Supporting Information for:

A Mechanistic Study of Isotactic Poly(propylene oxide) Synthesis by a Tethered Bimetallic Chromium Salen Catalyst

Bryce M. Lipinski,[‡] Katherine L. Walker,[‖,†] Naomi E. Clayman,[‖,†] Lilliana S. Morris,[‡,†] Timothy M. E. Jugovic,[§] Allison G. Roessler,[§] Yutan D. Y. L. Getzler,[‡] Samantha N. MacMillan,[‡] Richard N. Zare,[‖,*] Paul M. Zimmerman,[§,*] Robert M. Waymouth,[‖,*] and Geoffrey W. Coates[‡,*]

[‡]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853-1301, United States

[‖]Department of Chemistry, Stanford University, Stanford, California 94305-5080, United States

[§]Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109-1382, United States

[†]K.L.W., N.E.C., and L.S.M. contributed equally

* E-mail: coates@cornell.edu

* E-mail: waymouth@stanford.edu

* E-mail: paulzim@umich.edu

* E-mail: zare@stanford.edu

Table of Contents

I. General Considerations

All reactions and subsequent manipulations were performed under N_2 using a glovebox or Schlenk line. All NMR spectra were recorded on a 500 MHz Bruker AV III HD spectrometer with broadband Prodigy Cryoprobe (^{1}H, 500 MHz). ^{1}H and ^{13}C chemical shifts are referenced to the solvent residual peaks. All NMR spectra were processed using MestReNova (*V. 10.0.1-14719*) software package. Mass spectrometry (MS) experiments were conducted on an LTQ-Orbitrap XL instrument, with a resolution of 60,000 at *m/z* 400 and mass accuracy of less than 5 ppm, manufactured by Thermo Fisher Scientific (San Jose, CA). Collision induced dissociation (CID) spectra were taken in tandem MS mode by colliding desired ions with helium. Data was preliminarily analyzed in Thermo Fisher's Qual Browser tool, and exported as text files for further processing in Matlab. Data was recorded with the following parameters unless otherwise specified: -2 kV spray voltage, 275 °C capillary temperature, -60 V capillary voltage, -100 V tube voltage, flow rate of 5 uL/min. Gel permeation chromatography (GPC) was performed using an Agilent 1260 Infinity system, equipped with UV and refractive index detectors, and two Agilent PolyPore columns (5 micron, 4.6 mm ID). The GPC columns were eluted with THF at 30 °C at 0.3 mL/min and were calibrated with monodisperse polystyrene standards.

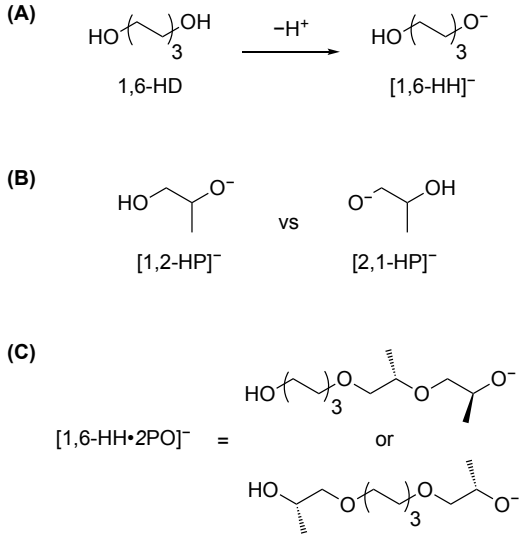
II. Materials and Synthesis

All reagents and materials were purchased from commercial vendors and were used as received unless otherwise noted. 1,2-Dimethoxyethane (DME), propylene oxide (PO), 1,4-butanediol (1,4-BD), 1,2-butanediol (1,2-BD), 1,2-propanediol (1,2-PD), 1,6-hexanediol (1,6-HD), and bis(triphenylphosphine)iminium chloride ([PPN]Cl) were purchased from Sigma-Aldrich. Deuterated solvents were purchased from Cambridge Isotope Laboratory. 3 Å molecular sieves were purchased from Alfa Aesar and activated by heating at 200 °C under vacuum for 18 hours, and stored in a nitrogen filled glove box. [PPN]Cl was recrystallized at room temperature over 5 days from anhydrous methylene chloride/hexane and dried at 80 °C under vacuum overnight. DME was dried over sodium/benzophenone for 72 hours, then vacuum transfer to a Straus storage flask. Residual oxygen was removed by three freeze-pump-thaw cycles. DME was further dried and stored over activated 3 Å molecular sieves. PO was dried by stirring over calcium hydride for 72 hours, followed by vacuum transfer into a Straus storage flask. Residual oxygen was removed by three freeze-pump-thaw cycles. 1,4-BD, 1,2-BD, and 1,2-PD were dried stirring over 3 rounds of activated 3 Å molecular sieves and degassed with three freeze-pump-thaw cycles. 1,6-HD was dried by heating at 60 °C and pulling full vacuum for 18 hours. Chromium complexes **1** and **8**,[1,2] Bis(triphenylphosphine)iminium trifluoroacetate ([PPN][OAc^{F3}]),[1,3] and (*R,R*)-N,N′-Bis(3,5-di-tert-butylsalicylidene)-1,2-cyclohexanediamino-chromium(III) chloride ((*R,R*-salcy)CrCl)[4] were synthesized according to reported procedures.

