Synthesis and Characterization of Si-Supported and Unsupported Chromium(0) Fischer Aminocarbene complexes

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Supporting information

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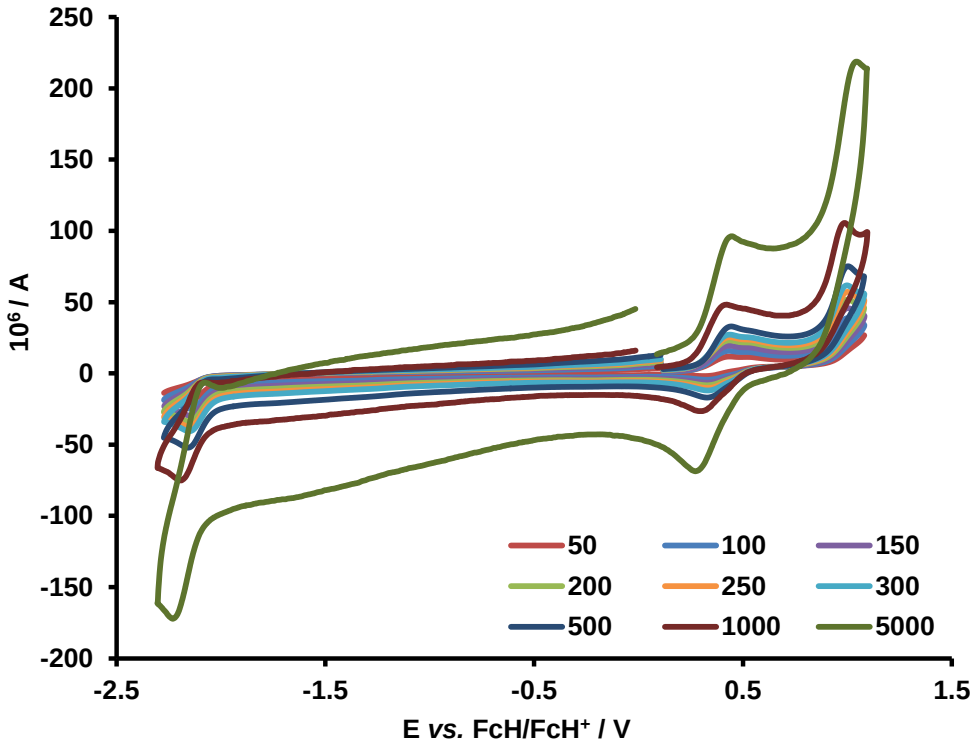
Electrochemistry

