.12923859493087	1.94885383348747	2.10710293024041
H	-5.00430231164567	2.88901890624153	2.66201104800225
H	-6.20254145005632	1.74082943770760	1.99495302378061
H	-4.70015258902575	2.08060051559265	1.10491645585411
C	-4.85599978318762	0.58043493096323	4.25845878499148
C	-6.04482982176904	1.12615305602174	4.76583848302614
H	-6.67176705842028	1.75629848120352	4.13484089203563
C	-6.44999721665345	0.87316637833112	6.08187498852876
H	-7.37741478863753	1.31308508945348	6.45387821189680
C	-5.67323608956792	0.06590582739099	6.91584055408338
H	-5.98780312558004	-0.13034665687756	7.94239202890359
C	-4.48611556173019	-0.48641012395367	6.42243794252277
H	-3.86769571605156	-1.11693744328505	7.06397179765509
C	-4.08525249996165	-0.23207108273882	5.10947604629373
H	-3.15320765066675	-0.66402730178370	4.74166541135033
O	-2.98308716946482	1.09753476315311	2.75934380255710

GANNIU[62]

Tetracarbonyl-((1,1,3,3-tetramethyldisiloxane-1,3-diyl)bis(diphenylphosphine))-chromium

Charge = 0
Spin Multiplicity = 1

C	5.939692	10.261805	14.811418

C	7.295912	9.958139	14.627952
H	7.703621	9.027924	15.017600
C	8.143917	10.847857	13.959644
H	9.197193	10.593070	13.831451
C	7.648364	12.057596	13.469115
H	8.310363	12.753606	12.951454
C	6.298187	12.375797	13.653547
H	5.901037	13.321534	13.280785
C	5.451548	11.486393	14.316889
H	4.404940	11.756329	14.462407
C	3.703198	10.207135	16.601883
C	4.309682	11.163233	17.435779
H	5.396196	11.260864	17.456494
C	3.533076	12.001758	18.237000
H	4.021304	12.740486	18.874928
C	2.137960	11.895755	18.224822
H	1.531880	12.552975	18.850257
C	1.526439	10.942809	17.407184
H	0.439146	10.851778	17.388239
C	2.304263	10.104453	16.601681
H	1.805151	9.367933	15.971347
C	4.799795	7.859776	12.487716
H	4.268000	7.381632	11.650337
H	5.520105	7.139153	12.895984
H	5.360906	8.716105	12.087439
C	2.469707	9.790738	13.012726
H	1.760648	10.218072	13.732873
H	1.893877	9.345210	12.185813
H	3.082227	10.603254	12.598503
C	1.183304	6.581213	16.725845
H	0.271164	7.047521	16.321847
H	1.692941	7.314933	17.363650
H	0.879449	5.732492	17.355026
C	1.351314	4.613169	14.375689
H	1.957541	4.166607	13.577517
H	0.448675	5.049858	13.919173
H	1.030964	3.816643	15.061090
C	3.670366	4.193372	17.522343
C	3.108811	2.964361	17.126758
H	3.089996	2.686297	16.072373
C	2.587460	2.081393	18.073526
H	2.159328	1.132119	17.746981
C	2.614641	2.410715	19.433334
H	2.207429	1.719984	20.173377
C	3.174521	3.624507	19.837035
H	3.211582	3.887773	20.895356

C	3.700852	4.507530	18.888182
H	4.148017	5.441074	19.222399
C	5.094824	4.241854	15.032945
C	6.017040	3.292300	15.506956
H	6.200391	3.194478	16.578066
C	6.701671	2.461839	14.618037
H	7.411825	1.728818	15.004509
C	6.482171	2.569561	13.240446
H	7.017544	1.919572	12.546673
C	5.573990	3.515214	12.759165
H	5.393278	3.607215	11.686905
C	4.885482	4.345494	13.649667
H	4.181978	5.077211	13.251302
C	6.943414	8.464254	17.619471
C	6.928039	6.736701	15.591139
C	6.591819	6.025704	18.064367
C	4.566751	7.728467	18.352690
Cr	5.743826	7.233805	16.968744
O	2.538361	7.201991	14.212133
O	7.730293	9.188811	18.099098
O	7.713386	6.397501	14.799254
O	7.200830	5.319552	18.774770
O	3.908016	8.064600	19.253864
P	4.773253	9.060579	15.620294
P	4.280447	5.387918	16.235487
Si	3.547244	8.446284	13.752958
Si	2.243619	5.977189	15.302986

GEBXIU[63]

trans-Hydrido-(tetrahydroborato-H,H')-bis(1,2-bis(dimethylphosphino)ethane-P,P')-chromium(II)

Charge = 0
Spin Multiplicity = 3

Cr	2.090562	10.337677	3.229031
P	0.497190	8.709953	3.857618
P	0.303180	11.802583	3.683909
P	3.420803	11.930787	2.101765
P	3.556002	8.829764	2.166716
C	0.881774	7.355342	5.056625
C	-0.389698	7.774581	2.528277
C	-0.960032	9.533721	4.703372
C	-0.324126	13.079314	2.499416
C	0.389000	12.803940	5.240375

C	-1.282720	10.835332	3.970284
C	4.115369	13.419640	2.950771
C	2.779032	12.674206	0.532397
C	4.987719	11.120026	1.464333
C	4.838175	7.992205	3.209295
C	3.001713	7.410642	1.115398
C	4.640650	9.733061	0.925057
H	1.324367	10.241363	1.784865
H	-0.649903	9.739334	5.740405
H	-1.825105	8.852953	4.742938
H	-1.715397	10.625871	2.979101
H	-2.006182	11.456213	4.521154
H	5.674950	11.041805	2.321903
H	5.473110	11.752559	0.704357
H	4.061911	9.813241	-0.008847
H	5.538286	9.134176	0.706107
H	-0.029033	6.815327	5.353849
H	1.358741	7.789457	5.944941
H	1.585101	6.647160	4.597995
H	0.316988	7.135570	1.985327
H	-0.823741	8.484973	1.813067
H	-1.187610	7.150338	2.956021
H	0.400138	13.900450	2.415056
H	-1.284037	13.490697	2.845260
H	-0.460109	12.625382	1.509218
H	-0.556066	13.336921	5.418665
H	1.208155	13.530642	5.158123
H	0.610903	12.143641	6.088207
H	4.596750	13.104516	3.885693
H	3.301817	14.115137	3.197655
H	4.848795	13.935895	2.314289
H	3.550238	13.290624	0.047952
H	1.901065	13.295839	0.745372
H	2.469685	11.871208	-0.148800
H	4.343670	7.306425	3.910004
H	5.376787	8.743823	3.800028
H	5.546164	7.428690	2.584608
H	2.566422	6.624302	1.746336
H	3.849945	6.985622	0.558496
H	2.239188	7.756927	0.405692
B	3.262803	10.482407	5.416829
H	2.855398	11.438865	4.731663
H	2.964521	9.422677	4.841932
H	2.694365	10.517120	6.499865
H	4.481558	10.555534	5.501669

GEKBIH[64]

cis-bis(η^4-1-(Di-isopropylamino)borole)-dicarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	0.334265	2.120965	6.700304
C	1.615419	1.204238	5.740632
C	-0.321750	0.531982	7.378899
O	2.499912	0.628073	5.242546
O	-0.746695	-0.504144	7.707893
C	0.205176	3.313773	4.696185
C	-0.742261	3.728730	5.667205
C	-1.633678	2.649428	5.990588
C	-1.296439	1.511293	5.198046
B	-0.270948	1.943834	4.095487
N	0.098501	1.322804	2.871718
C	1.068666	1.974940	1.959582
C	0.407627	2.464166	0.660362
C	2.298335	1.101609	1.663168
C	-0.503126	0.058715	2.377499
C	-2.019117	0.177120	2.155667
C	-0.149024	-1.146269	3.260589
C	1.852793	1.797375	8.359041
C	2.046365	3.020466	7.634486
C	0.924368	3.877147	7.875258
C	-0.026581	3.235233	8.714494
B	0.640791	1.970377	9.342282
N	0.302447	1.199022	10.489671
C	1.169666	0.080658	10.929958
C	0.427575	-1.263033	11.016525
C	1.902412	0.394216	12.245277
C	-0.854262	1.503715	11.367619
C	-2.199010	1.317718	10.650435
C	-0.746541	2.889379	12.023947
H	1.007106	3.990640	4.396889
H	-0.812917	4.721265	6.103572
H	-2.451831	2.710666	6.705187
H	-1.857264	0.585691	5.323736
H	1.424428	2.863651	2.498874
H	0.029339	1.626090	0.055407
H	1.138481	3.010850	0.045824
H	-0.432617	3.138268	0.879184
H	2.034069	0.201534	1.087686
H	2.788102	0.785709	2.593536