III. Nomenclature Assignment

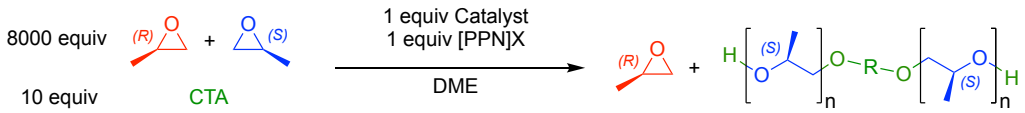
This section is here to provide clarification about small molecule and anion nomenclature assignments made here and in the main text. While the conjugate base of an alcohol is commonly referred to as an alkoxide, this assignment is not specific enough for our system that contains numerous diols. Instead, we opted to use the term "hydroxyalkanolate" to describe a diol that has been singly deprotonated (Scheme S1A). In the case of 1,2-diols, we did not differentiate between 1,2- and 2,1-hydroxyalkanolates in our assignments due to the lack of mechanistic pertinence to the induction period. While the secondary alcohol is more susceptible to deprotonation, we assigned all singly deprotonated 1,2-diols as 1,2-hydroxyalkanolates (Scheme S1B). As oligomers are generated from these hydroxyalkanolates, PO enchainment occurs on both sides of the anion as a result of rapid chain transfer. This systematic naming does not claim the exact enchainment order of the oligomers (Scheme S1C).[5]

Scheme S1. General Clarifications for Nomenclature Assignments



IV. Kinetic Polymerization Conditions and Analysis

Scheme S2. General Conditions for Kinetic Analysis



General polymerization setup: A 20 mL scintillation vial and stir bar was charged with **1**/**8** (0.0018 mmol), [PPN][OAc^{F3}]/[PPN]Cl (0.0018 mmol) and the appropriate CTA (0.018 mmol, 1,6-HD: 2.1 mg; 1,2-BD: 1.6 µL; 1,2-PD: 1.4 mg; water: 0.3 µL*). DME (2.0 mL) was added and mixture was stirred until all reagents were dissolved. Lastly, PO (1.0 mL, 14.3 mmol) was added to initiate the reaction.

*For water CTA reactions, a stock solution of the CTA in DME was made using standard Schlenk technique. The stock solution was used in the glovebox followed by extended periods of purging.

Conversion was measured hourly by taking 200 µL aliquots, removing PO and DME under vacuum, and undergoing ^{1}H NMR analysis against mesitylene as an internal standard. Each data point reported is the average of three experiments and the error bars provided show a standard deviation above and below that average.

A gel permeation chromatogram was provided to show the water content for a polymerization under these standard conditions (Figure S1). This trace is the result of a polymerization using **8** and [PPN]Cl in the absence of CTA. The high molecular weight shoulder is the result of adventitious water reacting to form 1,2-PD, which then acts as a CTA. The low molecular weight peak is the result of $[Cl]^-$ initiated chains.

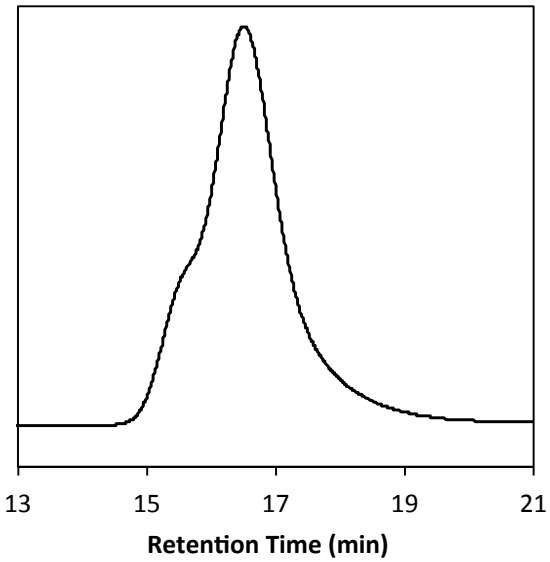


Figure S1. GPC chromatogram of PO polymerization at 45% conversion using **8** without CTA under these standard kinetic conditions.

From the text, it is clear that the presence of 1,2-diols resulted in a longer induction period, while polymerizations with 1,6-HD did not. For curiosity purposes, preliminary experiments were performed with 1,3- and 1,4-diols. We found that 1,3-diols behave like 1,2-diols (have an additional induction period) and 1,4-diols behave more like 1,6-diols (no additional induction period). These results agree with the coordination behavior observed by mass spectrometry.

Representative ^{1}H NMR spectra for polymerization conversion are presented Figures S2–S7.