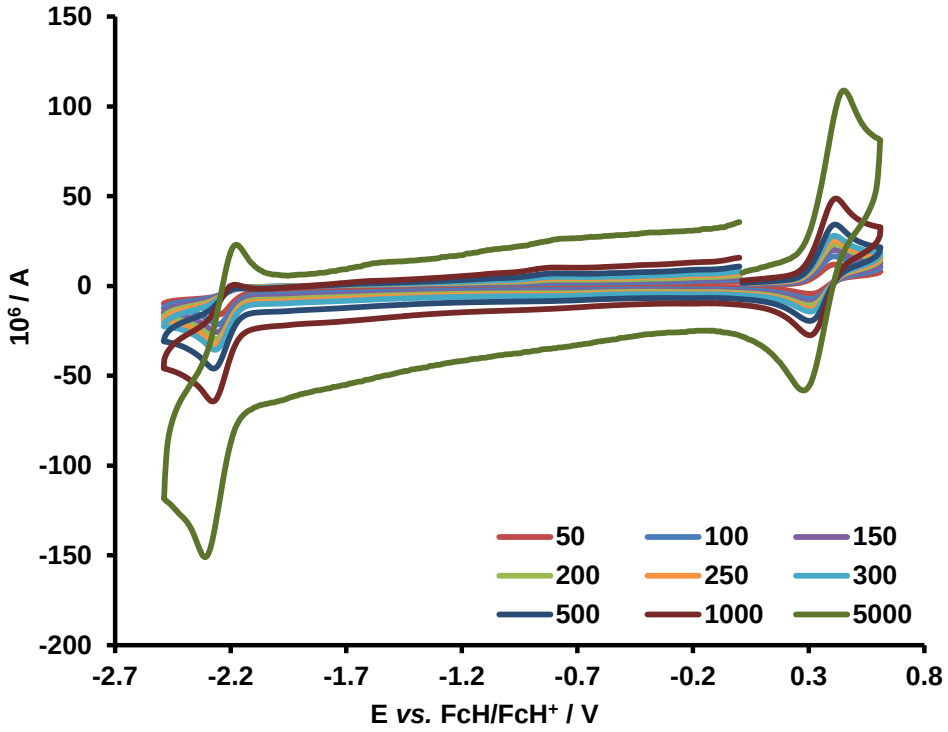
Complex 3: $[Cr(CO)_5{=}C(NHCy)(Th)]$

Scan Rate ($mV.s^{-1}$)	Oxidation						First Reduction				
	1st					2nd					
	E_{pa} (V)	E_{pc} (V)	ΔE (V)	$E^{0'}$ (V)	i_{pa}/i_{pc}	E_{pa} (V)	E_{pc} (V)	E_{pa} (V)	ΔE (V)	$E^{0'}$ (V)	i_{pc}/i_{pa}
50	0.455	0.323	0.131	0.389	0.41	0.563	-2.147	-	-	-	-
100	0.456	0.323	0.133	0.389	0.50	0.569	-2.148	-	-	-	-
150	0.458	0.320	0.138	0.389	0.61	0.578	-2.149	-	-	-	-
200	0.458	0.318	0.140	0.388	0.61	0.581	-2.154	-	-	-	-
250	0.459	0.317	0.142	0.388	0.40	0.582	-2.153	-2.058	0.095	-2.106	0.363
300	0.460	0.316	0.144	0.388	0.40	0.582	-2.158	-2.058	0.100	-2.108	0.410
500	0.469	0.312	0.157	0.391	0.43	0.591	-2.160	-2.060	0.100	-2.110	0.472



Complex 4: $[Cr(CO)_5=C(NHCy)(Fu)]$

Scan Rate ($mV.s^{-1}$)	First oxidation					First Reduction				
	E_{pa} (V)	E_{pc} (V)	ΔE (V)	$E^{0'}$ (V)	i_{pa}/i_{pc}	E_{pc} (V)	E_{pa} (V)	ΔE (V)	$E^{0'}$ (V)	i_{pc}/i_{pa}
50	0.430	0.297	0.133	0.363	0.70	-2.268		-	-	-
100	0.432	0.287	0.145	0.359	0.69	-2.278		-	-	-
150	0.434	0.282	0.152	0.358	0.66	-2.279		-	-	-
200	0.439	0.264	0.175	0.351	0.64	-2.284		-	-	-
250	0.445	0.273	0.172	0.359	0.63	-2.284	-2.186	0.098	-2.235	0.23
300	0.446	0.268	0.177	0.357	0.65	-2.286	-2.186	0.099	-2.236	0.27
500	0.456	0.254	0.202	0.355	0.66	-2.288	-2.188	0.101	-2.238	0.31



Optimized Cartesian coordinates (Å)

All compounds were optimized B3LYP as implemented in the Gaussian 09 program package. Geometries of the neutral complexes were optimized in gas phase with the triple-ζ basis set 6-311G(d,p) on all atoms except Cr, where def2-TZVPP was used.

1. **[Cr(CO)$_5$=C(NHCy)(Fu)]** ***Z-syn***

Cr	2.708322000	3.922709000	4.086355000
C	4.020177000	2.589522000	3.824044000
O	4.818614000	1.778896000	3.663541000
C	4.045054000	5.250416000	3.737141000
O	4.883121000	6.010059000	3.542349000
C	3.215425000	4.000739000	5.935482000
O	3.565770000	4.020023000	7.026725000
C	1.427013000	2.536717000	4.432447000
O	0.697396000	1.671919000	4.616037000
C	2.252368000	3.782846000	2.230514000
O	1.999577000	3.649416000	1.118916000
C	1.189622000	5.435552000	4.419797000
C	0.282993000	5.371003000	5.561714000
C	0.121985000	4.495363000	6.606529000
H	0.701293000	3.607157000	6.782474000
C	-0.947217000	4.973940000	7.412686000
H	-1.337694000	4.527271000	8.312561000
C	-1.383834000	6.117429000	6.818265000
H	-2.162344000	6.823357000	7.057027000
O	-0.664441000	6.381111000	5.705199000
N	0.936239000	6.504990000	3.679664000
H	0.180881000	7.117497000	3.981844000
C	1.583177000	6.975599000	2.451725000
H	2.368587000	6.264243000	2.210029000
C	2.214030000	8.359943000	2.681173000
H	2.958068000	8.293712000	3.479235000
H	1.435265000	9.054924000	3.024157000
C	2.851513000	8.899933000	1.392824000
H	3.256595000	9.899570000	1.575758000
H	3.704157000	8.265246000	1.122779000
C	1.848442000	8.931339000	0.231655000
H	1.062730000	9.665933000	0.451075000
H	2.342586000	9.268446000	-0.684506000
C	1.207595000	7.554352000	0.011036000
H	1.970903000	6.846539000	-0.334093000
H	0.453773000	7.605395000	-0.780150000
C	0.567207000	7.011993000	1.296950000
H	-0.277523000	7.652984000	1.584480000