H	3.024473	1.671299	1.064280
H	-0.054044	-0.128853	1.390491
H	-2.551657	0.347153	3.101724
H	-2.412000	-0.748164	1.707467
H	-2.250792	1.012137	1.479758
H	-0.578198	-1.045848	4.267245
H	0.939623	-1.247981	3.364897
H	-0.542973	-2.072871	2.816260
H	2.586318	0.994676	8.268176
H	2.920665	3.289709	7.045134
H	0.840032	4.881736	7.467878
H	-0.975278	3.728643	8.927228
H	1.934355	-0.021919	10.147625
H	-0.332912	-1.262403	11.812130
H	1.140781	-2.068458	11.247207
H	-0.067053	-1.499617	10.065501
H	1.199818	0.503159	13.085592
H	2.481399	1.324505	12.157372
H	2.595472	-0.422167	12.498343
H	-0.824555	0.765500	12.183420
H	-2.308712	2.027937	9.818852
H	-3.031888	1.483219	11.350683
H	-2.286296	0.301861	10.241838
H	-0.786975	3.692084	11.274578
H	0.198287	2.987058	12.576687
H	-1.576338	3.042141	12.730875

HAGJEG[65]

trans-bis(1,3-Di-isopropyl-4,5-dimethyl-2,3-dihydro-1H-imidazol-2-ylidene)-nitrido-diphenyl-chromium(V)

Charge = 0
Spin Multiplicity = 2

Cr	0.15872589877950	4.49249551793922	7.55251341847485
N	-2.46049882805821	6.16137112903200	8.13633941031226
N	-0.80720919179855	6.97141480368136	9.27999972871557
N	2.51564242344838	2.67074008241272	6.48200364466957
N	2.64811590271525	2.87081946237879	8.63671765521453
N	-0.54993474547160	4.11929254275272	6.23135823766361
C	1.43365620470036	6.07700509206946	6.89796551756227
C	2.82322661895858	6.19125047974556	7.12522689543140
H	3.33881494322910	5.43025110345420	7.71738590528558
C	3.59975769444973	7.24127130512058	6.61241193719607
H	4.67155712207435	7.28094832650823	6.82729731114837

C	3.01043685967880	8.22812560981791	5.81826427394683
H	3.60881067055048	9.04419409547699	5.40701380469866
C	1.63796820128168	8.14607424240069	5.55430632493266
H	1.15711449891401	8.90284765862149	4.92763452393534
C	0.87846897289824	7.09862420681065	6.08968092508321
H	-0.19109154605456	7.07590483516516	5.86327623013978
C	-0.73113976479496	3.09622082019593	8.90290810960500
C	-1.33799969957733	3.39082636323125	10.14400680766956
H	-1.36009026331208	4.42301630887408	10.50453452502505
C	-1.93977589624326	2.41501803297161	10.95299176221371
H	-2.38797149947070	2.70153683556134	11.90874865233743
C	-1.97871073694880	1.08225164926381	10.53568851750391
H	-2.45196813482662	0.31749108223334	11.15561420085536
C	-1.40367102183017	0.74770320586059	9.30370543562204
H	-1.42979370811194	-0.28818982395238	8.95321974181959
C	-0.79359787662125	1.73453521995634	8.51996485660530
H	-0.34837891477355	1.43007889631164	7.56896250452568
C	1.89451676176427	3.25581782635617	7.55680096471687
C	3.62897568895405	1.92379227842445	6.88614395197764
C	3.71362540386814	2.04913182362513	8.24973724553891
C	4.54527805612966	1.16642757390593	5.98116731846881
H	5.20797367426499	0.52776624557078	6.57784119736194
H	5.18151698419709	1.83373206629772	5.38161177748490
H	4.00304326340960	0.51211999554745	5.28646499404167
C	4.70795778956909	1.41448135125640	9.16660387297939
H	5.52817476635526	0.98850041182775	8.57626883512583
H	4.26621489696050	0.59640926659120	9.75513010488997
H	5.15185057362213	2.12841929211906	9.87239217662521
C	2.03193709254150	2.83145420431651	5.08670674856235
H	1.21950092799789	3.55938671890327	5.19377261874765
C	2.35350803667550	3.33283997880867	10.01541118374164
H	1.41584570129270	3.89400664437221	9.89433016079637
C	-1.12610817528755	5.97315298968405	8.39416725302638
C	-1.91384688096316	7.78299680865717	9.55567115523799
C	-2.95831302367125	7.27237786537761	8.82697985549797
C	-1.92093310734812	8.98224680247354	10.44760706652619
H	-2.95345995510227	9.31977760178964	10.59776114259433
H	-1.35576069192842	9.82319228725532	10.01897552118284
H	-1.50100264121138	8.77385094893098	11.44081659945121
C	-4.36461205944958	7.77643608831994	8.77303124692116
H	-4.40058335815138	8.80647070119808	9.14816380837942
H	-5.04790939107832	7.17546006999620	9.39154996066134
H	-4.76603317274353	7.78762041794976	7.75178632246277
C	-3.23918814557810	5.27317183796083	7.23501872751217
H	-2.54171886330625	4.45218240740332	7.03614396920720
C	0.53879614179706	7.08849484280628	9.89234753123454

H	1.12492752129529	6.33233645722647	9.35151560863079
C	1.41551351600645	1.53960767125372	4.54022530893460
H	0.63457079877536	1.16517590957821	5.21603029612112
H	2.15551301673510	0.74220756440823	4.38471293285670
H	0.94746641669084	1.75056728111529	3.56784133980408
C	3.08877659676389	3.43594645043409	4.15737047946401
H	3.54094387537381	4.33003656098838	4.60806581519020
H	2.59744820076597	3.74073484716437	3.22230397722147
H	3.88504431825125	2.72729358532757	3.89548605394721
C	2.05908343181945	2.17441540217121	10.97190008196796
H	1.28183280196684	1.51969068225559	10.55666336513077
H	1.68750105369838	2.58498993265053	11.92114247015235
H	2.95505956759721	1.58079496909204	11.19505261722708
C	3.42501727149362	4.28900402182820	10.55195646756595
H	3.57700172614287	5.13775969929732	9.87212178196497
H	4.39156448625987	3.79258451430411	10.70782213323796
H	3.09768587897654	4.68226335912540	11.52442849368978
C	-4.47845753526018	4.67995431141008	7.91241330214769
H	-4.22287759229848	4.25838195836557	8.89430481581101
H	-4.85865294345261	3.86207590977811	7.28386888746792
H	-5.29301372004119	5.40475826808375	8.03744221616402
C	-3.54101004701822	5.95343362817407	5.89665602319045
H	-2.60890770310759	6.28649087584218	5.42070590443676
H	-4.21121668756934	6.81760585036089	6.00158279060042
H	-4.02685000018623	5.23168758676792	5.22449004195444
C	1.19972932932926	8.44164102683756	9.61701181598915
H	1.15767345214660	8.68281882535458	8.54696757536720
H	2.25713329786177	8.38328628009227	9.91007417581034
H	0.74073867858454	9.25611150787384	10.19186225682501
C	0.52722871747077	6.72537138189304	11.38132452255907
H	0.10929542987251	5.72290289069702	11.54477908013600
H	-0.05107199307640	7.44028887336892	11.98081745125876
H	1.55806436076701	6.73418948525867	11.76206474802687

HAJVET[66]

(η^6-Cycloheptatriene)-tricarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	0.783382	0.748058	5.994157
O	1.680765	-0.199479	3.287913
O	2.350407	-1.448591	7.328989
O	-1.459186	-1.171774	5.436827
C	1.354818	0.197278	4.341066

C	1.743470	-0.597322	6.806542
C	-0.605615	-0.407136	5.681431
C	0.528082	1.555086	8.200294
C	-0.565888	1.844967	7.395612
C	-0.549795	2.541307	6.141931
C	0.576476	2.888603	5.368773
C	1.954305	2.622079	5.664913
C	2.472315	2.154604	6.865373
C	1.812024	2.351835	8.209963
H	0.362569	0.848881	9.015048
H	-1.523806	1.396338	7.666582
H	-1.519012	2.690120	5.664008
H	0.366809	3.271460	4.369021
H	2.632313	2.678885	4.810892
H	3.510451	1.820153	6.852477
H	2.471265	1.972567	8.999906
H	1.627162	3.419072	8.419993

HARZAD[67]

((η^6-2-(3-(diphenylphosphino)-2-methylprop-1-en-1-yl)phenyl)(diphenyl)phosphine)-dicarbonyl-chromium benzene solvate

Charge = 0
Spin Multiplicity = 1

Cr	1.931161	6.758305	9.404353
P	3.620469	5.557379	10.403193
P	3.346947	9.860998	10.980570
O	0.311393	6.600322	11.921926
O	0.476015	4.244104	8.661434
C	4.984134	6.651653	11.070309
H	4.507471	7.340297	11.788442
H	5.710278	6.041888	11.626080
C	5.679916	7.446978	9.995375
C	7.180554	7.494546	10.091125
H	7.620468	8.095456	9.284244
H	7.604374	6.478108	10.046413
H	7.493717	7.922640	11.057511
C	5.030435	8.098862	9.010888
H	5.629662	8.629428	8.263246
C	3.568320	8.117620	8.761498
C	3.074763	7.430712	7.605767
H	3.774692	6.864801	6.993649
C	1.697072	7.427227	7.296107
H	1.335746	6.843425	6.450282