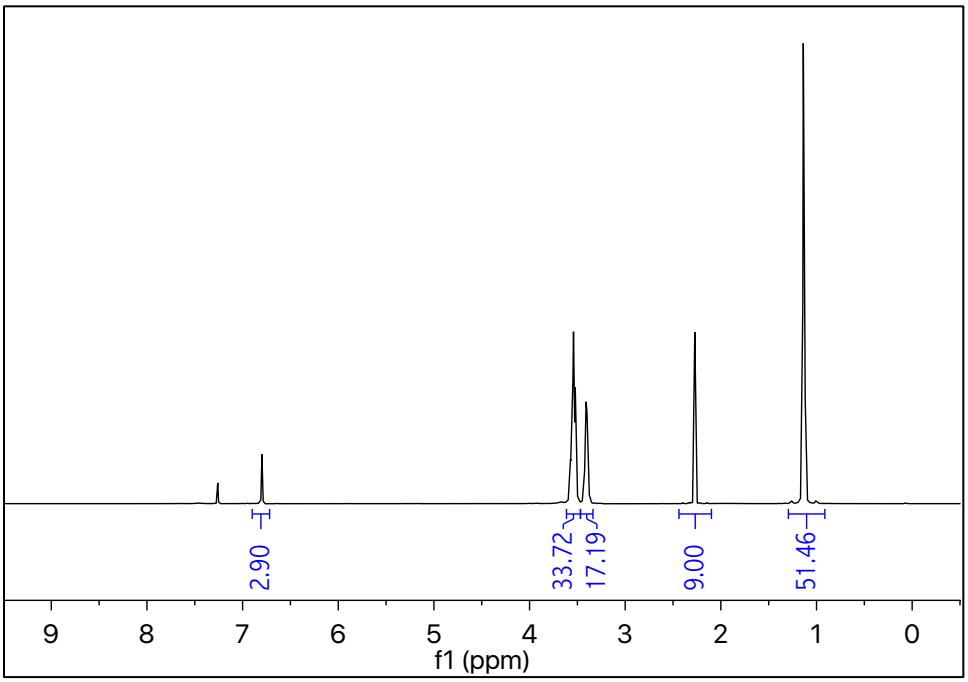


Figure S2. ^{1}H NMR spectrum in $CDCl_3$ of polymerization using **1** after 4 hours with no CTA (26.1% conversion of PO).

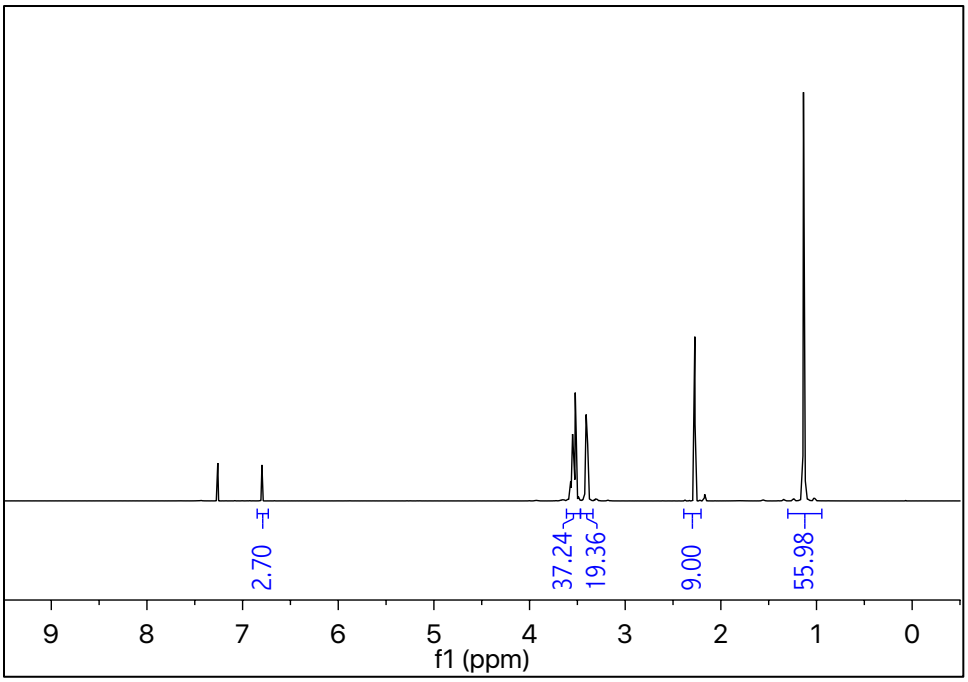


Figure S3. ^{1}H NMR spectrum in $CDCl_3$ of polymerization using **1** after 4 hours with 1,6-HD as the CTA (28.0% conversion of PO).

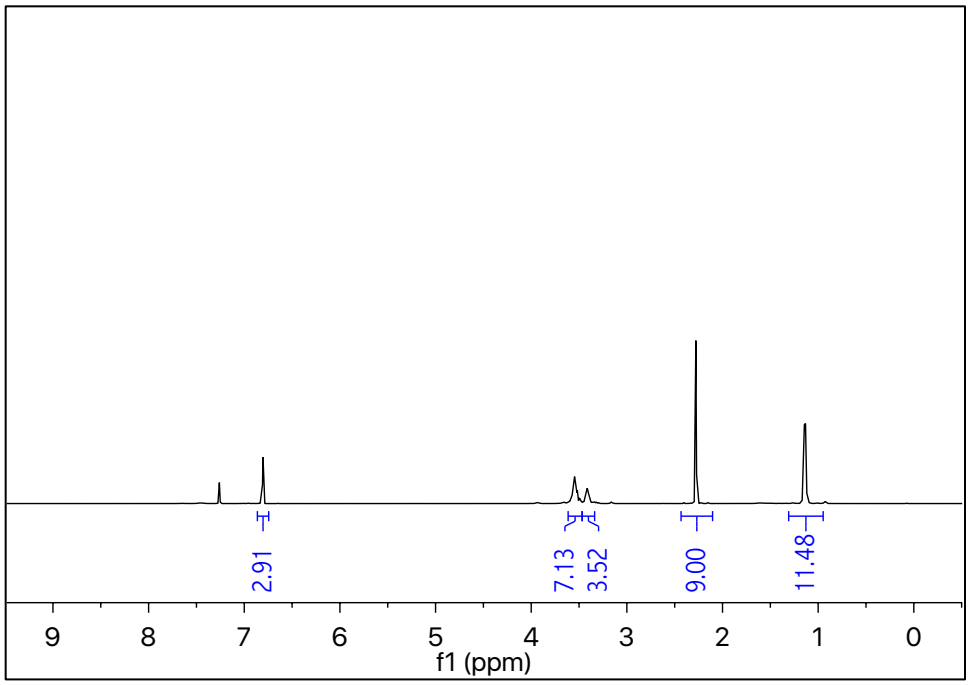


Figure S4. ^{1}H NMR spectrum in $CDCl_3$ of polymerization using **1** after 4 hours with 1,2-BD as the CTA (5.8% conversion of PO).