H	0.166164000	6.008495000	1.132516000

2. **[Cr(CO)$_5$=C(NHCy)(Fu)]** ***Z-anti***

Cr	2.710031000	3.898789000	4.073876000
C	3.972889000	2.520118000	3.789287000
O	4.739924000	1.683361000	3.611475000
C	4.068140000	5.172830000	3.640399000
O	4.923461000	5.900101000	3.397525000
C	3.293935000	4.007028000	5.908459000
O	3.701169000	4.041063000	6.977293000
C	1.417022000	2.554777000	4.554534000
O	0.683241000	1.719289000	4.826932000
C	2.167207000	3.741727000	2.247336000
O	1.853991000	3.617861000	1.149301000
C	1.242574000	5.427898000	4.432601000
C	0.265413000	5.307963000	5.513001000
C	-1.024274000	5.769365000	5.663026000
H	-1.580320000	6.363453000	4.954299000
C	-1.513917000	5.254841000	6.895056000
H	-2.490986000	5.400735000	7.326791000
C	-0.496414000	4.515420000	7.418111000
H	-0.385170000	3.946520000	8.325862000
O	0.574838000	4.527385000	6.595445000
N	1.025910000	6.545786000	3.751786000
H	0.324370000	7.193831000	4.106156000
C	1.631039000	7.009316000	2.497542000
H	2.380825000	6.272946000	2.219918000
C	2.312647000	8.372240000	2.699603000
H	3.093681000	8.280788000	3.458755000
H	1.573570000	9.090214000	3.081693000
C	2.900851000	8.897985000	1.381193000
H	3.342522000	9.885048000	1.546050000
H	3.720776000	8.240070000	1.069175000
C	1.844143000	8.961165000	0.270407000
H	1.090886000	9.717026000	0.528079000
H	2.303590000	9.287138000	-0.667454000
C	1.155746000	7.603313000	0.077644000
H	1.882062000	6.875573000	-0.303562000
H	0.366799000	7.677088000	-0.676523000
C	0.562871000	7.075891000	1.392439000
H	-0.248975000	7.740480000	1.719293000
H	0.127781000	6.083853000	1.246223000

3. **[Cr(CO)$_5$=C(NHCy)(Fu)]** ***E-syn***

Cr	2.936007000	3.699993000	4.190693000
C	4.225508000	2.320112000	4.136902000
O	5.009770000	1.480883000	4.102315000
C	4.302874000	4.950410000	3.714191000
O	5.143213000	5.679030000	3.429504000

C	3.356151000	4.029550000	6.031742000
O	3.637775000	4.215130000	7.127855000
C	1.614949000	2.387812000	4.662413000
O	0.861668000	1.566205000	4.928493000
C	2.518042000	3.402430000	2.345540000
O	2.273033000	3.226300000	1.238766000
C	1.454925000	5.297557000	4.195163000
C	0.365458000	5.375692000	5.142506000
C	0.149743000	4.695386000	6.320218000
H	0.808361000	3.962648000	6.750412000
C	-1.083563000	5.138285000	6.861423000
H	-1.553085000	4.812491000	7.775267000
C	-1.569437000	6.056129000	5.979387000
H	-2.474812000	6.640407000	5.949463000
O	-0.721913000	6.225744000	4.944561000
N	1.553137000	6.230612000	3.256896000
H	2.319656000	6.082400000	2.612837000
C	0.805048000	7.472196000	2.942800000
H	0.358923000	7.836583000	3.866119000
C	-0.306177000	7.203952000	1.914132000
H	-1.015710000	6.484165000	2.327406000
H	0.141308000	6.742031000	1.025049000
C	-1.019570000	8.504749000	1.516621000
H	-1.777402000	8.291351000	0.757044000
H	-1.556025000	8.903421000	2.387217000
C	-0.029735000	9.559815000	1.004198000
H	0.414035000	9.212724000	0.062535000
H	-0.554606000	10.492402000	0.776050000
C	1.087139000	9.818300000	2.024366000
H	0.659993000	10.284569000	2.921093000
H	1.815365000	10.529127000	1.623355000
C	1.802061000	8.518970000	2.423392000
H	2.326193000	8.111788000	1.547506000
H	2.561787000	8.715097000	3.185862000