C	0.782091	8.139061	8.106732
H	-0.284895	8.114752	7.893145
C	1.264201	8.831868	9.241652
H	0.556558	9.353576	9.883392
C	2.659467	8.886813	9.558328
C	0.977256	6.665100	10.952964
C	1.075340	5.219180	8.950224
C	4.597244	4.324446	9.413013
C	5.695922	3.654658	9.980878
H	5.975424	3.837687	11.020034
C	6.434489	2.737526	9.231340
H	7.286317	2.228225	9.685552
C	6.080580	2.467601	7.903893
H	6.656774	1.748389	7.319330
C	4.984083	3.118305	7.334272
H	4.695729	2.907587	6.302967
C	4.248510	4.041727	8.086401
H	3.390419	4.546754	7.641781
C	3.178041	4.535455	11.877378
C	2.638948	3.251811	11.684692
H	2.547451	2.844209	10.676528
C	2.223458	2.482657	12.773438
H	1.810065	1.486756	12.604450
C	2.340239	2.984094	14.074347
H	2.019201	2.381934	14.925860
C	2.870076	4.261039	14.276021
H	2.964542	4.662252	15.286636
C	3.281901	5.033720	13.185475
H	3.685507	6.029859	13.369307
C	4.061249	11.330984	10.109409
C	3.809225	11.672934	8.771307
H	3.134614	11.062648	8.168993
C	4.417497	12.793969	8.196887
H	4.211710	13.045707	7.154783
C	5.280463	13.592351	8.953567
H	5.754264	14.466736	8.504270
C	5.539533	13.260356	10.287875
H	6.217049	13.874271	10.884046
C	4.941830	12.133260	10.856940
H	5.164559	11.870287	11.894105
C	1.819916	10.583104	11.742290
C	1.297628	9.927015	12.870554
H	1.781018	9.020812	13.240796
C	0.165707	10.421083	13.524675
H	-0.229810	9.895632	14.395504
C	-0.449454	11.591866	13.070614

H	-1.327124	11.985180	13.586292
C	0.069523	12.261437	11.957260
H	-0.403260	13.178393	11.600528
C	1.194574	11.759996	11.296431
H	1.590875	12.292937	10.430753

HAWDUF[68]

((η^6-1,2,3,4,4a,8a)-1-(t-Butyl-dimethylsiloxy)-2,3-diethyl-4-methoxynaphthalene)-dicarbonyl-(triphenylphosphine)-chromium(0)

Charge = 0
Spin Multiplicity = 1

C	3.343936	14.325626	2.646559
O	3.805545	15.031439	1.579520
Si	3.492931	16.530337	0.825015
C	3.066229	16.114332	-0.960419
H	3.793339	15.388960	-1.355170
H	3.121925	17.017086	-1.586991
H	2.060410	15.687598	-1.077823
C	2.101626	17.559261	1.659984
C	2.029355	18.905218	0.900127
H	2.965646	19.477620	0.976898
H	1.798660	18.768911	-0.167404
C	2.410219	17.845620	3.142436
H	3.376513	18.355151	3.275681
H	2.420747	16.925867	3.745401
H	1.631984	18.505455	3.564609
C	0.730016	16.863816	1.556359
H	0.448020	16.656580	0.513407
H	-0.050495	17.516922	1.984806
H	0.703732	15.913266	2.107575
C	3.995424	14.435894	3.905241
C	5.167032	15.394294	4.045113
H	5.407572	15.516592	5.107454
H	4.820607	16.383721	3.705395
C	6.453687	15.034974	3.286476
H	7.178755	15.857235	3.380564
H	6.258676	14.867527	2.221045
H	6.912761	14.127715	3.696844
C	3.447897	13.724844	5.035033
C	4.051403	13.866336	6.417964
H	5.147194	13.847221	6.341936
H	3.761455	12.988150	7.008435
C	3.613631	15.145245	7.155961

H	4.081770	15.184256	8.149976
H	2.524630	15.180174	7.296027
H	3.905242	16.053993	6.610845
C	2.301301	12.906970	4.864481
O	1.748810	12.251356	5.951040
C	0.605932	12.925549	6.525131
H	0.230990	12.262806	7.313259
H	-0.183293	13.089478	5.775339
H	0.894614	13.892928	6.962842
C	1.660188	12.757042	3.583467
C	0.497217	11.947030	3.395517
H	0.118390	11.379829	4.243818
C	-0.133535	11.891208	2.173131
H	-1.029477	11.280679	2.052646
C	0.386512	12.603439	1.062680
H	-0.110355	12.535638	0.094103
C	1.529784	13.360179	1.196500
H	1.947187	13.889858	0.342338
C	2.181727	13.487224	2.458673
Cr	3.939099	12.246417	3.400709
C	4.862506	12.093030	1.852426
O	5.493748	12.079805	0.851761
C	5.490654	11.965703	4.274129
O	6.510649	11.814117	4.853076
P	3.652541	9.919651	3.493923
C	2.925784	9.039944	2.021654
C	2.861088	7.635592	1.967787
H	3.216525	7.038293	2.809068
C	2.354806	6.990422	0.838399
H	2.312140	5.900031	0.811318
C	1.913704	7.738964	-0.259997
H	1.525093	7.233916	-1.146097
C	1.980780	9.133088	-0.217923
H	1.644771	9.723679	-1.072077
C	2.484441	9.777969	0.918010
H	2.542133	10.866685	0.946578
C	2.628340	9.284917	4.902482
C	3.082465	9.513400	6.213402
H	4.032886	10.024323	6.378124
C	2.332296	9.095394	7.312915
H	2.709501	9.269867	8.322220
C	1.096038	8.468627	7.123152
H	0.505650	8.146630	7.982835
C	0.620954	8.261697	5.825882
H	-0.345449	7.779739	5.665810
C	1.383849	8.662386	4.723323

H	1.002600	8.483083	3.718002
C	5.207880	8.896196	3.652043
C	5.385604	7.894297	4.617653
H	4.604359	7.692446	5.349705
C	6.562030	7.136189	4.655309
H	6.679213	6.364488	5.418542
C	7.576017	7.361203	3.722437
H	8.492645	6.769570	3.751079
C	7.404860	8.351083	2.748698
H	8.187370	8.535412	2.010328
C	6.235081	9.111952	2.716795
H	6.123565	9.877960	1.949834
C	5.129163	17.458493	0.836831
H	5.426946	17.789689	1.841337
H	5.069347	18.346376	0.190099
H	5.927217	16.812003	0.443103
H	1.226634	19.527687	1.332242

JILVAB[69]

Tetracarbonyl-norbornadienyl-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	1.750998	5.765518	7.933556
C	2.173835	7.558148	7.809975
O	2.434842	8.692928	7.730360
C	0.707146	6.285929	9.412529
O	0.027703	6.678966	10.269903
C	2.563853	5.622279	6.239907
O	3.012034	5.609489	5.167486
C	0.173703	5.890005	6.982388
O	-0.821376	5.973165	6.378118
C	3.834132	4.953925	8.506825
C	3.577254	3.474108	8.154481
C	3.514449	2.853088	9.576952
C	2.455388	3.875925	10.072067
C	3.144798	5.200963	9.685291
C	1.389180	3.731369	8.966312
C	2.078560	3.484890	7.787874
H	4.623177	5.567181	8.079396
H	4.250315	3.031790	7.415005
H	4.468512	2.923873	10.120385
H	3.145940	1.816414	9.578774
H	2.093869	3.804482	11.101502

H	3.290430	6.044899	10.354801
H	0.329091	3.567377	9.141730
H	1.661224	3.090280	6.864892

KUVGEN[70]

(η^4-Norbornadiene)-(ethoxy(p-tolyl)methylidene)-tricarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	8.343514	8.545205	4.849775
C	8.389263	7.703027	6.530613
C	8.071632	9.621009	3.330612
C	7.851140	10.043775	5.799378
O	6.094511	6.849277	5.472634
C	6.508027	7.862936	4.685886
C	4.689537	6.392762	5.520119
C	4.501626	5.666062	6.835195
C	5.500362	8.331056	3.690631
C	4.910380	9.601712	3.777448
C	3.998104	10.032926	2.811158
C	3.661401	9.228632	1.713278
C	4.263825	7.961565	1.623626
C	5.154848	7.512207	2.596426
C	2.696144	9.702881	0.656102
O	8.409596	7.268648	7.611758
O	7.935203	10.363724	2.440866
O	7.548267	10.998407	6.409059
C	10.524353	8.467150	5.383786
C	10.816533	7.003650	4.981022
C	9.470321	6.576739	4.360732
C	9.345738	7.284553	3.176245
C	10.613533	8.154994	3.050730
C	10.403966	9.185454	4.183956
C	11.667164	7.217586	3.700125
H	4.032291	7.267213	5.431543
H	4.514414	5.729590	4.662173
H	3.470716	5.288228	6.895033
H	4.673882	6.337928	7.687034
H	5.185787	4.810429	6.916492
H	5.162173	10.256160	4.613163
H	3.543995	11.021802	2.910788
H	4.028976	7.312606	0.776042
H	5.605059	6.522325	2.496110
H	2.271885	10.682303	0.913526