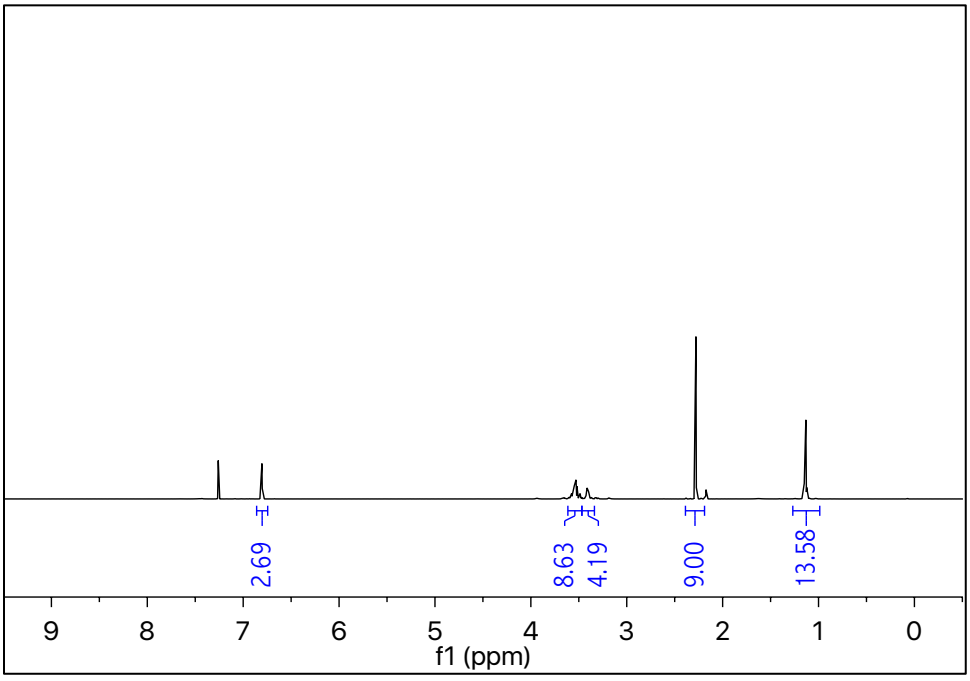


Figure S5. ^{1}H NMR spectrum in $CDCl_3$ of polymerization using **1** after 4 hours with H_2O as the CTA (6.6% conversion of PO).

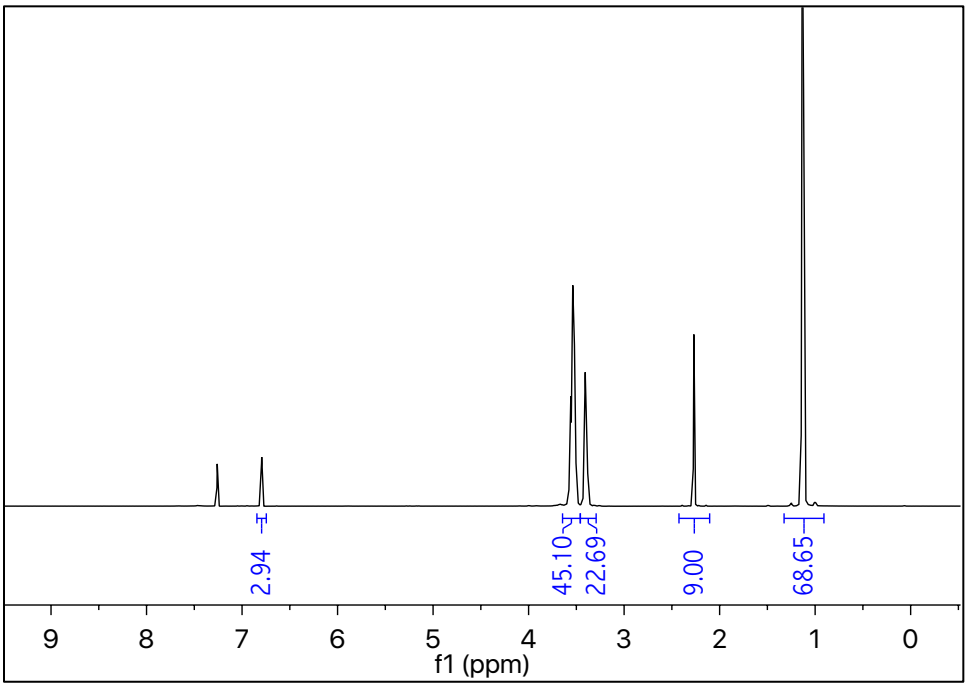


Figure S6. ^{1}H NMR spectrum in $CDCl_3$ of polymerization using **8** after 4 hours with no CTA (34.8% conversion of PO).