4. **[Cr(CO)$_5$=C(NHCy)(Fu)]** ***E-anti***

Cr	2.930444000	3.656286000	4.163465000
C	4.205141000	2.256993000	4.179228000
O	4.979608000	1.408195000	4.185381000
C	4.278711000	4.835096000	3.504852000
O	5.105635000	5.527108000	3.107358000
C	3.426531000	4.148968000	5.958291000
O	3.759759000	4.428927000	7.016974000
C	1.623481000	2.418672000	4.849487000
O	0.879515000	1.645374000	5.248890000
C	2.416452000	3.205482000	2.378828000
O	2.106961000	2.947973000	1.303771000
C	1.473803000	5.236357000	4.118134000
C	0.376033000	5.340443000	5.065476000
C	-0.939940000	5.754208000	5.017543000

H	-1.438988000	6.202152000	4.175401000
C	-1.538106000	5.422119000	6.262286000
H	-2.558780000	5.590185000	6.566039000
C	-0.553603000	4.837571000	7.001301000
H	-0.517043000	4.443499000	8.003254000
O	0.592188000	4.764181000	6.297932000
N	1.520199000	6.147380000	3.153814000
H	2.267405000	6.006088000	2.485123000
C	0.762626000	7.389397000	2.901970000
H	0.225385000	7.633819000	3.819647000
C	-0.237290000	7.210024000	1.746102000
H	-0.945509000	6.409977000	1.980127000
H	0.313132000	6.881981000	0.855365000
C	-0.976097000	8.521438000	1.439576000
H	-1.654292000	8.372322000	0.594370000
H	-1.604925000	8.793909000	2.297120000
C	0.003866000	9.665489000	1.145672000
H	0.540454000	9.450242000	0.213033000
H	-0.543186000	10.598658000	0.982153000
C	1.017149000	9.838472000	2.285119000
H	0.495867000	10.183073000	3.187091000
H	1.745679000	10.614776000	2.034438000
C	1.751748000	8.526381000	2.597629000
H	2.369276000	8.240657000	1.735285000
H	2.431057000	8.656277000	3.444830000

5. **[Cr(CO)$_5$=C(NHCy)(Th)]** ***Z-syn***

Cr	2.700692000	3.972859000	4.109660000
C	4.075271000	2.685521000	3.953370000
O	4.914772000	1.907139000	3.859047000
C	4.019592000	5.361014000	4.002375000
O	4.824298000	6.176261000	3.941780000
C	2.952951000	3.898700000	6.019935000
O	3.154777000	3.808860000	7.142606000
C	1.412255000	2.557279000	4.182619000
O	0.679268000	1.674793000	4.196796000
C	2.509679000	3.906355000	2.206855000
O	2.429125000	3.789802000	1.067165000
C	1.173500000	5.485442000	4.391035000
C	0.333900000	5.494497000	5.597440000
C	-0.241209000	4.448223000	6.282191000
H	-0.123343000	3.417874000	5.985441000
C	-1.029283000	4.846350000	7.392419000
H	-1.552720000	4.152108000	8.035862000
C	-1.038152000	6.199172000	7.582407000
H	-1.505999000	6.761653000	8.375993000
S	-0.099287000	7.019918000	6.390116000
N	0.923132000	6.536460000	3.624430000
H	0.154283000	7.150419000	3.894366000
C	1.585100000	6.986762000	2.393775000