H	1.864705	8.993232	0.527467
H	3.193026	9.795538	-0.322205
H	10.782784	8.893037	6.350767
H	11.209857	6.354724	5.769056
H	8.878454	5.717916	4.668340
H	8.639872	7.086281	2.373638
H	10.818308	8.565212	2.057532
H	10.556188	10.256034	4.069451
H	11.829991	6.290240	3.129282
H	12.625705	7.720068	3.899148

LIBCRB[71]

tetrakis(bis(*t*-Butyl)-methoxo)-chromium(IV)

Charge = 0
Spin Multiplicity = 3

Cr	-2.275714	4.709011	4.528912
O	-2.373246	3.719695	6.023211
O	-3.770996	5.697234	4.430505
C	-2.934379	2.475678	6.482499
C	-4.306364	2.774287	7.208207
C	-4.898777	1.548711	7.929545
C	-4.204853	3.935085	8.216641
C	-5.317456	3.175264	6.111830
C	-1.786783	1.668622	7.215241
C	-0.513122	1.752560	6.350195
C	-1.443115	2.212575	8.612487
C	-2.137740	0.166781	7.308133
C	-4.229990	6.941337	3.869265
C	-4.954370	6.643117	2.496491
C	-3.857050	6.242570	1.486222
C	-5.963116	5.482456	2.596876
C	-5.675304	7.868793	1.903844
C	-4.964237	7.747622	5.016322
C	-4.100847	7.662943	6.290993
C	-5.056907	9.249707	4.666305
C	-6.361813	7.202981	5.357534
H	-3.187594	1.861720	5.596635
H	-4.319279	1.253220	8.814436
H	-5.913171	1.802839	8.275237
H	-4.987366	0.678794	7.262222
H	-3.653325	3.657731	9.123465
H	-3.710957	4.806539	7.769588
H	-5.217670	4.237188	8.524828

H	-5.486181	2.346785	5.406773
H	-6.285900	3.421703	6.573894
H	-4.980009	4.051163	5.543397
H	-0.699187	1.378398	5.331987
H	-0.140166	2.780080	6.274197
H	0.274549	1.125796	6.795005
H	-2.248408	2.038645	9.337939
H	-0.543287	1.704782	8.993673
H	-1.231315	3.290020	8.576223
H	-1.247565	-0.386226	7.645017
H	-2.945482	-0.050297	8.014053
H	-2.422985	-0.236694	6.323946
H	-3.344046	7.555648	3.617310
H	-3.151571	7.070987	1.318932
H	-4.318238	5.997130	0.517100
H	-3.289203	5.366285	1.823469
H	-6.872182	5.761756	3.143792
H	-6.267350	5.177638	1.583696
H	-5.518457	4.612269	3.095132
H	-6.560495	8.164142	2.482944
H	-5.007917	8.738722	1.815812
H	-6.020496	7.614828	0.889242
H	-3.082638	8.038109	6.106805
H	-4.547159	8.288520	7.078753
H	-4.024525	6.635085	6.662917
H	-5.394902	9.802156	5.556400
H	-4.072327	9.653281	4.382496
H	-5.761718	9.467345	3.857752
H	-6.325808	6.125153	5.567439
H	-7.086243	7.378113	4.551552
H	-6.744168	7.709166	6.257765
O	-2.177673	3.720121	3.034365
O	-0.780966	5.697992	4.627515
C	-1.616597	2.476087	2.575034
C	-0.322617	6.942077	5.189329
C	-0.244206	2.774486	1.850067
C	-2.764079	1.669721	1.841409
H	-1.364023	1.861780	3.460825
C	0.401563	6.643396	6.562105
C	0.411390	7.749268	4.042720
H	-1.208860	7.555872	5.441526
C	0.348218	1.548852	1.128845
C	-0.345080	3.935365	0.841704
C	0.766456	3.175106	2.946987
C	-4.038072	1.753701	2.705966
C	-3.106915	2.214519	0.444283

C	-2.413556	0.167817	1.747958
C	-0.695923	6.241795	7.571766
C	1.410773	5.483169	6.461391
C	1.121810	7.869026	7.155717
C	-0.452220	7.665479	2.768151
C	0.504003	9.251121	4.393725
C	1.808927	7.204959	3.700813
H	-0.230990	1.253602	0.243675
H	1.362816	1.802781	0.783604
H	0.436326	0.678856	1.796119
H	-0.896821	3.658383	-0.065102
H	-0.838450	4.807104	1.288772
H	0.667911	4.236874	0.533499
H	0.934523	2.346520	3.652073
H	1.735218	3.421284	2.485439
H	0.428971	4.051097	3.515257
H	-3.852537	1.378947	3.724058
H	-4.410675	2.781320	2.782347
H	-4.825785	1.127442	2.260521
H	-2.301356	2.040663	-0.280901
H	-4.006790	1.707320	0.062421
H	-3.318263	3.292038	0.481069
H	-3.303713	-0.384748	1.410304
H	-1.605474	-0.049180	1.042406
H	-2.128993	-0.236194	2.732124
H	-1.401983	7.069702	7.739128
H	-0.234969	5.996253	8.540973
H	-1.263132	5.365329	7.233935
H	2.319956	5.763179	5.915048
H	1.714711	5.177830	7.474499
H	0.966655	4.613120	5.962407
H	2.007051	8.165059	6.577046
H	0.454051	8.738634	7.244057
H	1.466801	7.614605	8.170273
H	-1.470427	8.040427	2.952808
H	-0.006105	8.291707	1.980793
H	-0.528527	6.637907	2.395453
H	0.841714	9.804170	3.503896
H	-0.480533	9.654441	4.678040
H	1.209010	9.468313	5.202217
H	1.772912	6.127275	3.490176
H	2.533535	7.379567	4.506743
H	2.191063	7.711778	2.800844

NIDHAJ[72]

Nitrido-(N,N'-bis(salicylidene)ethylenediamine)-chromium(V)

Charge = 0
Spin Multiplicity = 2

Cr	4.52458782409923	2.34429436522947	0.49279432806952
O	6.40980547507858	2.44020943664538	0.86224235002649
O	4.37066795170433	1.26645856337063	2.08536526114413
N	3.85290684994411	3.70019459072172	0.81230497739790
N	4.94203400096939	2.56160611726606	-1.46792950951410
N	3.02717203306090	1.24155699798147	-0.30452962922689
C	7.31732273177636	3.03758835959857	-1.30596273142704
C	7.42013948763348	2.82571103605284	0.10863305676592
C	8.68950883346150	3.00809478802200	0.71364422716224
C	9.79277534984651	3.38749006049945	-0.03760871118351
C	9.69172831792751	3.59673746606342	-1.42807721444551
C	8.46606053406680	3.41510880667880	-2.04529211246826
C	6.08646075898771	2.84733593338912	-2.01370977305511
C	3.74097056040166	2.41279150778259	-2.30137581408323
C	2.98689131323552	1.19556611695065	-1.77860355433903
C	2.11151458790135	0.61681221111703	0.37697547568746
C	2.10914235219161	0.45000871578863	1.79931813275503
C	3.26694739832552	0.75430582560774	2.59183968831136
C	3.22691577586282	0.43450624803745	3.97270671618032
C	2.09192043615910	-0.12204974048268	4.54441619309625
C	0.94962987817575	-0.40930593385257	3.76872113470894
C	0.97339887730296	-0.13677564272990	2.41209475567857
H	8.77139401956843	2.84285517719044	1.78882097328446
H	10.75446549573914	3.52500835890151	0.46054638769773
H	10.56574006863636	3.89465950067993	-2.00698388823805
H	8.36276034223210	3.56500065658675	-3.12250860877507
H	6.12373563359240	2.95584037011101	-3.10678950740982
H	3.12841924055537	3.31900803318797	-2.17703164718787
H	4.00008386503225	2.29955430585067	-3.36390168961727
H	3.49669955160446	0.27642323787082	-2.10850330932302
H	1.95042331298201	1.16899382867980	-2.14492834754509
H	1.28449486339171	0.15070380759670	-0.17687853887663
H	4.11141245324862	0.65053591612314	4.57355663685848
H	2.08685728130760	-0.34166983731378	5.61384842235072
H	0.06563444687430	-0.84875400483052	4.23061096249379
H	0.10824109712257	-0.37029518037231	1.78732390704619