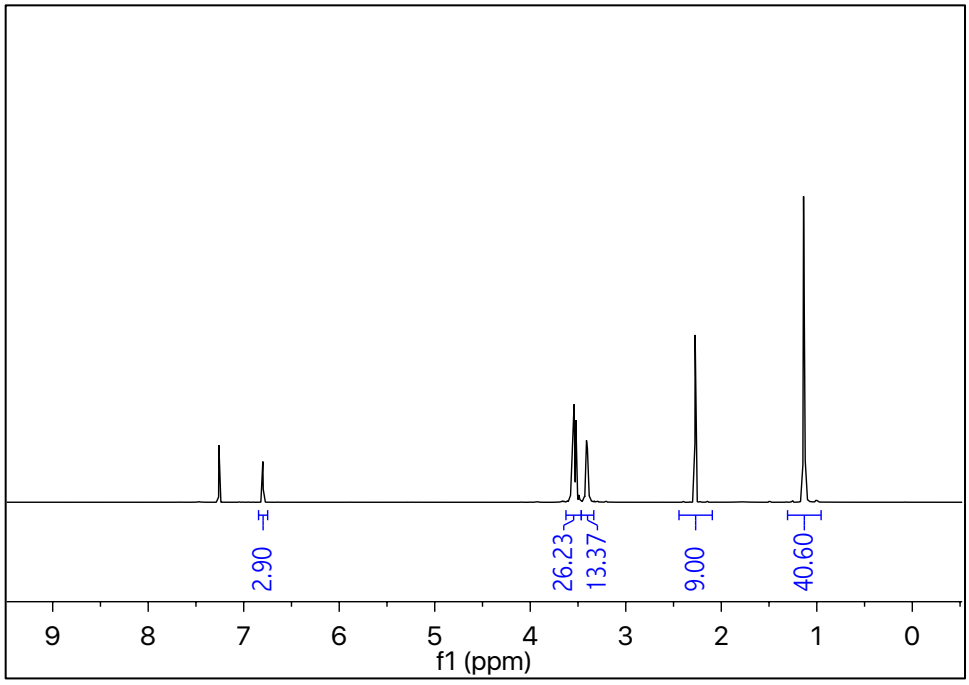


Figure S7. ^{1}H NMR spectrum in $CDCl_3$ of polymerization using **8** after 4 hours with 1,2-PD as the CTA (20.4% conversion of PO).

V. Mass Spectrometry Analysis

General sample preparation: A 20 mL scintillation vial and stir bar was charged with **1** (2.0 mg, 0.0013 mmol), [PPN][OAc^{F3}] (0.9 mg, 0.0013 mmol) and DME (2.25 mL). When appropriate, PO (0.75 mL, 10.7 mmol) and/or the corresponding CTA was added (0.013 mmol, 1,6-HD: 1.6 mg; 1,4-BD: 1.2 μL; 1,2-BD: 1.2 μL; 1,2-PD: 1.0 μL; water: 0.2 μL). Final sample preparation consisted of removing a 90 μL aliquot of the reaction mixture and diluting into 200 μL of DME. Solvents used in the MS experiments were dried by stirring over calcium hydride for 72 hours.

Data were preliminarily analyzed in Thermo Fisher's Qual Browser tool and then exported as text files for further processing in MatLab. Species were assigned by the primary ion clusters observed. Representative tables for all assignable species observed in Figures 1A and 1B are provided.

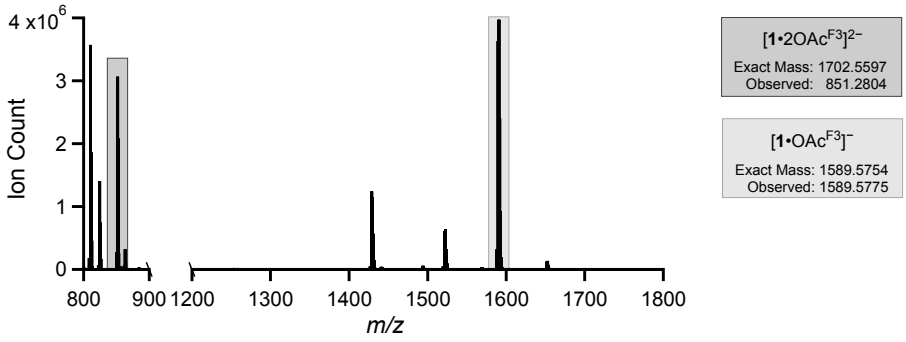


Figure S8. Mass spectrum of the activated complex ([**1**•OAc^{F3}][PPN]) in the presence of 1,6-HD and absence PO (extended *m/z* range for Figure 1A to show doubly ionized complex). Experiments in which 1,4-BD was substituted for 1,6-HD appears almost identical.

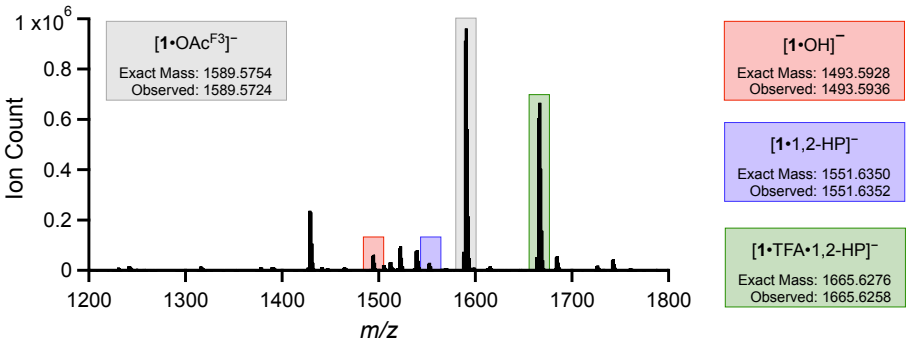


Figure S9. Mass spectrum of the activated complex ([**1**•OAc^{F3}][PPN]) in the presence of 1,2-PD and absence PO. The 1,2-HP complex is observed (TFA = Trifluoroacetic acid).