H	2.422160000	6.315624000	2.221370000
C	2.125190000	8.414688000	2.582223000
H	2.837947000	8.429278000	3.411092000
H	1.294896000	9.079241000	2.857949000
C	2.785385000	8.929356000	1.294760000
H	3.125609000	9.958176000	1.444298000
H	3.682591000	8.332856000	1.089816000
C	1.832362000	8.847456000	0.094478000
H	0.998098000	9.544709000	0.245385000
H	2.345826000	9.169115000	-0.816488000
C	1.280484000	7.426508000	-0.083565000
H	2.096120000	6.748877000	-0.362578000
H	0.558803000	7.396352000	-0.905013000
C	0.617576000	6.908454000	1.201344000
H	-0.273219000	7.511772000	1.423735000
H	0.281162000	5.876651000	1.071469000

6. **[Cr(CO)$_5$=C(NHCy)(Th)]** ***Z-anti***

Cr	2.794839000	3.875678000	4.030223000
C	4.023929000	2.489478000	3.651264000
O	4.767535000	1.647263000	3.412463000
C	4.108983000	5.131999000	3.436688000
O	4.949751000	5.835744000	3.094825000
C	3.594122000	4.032062000	5.774050000
O	4.155807000	4.092168000	6.770845000
C	1.567817000	2.520674000	4.648576000
O	0.883327000	1.667511000	4.984206000
C	2.085742000	3.685286000	2.262728000
O	1.671847000	3.551704000	1.200622000
C	1.310782000	5.385883000	4.442483000
C	0.338245000	5.253091000	5.543882000
C	-1.024751000	5.472866000	5.482660000
H	-1.535422000	5.740879000	4.566309000
C	-1.696628000	5.234718000	6.709686000
H	-2.764953000	5.338167000	6.844730000
C	-0.842742000	4.849523000	7.704822000
H	-1.072044000	4.627053000	8.735811000
S	0.788057000	4.734979000	7.148721000
N	1.036246000	6.479269000	3.747731000
H	0.305188000	7.090932000	4.109574000
C	1.627393000	6.979304000	2.499642000
H	2.345812000	6.233848000	2.168490000
C	2.353965000	8.310740000	2.749222000
H	3.146033000	8.161482000	3.487270000
H	1.643710000	9.029610000	3.180087000
C	2.931371000	8.879374000	1.444439000
H	3.406195000	9.844347000	1.644342000
H	3.724327000	8.212984000	1.084521000
C	1.853314000	9.025936000	0.362133000
H	1.129747000	9.791286000	0.671439000

H	2.301870000	9.380879000	-0.570477000
C	1.118048000	7.700407000	0.123010000
H	1.812525000	6.969643000	-0.308625000
H	0.315477000	7.833692000	-0.608233000
C	0.536922000	7.129403000	1.425382000
H	-0.246844000	7.801892000	1.800838000
H	0.068308000	6.158515000	1.242651000

7. [Cr(CO)$_5$=C(NHCy)(Th)] ***E-syn***

Cr	2.853808000	3.603827000	4.099028000
C	4.081005000	2.158039000	4.195976000
O	4.825885000	1.286228000	4.250518000
C	4.112569000	4.519335000	2.998690000
O	4.894729000	5.039846000	2.335874000
C	3.626722000	4.441327000	5.638664000
O	4.092154000	4.951765000	6.554527000
C	1.668929000	2.568441000	5.220166000
O	1.014812000	1.900031000	5.878417000
C	2.014100000	2.870179000	2.537366000
O	1.504008000	2.457959000	1.597573000
C	1.453147000	5.202352000	3.985443000
C	0.326933000	5.309788000	4.930003000
C	0.376898000	5.410062000	6.299191000
H	1.306825000	5.478186000	6.846039000
C	-0.903902000	5.422170000	6.918380000
H	-1.052341000	5.499229000	7.987100000
C	-1.927131000	5.289772000	6.026325000
H	-2.985842000	5.211845000	6.220420000
S	-1.345065000	5.189131000	4.398111000
N	1.508743000	6.118134000	3.035170000
H	2.267296000	6.002560000	2.372511000
C	0.747058000	7.369164000	2.824824000
H	0.062638000	7.472677000	3.666871000
C	-0.056271000	7.305130000	1.516279000
H	-0.768270000	6.476711000	1.562327000
H	0.630603000	7.088280000	0.687709000
C	-0.784770000	8.630130000	1.245225000
H	-1.312695000	8.568519000	0.289223000
H	-1.552237000	8.782629000	2.014283000
C	0.182871000	9.821208000	1.248379000
H	0.872408000	9.730735000	0.399522000
H	-0.368129000	10.755243000	1.103994000
C	0.989482000	9.879331000	2.552648000
H	0.313354000	10.095071000	3.389214000
H	1.712900000	10.699078000	2.519818000
C	1.723165000	8.557702000	2.824505000
H	2.483884000	8.397283000	2.048744000
H	2.249817000	8.597352000	3.782234000