NEVSAI[73]

Di-isopropylamido-nitrosyl-bis(trimethylsilylmethyl)-chromium(II)

Charge = 0
Spin Multiplicity = 1

Cr	-1.35467688864916	6.40261014882658	4.44907600590178
Si	-0.50353686621782	6.57571559133350	7.75149769885870
Si	1.19048890801217	7.24624775546190	2.15926344214610
O	-1.79999889158285	9.19393320598146	4.70583423144235
N	-1.60880343245268	8.00464229124276	4.59469116480475
N	-2.74472276955442	5.83392866460173	3.48267158334873
C	-1.46486134576499	5.75128554809306	6.35105011405506
C	0.42659564171072	6.26802339433125	3.57542819306912
C	1.30054175772528	6.93602174748612	7.29826532671057
C	-1.36019185869850	8.19080942869354	8.23362548698434
C	-0.49250049798240	5.41166212451039	9.25219270088396
C	3.01210728268762	6.74907839172180	1.96133316054041
C	1.11127254073709	9.09977941091296	2.51956202865150
C	0.30469854111113	6.86663887566925	0.53146454166844
C	-3.95919789753630	6.45957056665610	2.92625897012731
C	-3.61654233333564	7.52361643617285	1.87698639378368
C	-4.85467482387522	7.02810558339224	4.03622344185586
C	-2.59377352775761	4.36274030009928	3.35307161612872
C	-2.43419056809256	3.91784526536779	1.89220013084098
C	-3.70217167425921	3.58374631601349	4.07621113937003
H	-1.19211677812722	4.67947435100464	6.25300916286333
H	-2.53193403895166	5.79239464088406	6.63392461075392
H	0.98758978605507	6.51973617624434	4.50384349447314
H	0.53191152488243	5.17729337845927	3.39965677143499
H	1.38004803309450	7.71108923476895	6.52158462363316
H	1.81450675768451	6.03291644322347	6.93463005323821
H	1.84705710527454	7.29623398446068	8.18385223136316
H	-1.37496562555063	8.89941858415113	7.39287142177335
H	-0.84301271650022	8.67157779009617	9.07834340331761
H	-2.40231176227649	8.00677160544541	8.53669392557615
H	0.01657840107217	4.46488142991380	9.01494904935099
H	-1.51726123442409	5.17161219263975	9.57425305618059
H	0.03215068781220	5.87310231791504	10.10364997357184
H	3.48481431424250	7.30665033811448	1.13738851104677
H	3.10932779164581	5.67492163043000	1.74062426123256
H	3.58220544195338	6.95644229240168	2.87988354320773
H	1.58516606659436	9.66977122335322	1.70535875707603
H	1.64193830136476	9.34450336958217	3.45230770378442
H	0.07387719269961	9.44741415611117	2.62477505705594
H	0.77361618523325	7.41549162400188	-0.29989129608876
H	-0.75483035435515	7.15622289883819	0.57576058844044
H	0.35500801315080	5.79329022770431	0.29301149304882
H	-4.52478967570295	5.66150655506046	2.41596910106050

H	-3.03810187138388	8.34377595749097	2.32423328101255
H	-4.54087699455726	7.94393525435035	1.45382084455256
H	-3.02731675643770	7.09133578080371	1.05679585765889
H	-4.33881751622708	7.83568293052239	4.57373362199030
H	-5.12685156858868	6.24973745333437	4.76175872646304
H	-5.77990076930394	7.43507915316088	3.60203331621660
H	-1.63833940679085	4.11356457131892	3.86760983317308
H	-3.35593123510262	4.10288792010526	1.32115298897470
H	-2.22442042544019	2.83951210743788	1.84786171955982
H	-1.60992940215432	4.45626961281901	1.40695296402369
H	-4.67890062228179	3.76137254487899	3.60335221913884
H	-3.76681469544107	3.87481427000193	5.13306100740373
H	-3.49637344938674	2.50498495240306	4.02474675126490

NOHKUQ[74]

tris(Dicyclohexylamido)-chromium(III)

Charge = 0
Spin Multiplicity = 4

Cr	7.74819527996947	4.68695138563842	8.21600202888850
N	9.55766345310971	5.22464870094172	8.20579578527413
N	7.26686128825351	2.91212078727472	7.81248198231911
N	6.38676457160609	5.91686241575354	8.62704656656708
C	6.77430644262524	2.07244203731534	8.92075488729284
C	7.61668157324847	0.80378217022882	9.17511342051873
C	7.10982828254923	0.01809709604335	10.39489075656144
C	5.62539902015122	-0.34417072047012	10.25407772249590
C	4.77387366110209	0.90740446567356	10.00316428738623
C	5.27969572530237	1.70494345862330	8.79055844264086
C	7.28766886821985	2.27215666862131	6.48568996391776
C	6.54129087213717	3.10350089007307	5.42599121850814
C	6.53937555645629	2.42118217223451	4.04974539404878
C	7.96259351679838	2.10129695841705	3.57273396823927
C	8.72487492792518	1.27920824143825	4.62062572747573
C	8.71778955696712	1.96609208282701	5.99440037436499
C	10.11516842206969	6.21119699921227	7.26364832005033
C	10.22196305170856	7.62433020461980	7.87831811416538
C	10.86123773258788	8.62410966420600	6.90310891085587
C	10.07946202493102	8.68724097124369	5.58399326919404
C	9.92953109342963	7.29200380688223	4.96239927331398
C	9.31975579551140	6.28581561101539	5.95198685827473
C	10.56903981936975	4.71781411289917	9.14900329162302
C	11.47889979190442	3.63957477812819	8.51803818650558
C	12.55445553082086	3.15033864604925	9.49915842507988

C	11.92807223793962	2.61659120776157	10.79420177476008
C	9.94071407180560	4.16236276570716	10.43430610133792
C	10.99986225993407	3.66103113903175	11.42890234027358
C	5.50389379712523	6.33857578739539	7.52411927281955
C	4.05994377707348	5.80678197141186	7.66086957775819
C	3.18865998040706	6.18778479596384	6.45378255026490
C	3.19022453217987	7.70303131468989	6.21155767796560
C	4.62138736633399	8.23610171543036	6.06465394875967
C	5.49069729305554	7.86210093362481	7.27538394784991
C	6.05630315417472	6.45532196206267	9.95803414477782
C	7.07629859750811	7.50373062762940	10.44753187617289
C	6.71057524288522	8.06437695965578	11.83046834614537
C	6.54975651684737	6.94745584032905	12.86999545128373
C	5.53918525393352	5.89373062435631	12.39663266873598
C	5.90710014503292	5.34230383406984	11.01082085954828
H	6.86098239751822	2.69314738948943	9.83395858942255
H	7.57898237807964	0.15167072050559	8.28519665628169
H	8.67037573156549	1.09356515550569	9.31218204099118
H	7.71659854128325	-0.89063441832372	10.53614890034925
H	7.24739190692535	0.63164627473456	11.30326759678369
H	5.50205847409074	-1.04340917528757	9.40775609830183
H	5.27226526756799	-0.87230058674559	11.15414239847004
H	3.71770704769086	0.62954365986261	9.85555163301893
H	4.80389734171990	1.55067611005247	10.90076524073799
H	4.69821466555849	2.63151666495888	8.66452069961233
H	5.12830121766187	1.10452694614251	7.87713552088551
H	6.75992475048602	1.30169948554465	6.55586418205592
H	5.51220660611348	3.29130759587332	5.76929055232283
H	7.03181168391097	4.09181739840439	5.34792252017416
H	5.96194318871435	1.48134783634961	4.11628072042116
H	6.02034965580048	3.05552608326602	3.31328667104179
H	7.93148315710047	1.56334557922574	2.61160613097821
H	8.50458312704144	3.04563286449625	3.38726779120531
H	8.25557527690359	0.28249468162606	4.70879342962814
H	9.76222307838420	1.10565239728851	4.29128143748498
H	9.27446170412388	2.91800926844760	5.94469256276644
H	9.23263950673706	1.34290444456667	6.74096007672151
H	11.14417369523794	5.89446973556476	6.99406781432664
H	9.20320219205186	7.95750797440769	8.13918911993017
H	10.79561365410326	7.58419408435600	8.81765241794413
H	10.91432711449323	9.62308137339926	7.36524099563778
H	11.90238465912948	8.31874005806691	6.69454377510008
H	9.07695229214761	9.10726658054125	5.77938257259677
H	10.57437500960901	9.36918313638536	4.87411508517350
H	9.31146182879740	7.34256009788688	4.05186983169944
H	10.92342081389650	6.92843674430990	4.64590509398313