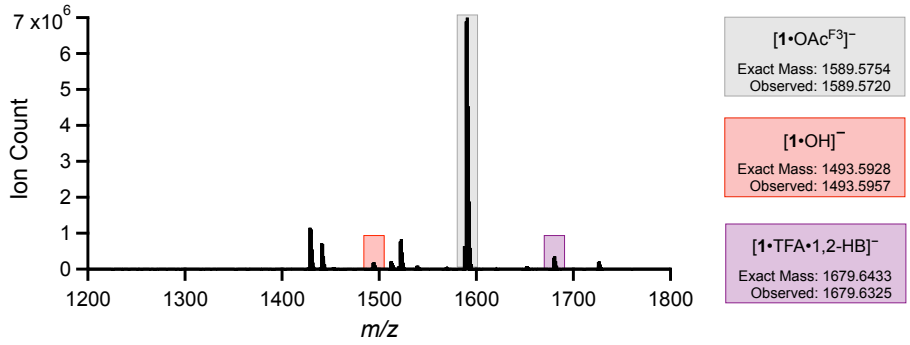


Figure S10. Mass spectrum of the activated complex ([**1**•OAc^{F3}][PPN]) in the presence of 1,2-BD and absence PO. A 1,2-HB complex is observed (TFA = Trifluoroacetic acid).

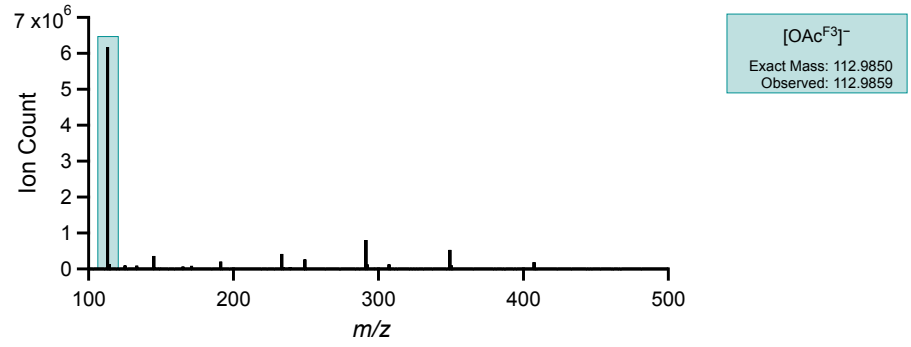


Figure S11. Low *m/z* mass spectrum of the activated complex ([**1**•OAc^{F3}][PPN]) in the presence of 1,6-HD and PO after 1.0 h (extended *m/z* range for Figure 1C to show off-scale [OAc^{F3}]$^-$ signal).

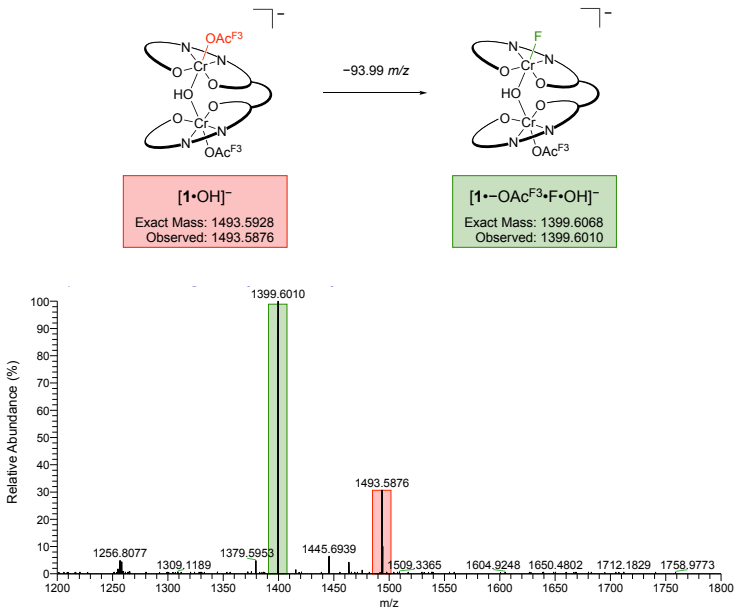


Figure S12. CID on [**1**•OH]⁻ (1493.5876 *m/z*) with normalized collision energy = 13. The primarily resulting fragment was 1399.6010 *m/z*, consistent with $[OAc^{F3}]^-$ fragmenting to F^-. No observed loss or fragmentation of $[OH]^-$.