8. **[Cr(CO)$_5$=C(NHCy)(Th)]** ***E-anti***

Cr	2.969792000	3.610744000	4.087008000
C	4.202115000	2.168299000	4.076186000
O	4.948672000	1.296048000	4.063279000
C	4.188827000	4.579840000	2.987806000
O	4.946559000	5.130977000	2.321451000
C	3.821155000	4.373534000	5.631943000
O	4.361200000	4.827941000	6.534647000
C	1.827986000	2.509030000	5.188927000
O	1.198913000	1.789564000	5.817622000
C	2.089051000	2.942726000	2.523266000
O	1.552975000	2.569483000	1.580795000
C	1.546871000	5.201755000	4.066581000
C	0.444443000	5.313807000	5.036127000
C	-0.912784000	5.269878000	4.803772000
H	-1.334179000	5.187107000	3.810654000
C	-1.693781000	5.285987000	5.991792000
H	-2.774851000	5.246878000	6.003419000
C	-0.930037000	5.361173000	7.120719000
H	-1.253351000	5.422760000	8.148466000
S	0.760256000	5.365140000	6.754189000
N	1.547043000	6.115525000	3.110769000
H	2.274255000	6.005025000	2.412903000
C	0.750512000	7.347095000	2.917109000
H	0.083037000	7.433199000	3.774518000
C	-0.080733000	7.258157000	1.627198000
H	-0.770015000	6.411198000	1.688625000
H	0.592026000	7.054370000	0.783726000
C	-0.847379000	8.563216000	1.364459000
H	-1.394619000	8.482723000	0.420774000
H	-1.601029000	8.704259000	2.149372000
C	0.092438000	9.776080000	1.338627000
H	0.763879000	9.696261000	0.474381000
H	-0.483487000	10.696039000	1.201327000
C	0.926636000	9.861260000	2.623717000
H	0.264430000	10.067244000	3.473866000
H	1.629528000	10.697470000	2.569219000
C	1.696726000	8.559144000	2.888578000
H	2.446060000	8.411129000	2.099289000
H	2.241205000	8.618081000	3.835251000

9. **[Cr(CO)$_5$=C(OEt)(Fu)]** ***syn***

Cr	0.966994000	-1.069837000	-1.058594000
C	1.283517000	0.087601000	-2.568125000
O	1.438974000	0.730220000	-3.501167000
C	2.177078000	-2.335491000	-1.840017000
O	2.853428000	-3.102104000	-2.360540000
C	0.543867000	-2.274380000	0.371164000
O	0.218615000	-3.013857000	1.185791000

C	-0.441163000	-1.880128000	-2.054100000
O	-1.290428000	-2.366161000	-2.652138000
C	2.473316000	-0.092545000	0.016140000
O	3.434947000	-0.578019000	0.793194000
C	3.602068000	-1.987734000	1.075808000
H	3.584510000	-2.542431000	0.139772000
H	2.766399000	-2.311887000	1.696513000
C	4.925223000	-2.146949000	1.797070000
H	5.082966000	-3.200463000	2.040819000
H	4.935941000	-1.574406000	2.726883000
H	5.754243000	-1.811757000	1.170339000
C	2.657406000	1.345936000	0.044078000
C	3.569837000	2.160129000	0.684464000
H	4.366448000	1.816429000	1.322885000
C	3.251851000	3.495829000	0.340320000
H	3.752222000	4.396694000	0.657336000
C	2.166261000	3.418168000	-0.487165000
H	1.573863000	4.160169000	-0.996700000
O	1.796070000	2.139367000	-0.676218000
C	-0.316094000	0.181689000	-0.348864000
O	-1.111374000	0.894614000	0.059796000