H	9.27007399958567	5.28419520149368	5.49647450958702
H	8.28156645141263	6.58726187760742	6.18592335082533
H	11.22471049469832	5.56231485779338	9.44980063158257
H	10.83801748541632	2.79666741026362	8.20744939888581
H	11.95138064401836	4.03465046826862	7.60502731882326
H	13.17428426655214	2.37322481991743	9.02358409685618
H	13.23333244132520	3.98706560951601	9.74434712244515
H	11.34650111557101	1.70537231285368	10.56756450446820
H	12.71261470519953	2.31996525897036	11.50870236352908
H	9.31485283790051	4.93972906507909	10.90101864041813
H	9.27101496097917	3.32476649164262	10.16296263892652
H	10.50649023981054	3.24513833375630	12.32177203813408
H	11.60285425851385	4.51884207119226	11.77611131866702
H	5.92056280112227	5.87341183885530	6.60909880048217
H	4.09787238835002	4.71322762310880	7.78501005058888
H	3.60459555690132	6.21719070896043	8.57895383385547
H	3.57255744085112	5.67754731758200	5.55239026266594
H	2.15926677716294	5.82357087873145	6.60233031251979
H	2.59642743490645	7.94805847749641	5.31641766890286
H	2.70041145759697	8.20690723526705	7.06393744458959
H	5.07266366005550	7.81311294737008	5.14912835735265
H	4.61228578444162	9.32991981182864	5.93142925441982
H	5.10149094092009	8.37526094799040	8.17176577074234
H	6.52551892334767	8.21168305248839	7.13308859484243
H	5.07779700211902	6.96883710616310	9.89535477360905
H	8.07172325555067	7.02703602617756	10.48085460160639
H	7.14397197105933	8.31741097550044	9.70943226502506
H	7.47552760024604	8.78676999130034	12.15839444822708
H	5.76226723260570	8.62663854511546	11.75489132618821
H	7.52825714186821	6.46246399463368	13.03519758883632
H	6.23857012794819	7.36725473351922	13.84005023203157
H	5.47416325332888	5.06921262197066	13.12479140023922
H	4.53385411194728	6.35002306121626	12.35186215850848
H	5.15681900002155	4.61470295137021	10.66440224038191
H	6.86717218723087	4.79798113008838	11.08102381117347

RIJQIK[75]

cis-Chloro-dicarbonyl-bis(di-isopropylamine)carbyne-bis(trimethylphosphine)-chromium

Charge = 0
Spin Multiplicity = 3

Cr	0.049393	3.222582	4.320390
Cl	1.811881	3.686260	2.663281
P	0.856125	0.949271	4.759558

C	2.400808	0.482794	3.872465
H	3.193285	1.193888	4.137005
H	2.237240	0.547917	2.790137
H	2.706505	-0.537146	4.146216
C	1.314350	0.598509	6.509326
H	0.431754	0.704279	7.152129
H	2.075788	1.315212	6.842540
H	1.709059	-0.422850	6.604632
C	-0.254809	-0.479484	4.402737
H	-1.198965	-0.346418	4.946522
H	0.214687	-1.424333	4.711408
H	-0.477713	-0.526467	3.329566
P	-1.138715	2.615761	2.183718
C	-2.833651	1.892371	2.283749
H	-2.795775	0.927590	2.806093
H	-3.258839	1.746617	1.280349
H	-3.479370	2.568963	2.858354
C	-0.329917	1.487996	0.963022
H	-0.252713	0.472904	1.374008
H	0.680526	1.864031	0.759762
H	-0.907228	1.448191	0.028153
C	-1.446121	4.097051	1.126438
H	-0.484701	4.583622	0.918252
H	-2.089292	4.805097	1.665523
H	-1.930313	3.813066	0.180849
C	-0.593077	4.968201	4.316091
O	-0.957641	6.078922	4.365539
C	1.197850	3.862595	5.598025
O	1.941324	4.334778	6.378698
C	-1.522726	2.769560	5.323646
N	-2.347247	2.765808	6.319327
C	-3.629955	1.960764	6.198624
H	-3.527215	1.475927	5.218826
C	-4.852714	2.879707	6.165594
H	-4.757489	3.636054	5.374570
H	-5.011561	3.392945	7.124999
H	-5.749899	2.278688	5.959444
C	-3.731647	0.877954	7.273729
H	-2.847046	0.226360	7.270634
H	-4.613271	0.254090	7.068875
H	-3.853296	1.299782	8.281717
C	-2.184416	3.512688	7.643173
H	-3.125474	3.332282	8.180107
C	-1.038210	2.923356	8.461848
H	-1.187888	1.852296	8.654055
H	-0.978832	3.437805	9.431875

H	-0.081081	3.060214	7.942447
C	-2.035556	5.016053	7.432669
H	-2.848252	5.420429	6.814825
H	-1.079291	5.256478	6.953632
H	-2.064116	5.518572	8.410238

ROPSEU[76]

(μ_2-Tetrachlorodiphosphido)-decacarbonyl-di-chromium

Charge = 0
Spin Multiplicity = 1

Cr	1.058927	0.538055	5.358186
P	2.888248	0.395608	6.743772
Cl	2.646836	-0.709227	8.493585
Cl	3.593770	2.200402	7.509831
C	-0.519923	0.740529	4.356997
O	-1.494846	0.876697	3.752319
C	1.831117	-0.315975	3.837814
O	2.222911	-0.817438	2.875276
C	0.433992	-1.155659	5.956538
O	0.030719	-2.183473	6.292779
C	0.160835	1.407868	6.788089
O	-0.415452	1.937995	7.636726
C	1.672846	2.208094	4.687171
O	2.021352	3.219133	4.252746
P	4.978102	-0.452230	6.225258
Cr	6.829100	-0.539057	7.586257
C	8.432730	-0.668624	8.559204
O	9.423370	-0.758042	9.146796
C	6.013101	0.155762	9.163569
O	5.596644	0.566499	10.158188
C	7.300979	1.235649	7.090812
O	7.612341	2.313273	6.818527
C	7.775613	-1.244444	6.096688
O	8.381739	-1.672983	5.212251
C	6.364432	-2.291933	8.160684
O	6.105556	-3.352177	8.536163
Cl	5.196477	0.635549	4.460573
Cl	4.279874	-2.269873	5.485661

TALYIO[77]

(η^6-3,4-Dimethylenecyclobutene)-tricarbonyl-chromium(0)

Charge = 0
Spin Multiplicity = 1

Cr	3.674666	6.023061	7.378274
C	3.342951	5.529976	9.497609
C	2.079844	5.717986	8.863965
C	2.322346	4.580483	7.955135
C	3.655247	4.382708	8.622991
C	4.842759	4.056989	7.984770
C	2.070553	4.466473	6.596298
C	4.998370	7.169864	7.952420
O	5.819843	7.911816	8.326927
C	4.478151	5.800693	5.714369
O	4.978589	5.645200	4.675109
C	2.735389	7.504337	6.812302
O	2.143368	8.452437	6.471691
H	3.846355	5.990601	10.342613
H	1.233582	6.377272	9.033735
H	4.841564	3.331394	7.171209
H	5.798884	4.258231	8.467652
H	2.544020	3.671639	6.019755
H	1.192029	4.940121	6.158594

XUJKAO[78]

(η^5-Cyclopentadienyl)-dicarbonyl-(N,N-dimethylaminocarbyne)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	4.497651	2.686362	4.886782
N	5.979720	2.683842	7.545164
O	2.554723	0.660347	5.934623
C	6.152032	1.970669	3.559642
C	4.903427	1.525822	3.033618
C	4.130021	2.676796	2.686694
C	5.350807	2.691144	6.404725
C	6.347269	1.428019	8.222279
C	3.314400	1.448504	5.505515
H	6.958088	1.334332	3.913406
H	4.599598	0.490729	2.905647
H	3.134742	2.673413	2.253227
H	7.438527	1.382697	8.350605
H	5.865611	1.387511	9.210074
H	6.012399	0.582783	7.613284
C	6.149646	3.396875	3.553671

C	4.899598	3.833243	3.024127
H	6.953328	4.038843	3.902662
H	4.592319	4.866240	2.887789
C	6.353776	3.930961	8.234785
H	7.445250	3.969559	8.363431
H	5.872364	3.964216	9.222970
H	6.023156	4.784020	7.634367
C	3.306491	3.922699	5.494657
O	2.541965	4.709704	5.916926

YIKSAM[79]

Pentacarbonyl-trichlorophosphine-chromium

Charge = 0
Spin Multiplicity = 1

Cr	4.693202	9.048770	1.378556
P	4.521761	11.212521	2.112006
Cl	2.725434	11.866385	2.916944
Cl	4.842123	12.701164	0.701749
Cl	5.834383	11.842569	3.591383
C	6.421175	9.455005	0.697884
C	5.454130	8.487539	3.028896
C	2.978402	8.577561	2.053317
C	3.895051	9.539294	-0.276414
C	4.889306	7.297961	0.722796
O	7.473590	9.671248	0.274623
O	5.904570	8.116147	4.024370
O	1.944906	8.262255	2.457849
O	3.408952	9.804142	-1.289343
O	5.014105	6.224230	0.314244