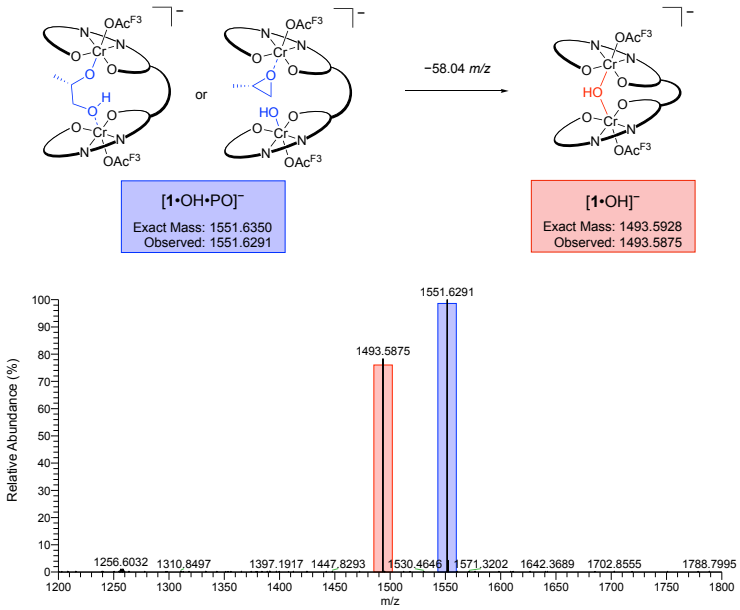


Figure S13. CID on [**1**•OH•PO]⁻ (1551.6291 *m/z*) with normalized collision energy = 11. The primarily resulting fragment was 1493.5875 *m/z*, consistent with the loss of PO.

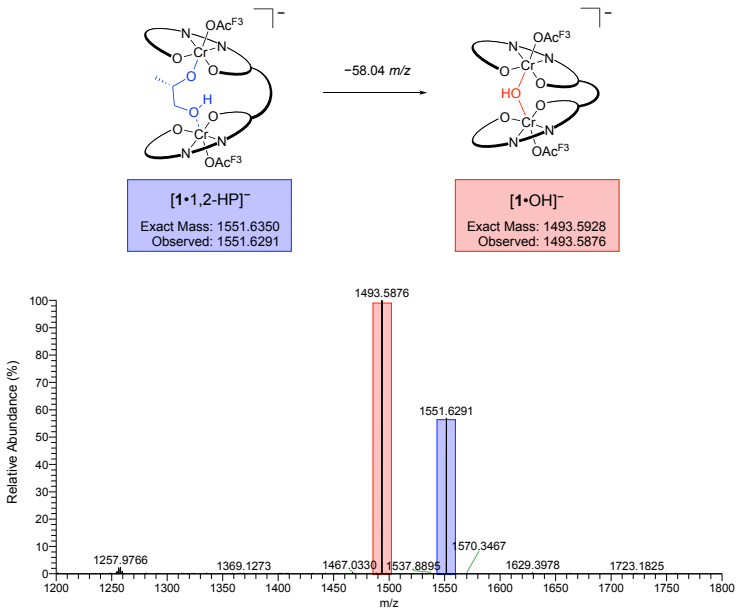


Figure S14. CID on [**1**•1,2-HP]⁻ (1551.6291 *m/z*) with normalized collision energy = 11. The primarily resulting fragment was 1493.5876 *m/z*, consistent with the loss of PO.

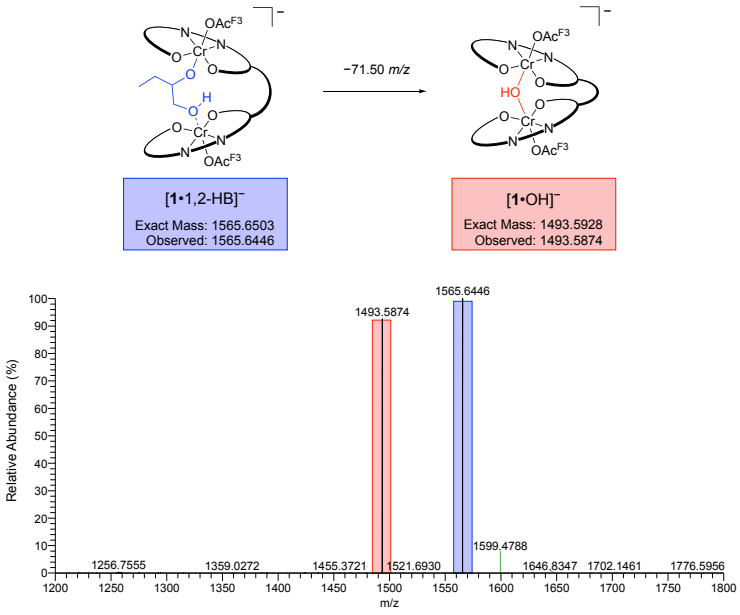
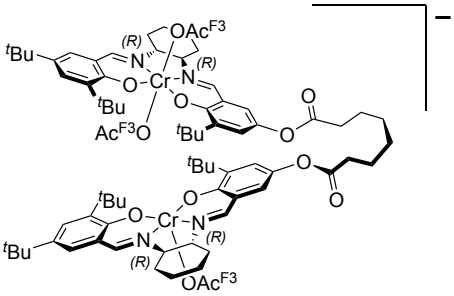


Figure S15. CID on [**1**•1,2-HB]⁻ (1565.6446 *m/z*) with normalized collision energy = 12. The primarily resulting fragment was 1493.5874 *m/z*, consistent with the loss of 1,2-butylene oxide.