10. **[Cr(CO)$_5$=C(OEt)(Fu)]** ***anti***

Cr	0.863475000	-1.133790000	-1.017171000
C	1.231862000	-0.110976000	-2.599347000
O	1.425767000	0.468157000	-3.568084000
C	1.963450000	-2.532347000	-1.741259000
O	2.555144000	-3.383718000	-2.230962000
C	0.406563000	-2.213694000	0.504436000
O	0.055208000	-2.872171000	1.374892000
C	-0.611686000	-1.915408000	-1.928716000
O	-1.502961000	-2.380975000	-2.480419000
C	2.475312000	-0.182365000	-0.034850000
O	3.437292000	-0.701663000	0.705779000
C	3.571540000	-2.112722000	0.999392000
H	3.675398000	-2.656144000	0.061339000
H	2.670956000	-2.450123000	1.510427000
C	4.800325000	-2.265809000	1.872899000
H	4.942718000	-3.320453000	2.121457000
H	4.689668000	-1.703172000	2.801889000
H	5.692594000	-1.908764000	1.355012000
C	2.713724000	1.249057000	-0.072820000
C	2.056145000	2.301126000	-0.678391000
H	1.169921000	2.233441000	-1.283468000
C	2.761207000	3.485050000	-0.357566000
H	2.526971000	4.491738000	-0.663084000
C	3.809348000	3.090363000	0.425486000
H	4.610149000	3.630834000	0.904165000
O	3.804314000	1.761702000	0.610724000
C	-0.331503000	0.209338000	-0.343956000

O	-1.080638000	0.981799000	0.047905000

11. **[Cr(CO)$_5$=C(OEt)(Th)]** ***syn***

Cr	2.140675000	-0.281192000	-0.000205000
C	1.548441000	-1.471131000	1.388100000
C	1.548374000	-1.470160000	-1.389320000
C	3.805636000	-1.200632000	-0.000458000
C	2.851545000	0.856903000	-1.373705000
C	2.851227000	0.856055000	1.374169000
O	1.246638000	-2.187122000	2.228830000
O	1.246374000	-2.185541000	-2.230496000
O	4.806951000	-1.759768000	-0.000614000
O	3.341545000	1.476423000	-2.204978000
O	3.340914000	1.475135000	2.205952000
C	0.244666000	0.659002000	0.000011000
C	-1.035598000	-0.031149000	-0.000162000
O	-0.037601000	1.955968000	0.000266000
S	-2.550037000	0.884836000	0.000307000
C	-3.475406000	-0.561142000	-0.000255000
C	-2.693992000	-1.689293000	-0.000823000
H	-3.091935000	-2.694718000	-0.001261000
C	-1.316383000	-1.387626000	-0.000776000
H	-0.550532000	-2.146207000	-0.001204000
C	0.943825000	3.021215000	0.000384000
H	1.565504000	2.921106000	-0.887784000
H	1.566439000	2.920136000	0.887780000
C	0.180345000	4.330304000	0.001492000
H	0.888233000	5.162854000	0.001545000
H	-0.450236000	4.414563000	0.888769000
H	-0.451204000	4.415495000	-0.885005000
H	-4.554276000	-0.507637000	-0.000148000

12. **[Cr(CO)$_5$=C(OEt)(Th)]** ***anti***

Cr	2.181155000	-0.268877000	-0.039171000
C	1.691928000	-1.533440000	1.330980000
C	1.654930000	-1.438303000	-1.478289000
C	3.881301000	-1.120114000	-0.063845000
C	2.878687000	0.927220000	-1.366943000
C	2.829301000	0.855077000	1.373818000
O	1.513976000	-2.285037000	2.175385000
O	1.424562000	-2.128714000	-2.361053000
O	4.906552000	-1.633811000	-0.080551000
O	3.377961000	1.578889000	-2.167920000
O	3.273556000	1.473711000	2.231229000
C	0.257007000	0.615913000	-0.016797000
C	-1.022488000	-0.091253000	0.031100000
O	-0.056003000	1.904957000	-0.034901000
S	-1.142718000	-1.837958000	0.017712000
C	-2.855110000	-1.778008000	0.080366000

C	-3.331760000	-0.489215000	0.112890000
H	-4.384306000	-0.243521000	0.155777000
C	-2.295785000	0.463314000	0.083030000
H	-2.452413000	1.531571000	0.099281000
C	0.902578000	2.986415000	-0.116284000
H	1.364966000	2.957593000	-1.102566000
H	1.669245000	2.842592000	0.641844000
C	0.139326000	4.277927000	0.099783000
H	0.829180000	5.123019000	0.035061000
H	-0.331072000	4.293894000	1.085102000
H	-0.634105000	4.408128000	-0.659977000
H	-3.422358000	-2.696852000	0.089886000