YIPMAL[80]

1-(Di-t-butylphosphino)-3-ethoxyindene-pentacarbonyl-chromium

Charge = 0
Spin Multiplicity = 1

Cr	3.303335	3.016421	10.572862
C	4.014528	4.193784	11.869544
O	4.279380	4.935849	12.724564
C	1.766919	3.159449	11.577426
O	0.792839	3.238997	12.213537
C	2.801864	4.556568	9.599093

O	2.433630	5.519451	9.065405
C	3.806777	1.523491	11.622776
O	4.036164	0.628708	12.325617
C	2.212926	1.946637	9.459811
O	1.406787	1.346156	8.876516
P	5.424772	2.736962	9.124545
C	5.852091	0.936515	8.552361
C	4.548712	0.192992	8.209424
C	6.754283	0.918756	7.304597
C	6.539032	0.153163	9.687865
C	6.978466	3.508405	9.980997
C	7.073267	3.009253	11.437331
C	6.770271	5.036259	10.003107
C	8.324833	3.185926	9.302351
C	4.178351	3.117036	5.458192
O	3.400643	2.689875	4.436329
C	2.041822	2.315753	4.791599
C	1.322113	1.895391	3.527730
C	3.912118	3.229635	6.787840
C	5.115590	3.776163	7.521370
C	6.116251	4.008627	6.390867
C	7.345570	4.666012	6.349957
C	8.007830	4.823663	5.122954
C	7.441498	4.351565	3.932940
C	6.181539	3.745224	3.945820
C	5.528611	3.593685	5.171755
H	3.913867	0.050651	9.092037
H	4.816254	-0.805941	7.828984
H	3.968867	0.703829	7.431154
H	6.985371	-0.132774	7.067915
H	7.705468	1.440742	7.452457
H	6.251866	1.351388	6.431870
H	5.960751	0.161643	10.619925
H	7.553904	0.507776	9.900223
H	6.622539	-0.897461	9.366335
H	6.173309	3.226480	12.020609
H	7.915783	3.529461	11.920454
H	7.270825	1.933282	11.500528
H	5.805597	5.320713	10.442690
H	6.833429	5.489683	9.006558
H	7.560644	5.488369	10.622466
H	8.338467	3.399242	8.229816
H	8.618430	2.139435	9.447028
H	9.101844	3.807955	9.775693
H	1.554570	3.182997	5.266744
H	2.084076	1.493535	5.524388

H	1.286316	2.719638	2.802109
H	0.290298	1.609183	3.775097
H	1.816337	1.032426	3.060603
H	2.973240	2.996023	7.274744
H	4.878599	4.755866	7.971330
H	7.802378	5.081065	7.246275
H	8.973771	5.330468	5.099875
H	7.973273	4.482332	2.989161
H	5.705885	3.418885	3.019987

YIZBOY[81]

Pentacarbonyl-(phosphinoformic acid)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	2.077472	3.370160	4.787846
C	0.625402	4.299633	5.491841
O	-0.281706	4.878815	5.928087
C	2.792318	4.981907	4.098478
O	3.219536	5.975427	3.684688
C	1.111720	3.102989	3.179946
O	0.505318	2.950570	2.205025
C	1.390053	1.745067	5.478604
O	0.949226	0.764239	5.907776
C	3.029419	3.654346	6.403342
O	3.586766	3.846639	7.399702
P	3.860113	2.170258	3.801928
H	3.576988	0.923698	3.195732
H	4.598391	2.776834	2.755454
C	5.277498	1.578088	4.892897
O	5.307462	0.487702	5.424101
O	6.199362	2.549088	5.048383
H	6.892491	2.220028	5.667049

YOKXEB[82]

(bis(Diphenylphosphinoxy)-di-t-butylsilane-P,P')-tetracarbonyl-chromium toluene solvate

Charge = 0
Spin Multiplicity = 1

Cr	1.132844	1.502296	2.293405
Si	4.764555	2.320350	4.127804
C	4.911242	3.703154	5.442951

C	5.973192	4.749718	5.042346
H	5.789442	5.169369	4.042691
H	6.991363	4.337503	5.059091
H	5.947432	5.586587	5.761078
C	5.280522	3.122564	6.825679
H	6.295234	2.702083	6.842779
H	4.585872	2.335469	7.152475
H	5.246079	3.927954	7.579032
C	3.545340	4.417409	5.552509
H	3.263178	4.913306	4.613795
H	3.606373	5.195070	6.332754
H	2.731696	3.734486	5.833672
C	6.315820	1.301738	3.660226
C	5.901588	0.230627	2.626480
H	5.167920	-0.476937	3.036230
H	6.792281	-0.350267	2.332434
H	5.478602	0.668416	1.711698
C	7.411816	2.193634	3.037191
H	7.046853	2.777328	2.179864
H	8.236371	1.556102	2.675261
H	7.838266	2.897732	3.764319
C	6.902392	0.584384	4.894959
H	7.728948	-0.072879	4.574992
H	6.158439	-0.046055	5.402691
H	7.313257	1.289937	5.630271
O	3.595892	1.253182	4.712954
P	2.237141	0.511030	4.154584
C	2.767231	-1.257874	4.094604
C	3.600933	-1.755225	5.112650
H	3.951335	-1.090105	5.903023
C	3.983505	-3.096233	5.119442
H	4.635933	-3.468913	5.910751
C	3.525632	-3.962838	4.119109
H	3.822619	-5.012703	4.127290
C	2.685111	-3.479964	3.114260
H	2.320299	-4.149161	2.333697
C	2.309535	-2.131800	3.100943
H	1.653570	-1.769097	2.311190
C	1.245401	0.448382	5.712689
C	1.594106	1.193494	6.845557
H	2.486809	1.816060	6.829036
C	0.811454	1.133897	8.003888
H	1.097894	1.720060	8.878680
C	-0.328137	0.327992	8.040849
H	-0.939267	0.281742	8.943495
C	-0.678738	-0.425491	6.914918

H	-1.562357	-1.065302	6.936096
C	0.101954	-0.366748	5.759601
H	-0.181717	-0.973424	4.899038
O	4.216263	3.021016	2.694330
P	2.814982	3.125166	1.839245
C	2.427099	4.927558	1.969096
C	3.480695	5.858990	1.941134
H	4.513074	5.511645	1.883635
C	3.214468	7.227322	1.986272
H	4.040466	7.940176	1.970214
C	1.892080	7.684699	2.043892
H	1.684728	8.755455	2.075233
C	0.840517	6.766273	2.057597
H	-0.192798	7.113715	2.099587
C	1.107514	5.392939	2.023147
H	0.277269	4.688512	2.034995
C	3.490496	3.114983	0.118475
C	2.626849	3.389712	-0.954999
H	1.574958	3.614695	-0.776903
C	3.106051	3.394349	-2.265826
H	2.423058	3.612077	-3.088418
C	4.454645	3.123939	-2.523802
H	4.827916	3.126069	-3.549004
C	5.319847	2.856130	-1.461141
H	6.374534	2.649531	-1.650513
C	4.840190	2.852692	-0.146685
H	5.523417	2.654298	0.677036
C	2.040941	0.435070	1.033593
O	2.560240	-0.210208	0.216107
C	0.283374	2.593550	3.573281
O	-0.291241	3.237451	4.353847
C	-0.206868	0.233923	2.428823
O	-1.094219	-0.528383	2.421706
C	0.063843	2.219118	0.965568
O	-0.692550	2.605569	0.160777

YUBWAT[83]

Bromo-(η^5-cyclopentadienyl)-di-isopropylaminocarbyne-bis(t-butylisocyano)-chromium hexafluorophosphate

Charge = 1
Spin Multiplicity = 3

Br	-1.155425	0.719114	11.867920
Cr	0.328299	3.784775	10.983992

N	2.497057	5.100819	9.270661
N	2.285394	1.681971	12.290833
N	-0.911129	2.159491	8.580626
C	1.607384	4.534313	9.983736
C	3.874335	5.486760	9.800381
C	3.877542	6.979611	10.129826
C	4.299082	4.617634	10.972731
C	2.280321	5.404489	7.787884
C	2.691175	4.177247	6.976070
C	1.516772	2.417084	11.802727
C	2.964917	0.569680	12.941321
C	2.280197	0.357288	14.303229
C	2.785891	-0.659915	12.033173
C	4.447177	0.935238	13.109261
C	-0.462651	2.704819	9.514572
C	-1.576394	1.245019	7.660780
C	-0.841955	-0.103758	7.760447
C	-1.488291	1.831476	6.244036
C	-3.037179	1.117218	8.127178
C	-1.367124	4.080063	12.474892
C	-0.154538	4.600928	13.010036
C	0.284754	5.669964	12.171025
C	-0.643749	5.785484	11.090237
C	-1.650483	4.789608	11.273555
H	4.538255	5.295895	8.944458
H	4.901860	7.281546	10.387467
H	3.550300	7.593738	9.280520
H	3.229493	7.191712	10.991349
H	5.327604	4.887497	11.246944
H	3.660151	4.778499	11.851116
H	4.280765	3.552768	10.709221
H	2.980778	6.227562	7.590152
H	3.714599	3.855947	7.212051
H	2.006638	3.339026	7.165057
H	2.757003	-0.494914	14.805722
H	2.390521	1.245112	14.939994
H	1.212581	0.140900	14.166043
H	3.260838	-1.523878	12.517031
H	1.719203	-0.872258	11.882892
H	3.262507	-0.498762	11.057086
H	4.962940	0.102534	13.605386
H	4.924224	1.105971	12.134965
H	4.563286	1.834547	13.728585
H	-1.343929	-0.824807	7.101506
H	0.203745	-0.005326	7.440153
H	-0.869545	-0.479200	8.791827

H	-1.989882	1.148328	5.546045
H	-1.985718	2.809062	6.190347
H	-0.442785	1.942785	5.927021
H	-3.555641	0.410294	7.465695
H	-3.079301	0.740827	9.157718
H	-3.551886	2.085904	8.074867
H	-1.929395	3.239996	12.868355
H	0.346441	4.252890	13.908739
H	1.157502	6.293498	12.336855
H	-0.602067	6.510185	10.283633
H	-2.493825	4.610917	10.612865
C	0.861646	5.874489	7.503194
H	2.652770	4.426656	5.907012
H	0.790818	6.138668	6.439581
H	0.123734	5.088030	7.708585
H	0.607906	6.766036	8.091493

YUDHOU[84]

cis-Tetracarbonyl-(1-trimethylsilyl-2,4,4-triphenyl-4-phospha-1,3-diazabutene-N,P)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	-0.370457	2.237126	2.966444
P	-2.555709	1.513274	3.348779
Si	-0.483848	5.678180	2.560469
O	0.132701	2.663950	5.944046
O	2.505914	2.995081	2.476055
O	0.771062	-0.520653	3.291347
O	-0.547017	1.869324	-0.055197
N	-1.473155	4.171488	2.695556
N	-3.446218	2.955114	2.976388
C	-0.102824	2.532189	4.811648
C	1.366830	2.785191	2.660064
C	0.309652	0.553371	3.164506
C	-0.525281	2.003768	1.102041
C	-2.774258	4.111537	2.651540
C	-3.709957	5.197420	2.206228
C	-4.629787	5.767203	3.098985
C	-5.531748	6.735591	2.651399
C	-5.538309	7.120829	1.307183
C	-4.638254	6.537264	0.409990
C	-3.724223	5.580387	0.856606
C	-3.133908	1.080315	5.039266
C	-3.546630	2.073803	5.939229

C	-3.897843	1.736173	7.249231
C	-3.824852	0.406974	7.675579
C	-3.401917	-0.586342	6.786073
C	-3.059700	-0.253461	5.473654
C	-3.403959	0.239690	2.329516
C	-4.796815	0.066604	2.426711
C	-5.445702	-0.878086	1.631286
C	-4.708864	-1.675589	0.747364
C	-3.323342	-1.523262	0.660709
C	-2.672876	-0.565618	1.445988
C	-1.457502	7.294462	2.670755
C	0.688573	5.753200	4.033294
C	0.428248	5.647144	0.914003
H	-4.629371	5.468079	4.148536
H	-6.232069	7.188029	3.354995
H	-6.248002	7.872290	0.957878
H	-4.646634	6.826426	-0.641885
H	-3.025812	5.121617	0.155023
H	-3.600820	3.114815	5.618091
H	-4.228029	2.515947	7.937462
H	-4.096713	0.144821	8.699242
H	-3.342437	-1.625863	7.112301
H	-2.742332	-1.040246	4.786749
H	-5.382389	0.662054	3.130431
H	-6.527550	-0.998021	1.707040
H	-5.217022	-2.418593	0.130649
H	-2.743102	-2.148045	-0.019758
H	-1.592023	-0.449739	1.371481
H	-0.708411	8.100256	2.742109
H	-2.091995	7.499408	1.800265
H	-2.081495	7.343641	3.574304
H	1.439109	4.955925	4.058636
H	1.219147	6.717946	3.994151
H	0.122323	5.724759	4.976183
H	1.060310	4.758641	0.792399
H	-0.282055	5.680713	0.074592
H	1.073978	6.536263	0.842291
H	-4.457967	2.960657	2.855394

ZAGKIB[85]

Nitrido-tris(di-isopropylamino)-chromium

Charge = 0
Spin Multiplicity = 1

Cr	1.60047312385121	4.11511055944119	2.45663958073425
N	3.00475447592614	4.07859876888245	1.82068707595285
N	0.74156398822114	2.58716499055102	1.84239020283106
N	1.88699172346628	4.10883870164723	4.29126429023796
N	0.81857255346836	5.68341743523967	1.83702478434934
C	-0.45164826350952	2.13542861041701	2.59159185579744
C	-0.21532208651598	0.80374018641720	3.32552024407682
C	-1.72396295384601	2.06579604923440	1.72687064404946
C	1.17572580777780	1.68223590663492	0.75304080809846
C	2.49996693119711	0.96844880661803	1.06117977824737
C	1.25047454604181	2.41547194765827	-0.59269665797893
C	3.15459976276189	3.83966681184451	5.00996248558748
C	3.65439291336354	2.41094312732729	4.75735450155751
C	4.25010577192027	4.86764190348930	4.69461491463160
C	0.76528585528938	4.53867751857576	5.15520282202903
C	1.04177251086448	5.88290981215841	5.85172300400181
C	0.33826364687150	3.46629509888131	6.17474991657232
C	1.48012559771567	6.80493610801518	1.12958058660711
C	2.05313157819165	6.39246947142233	-0.23376300950853
C	2.55554582556235	7.46982553221858	1.99897039636510
C	-0.65369174293280	5.79300649477995	1.93367480621060
C	-1.11673900969461	6.99521946237092	2.77708231016413
C	-1.33983784127238	5.79447843127681	0.55555779965964
H	-0.63413458860173	2.90015105637447	3.36621538401503
H	0.67780904937458	0.86303060001868	3.96196817484054
H	-0.07953063837879	-0.02584878599879	2.61587611062450
H	-1.08130833119261	0.56093305618570	3.95947102923040
H	-1.90979207689489	3.01833791534882	1.21340906545152
H	-2.59393730114007	1.83929407570465	2.36114969341937
H	-1.65473325712801	1.27374612382898	0.96712349200567
H	0.40248341017881	0.90139902622708	0.65585108472278
H	2.43545661118030	0.39872251743064	1.99798006378635
H	3.31155954377532	1.70329449707477	1.15707836897838
H	2.75215176459160	0.27033723055440	0.24796053332828
H	0.29020824151712	2.89223219887439	-0.83483547517288
H	1.50189722096570	1.70951657991900	-1.39922755779626
H	2.02239383724102	3.19651581729133	-0.55639563750882
H	2.93372293972118	3.92091987543234	6.08778636580278
H	2.88987539764183	1.67126204478625	5.03439339754991
H	4.55991880968895	2.21223600441466	5.35103474238447
H	3.89531864577237	2.27414074094561	3.69389431122733
H	3.91745881119380	5.88807280481432	4.92910303510975
H	4.51102521942522	4.82459122268172	3.62787721968619
H	5.15286141339360	4.65313871387775	5.28732048884257
H	-0.09794881091629	4.70014306499804	4.48682760487492
H	1.30903571768176	6.65259936991451	5.11509042496660

H	1.86310053768065	5.79926474454066	6.57866149983869
H	0.14742823415831	6.21873637223304	6.39773304067325
H	0.10762979835367	2.51383538071626	5.67865782023269
H	-0.56021427231324	3.80113434234301	6.71422137407407
H	1.12254234801841	3.28074209123610	6.92327602631307
H	0.70266352890352	7.56364089959335	0.93597548339638
H	1.27245347887682	5.96591924631962	-0.87800895690589
H	2.84121797528864	5.63816828185920	-0.10108469816337
H	2.48546025637871	7.26710150871437	-0.74394604912970
H	2.13320552667995	7.81945015439131	2.95161255729262
H	2.98974401726673	8.33467094800883	1.47409005875541
H	3.35923027840569	6.75464724925950	2.22190315621037
H	-0.99808107373450	4.88458025043708	2.45735530904246
H	-0.65772061818281	6.97987787192186	3.77435073226483
H	-2.20979420727806	6.96771981464461	2.89947060398054
H	-0.86133754064587	7.95065028847963	2.29595959711208
H	-1.02865518320773	4.92388624707723	-0.03765744878971
H	-1.09846650004315	6.70400324208257	-0.01418684824886
H	-2.43288992841578	5.76061058034065	0.67801668140782

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