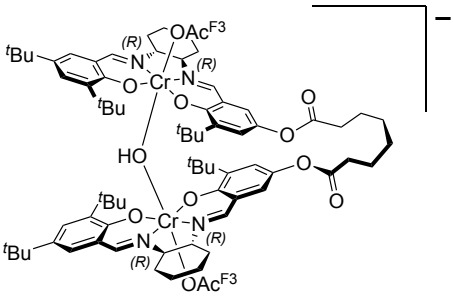
Table S1: Assignable Cr species from Figure 1A and Figure 1B

Proposed Structure:



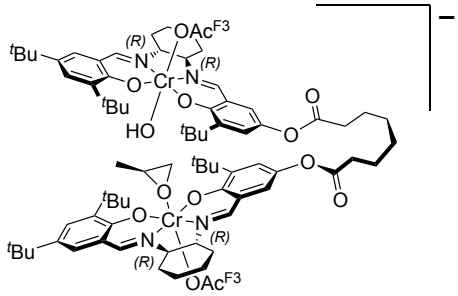
Experimental Mass	Experimental Relative Area	Simulated Mass	Simulated Relative Area	Δ ppm	Total Area
1587.5806	8.0	1587.5806	9.6	0.03	7872
1588.5846	7.6	1588.5838	9.3	0.47	7510
1589.5775	91.4	1589.5754	93.8	1.32	91765
1590.5774	100.0	1590.5780	100.0	-0.36	97533
1591.5782	60.5	1591.5803	58.1	-1.35	59062
1592.5800	23.4	1592.5822	24.1	-1.39	22870
1593.5827	4.8	1593.5842	7.9	-0.98	4910
1594.5863	1.0	1594.5861	2.1	0.13	1054

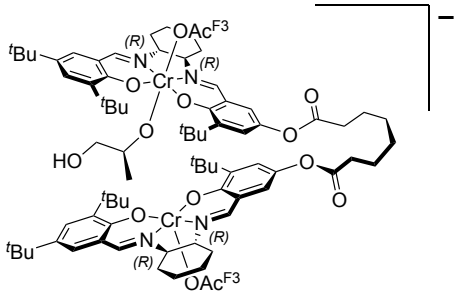
Proposed Structure:



Experimental Mass	Experimental Relative Area	Simulated Mass	Simulated Relative Area	Δ ppm	Total Area
1491.5962	8.2	1491.5984	9.8	-1.46	1159
1492.5976	7.3	1492.6014	9.3	-2.56	1072
1493.5891	94.4	1493.5928	95.9	-2.49	13483
1494.5925	100.0	1494.5957	100.0	-2.14	14096
1495.5970	55.9	1495.5978	56.7	-0.57	8079
1496.5970	20.1	1496.5998	22.9	-1.93	2808
1497.6034	4.0	1497.6018	7.3	1.09	617
1498.6054	0.8	1498.6036	1.9	1.18	134

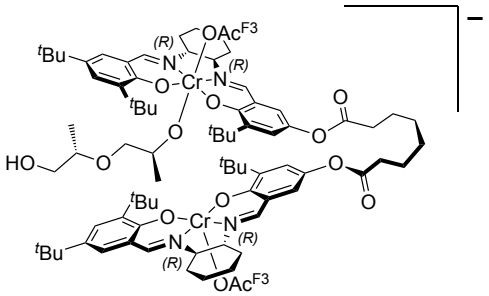
Proposed Structure:

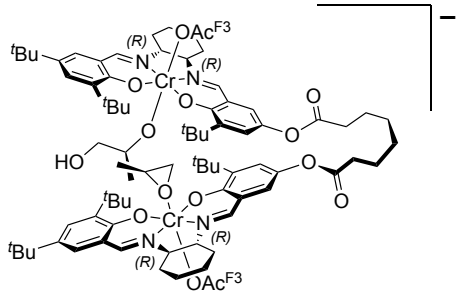




Experimental Mass	Experimental Relative Area	Simulated Mass	Simulated Relative Area	Δ ppm	Total Area
1549.6401	8.6	1549.6404	9.5	-0.20	1683
1550.6429	8.3	1550.6434	9.3	-0.29	1638
1551.6352	94.2	1551.6350	92.9	0.16	18792
1552.6400	100.0	1552.6376	100.0	1.49	20362
1553.6341	59.7	1553.6398	58.6	-3.66	12151
1554.6408	24.3	1554.6418	24.4	-0.65	4885
1555.6485	7.2	1555.6437	8.0	3.06	1519
1556.6455	1.8	1556.6459	2.2	-0.22	361

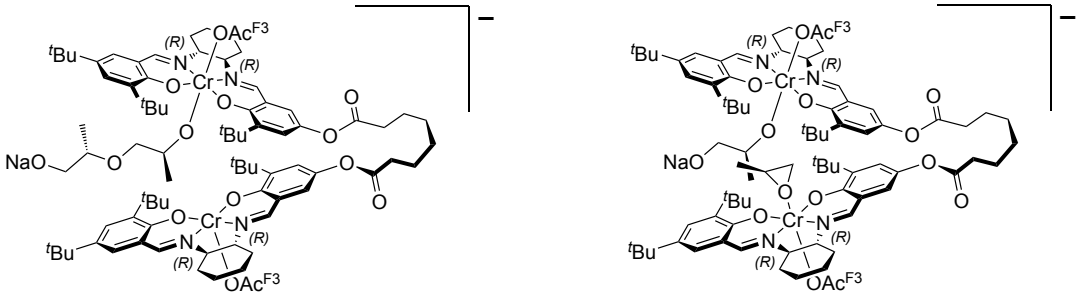
Proposed Structure:





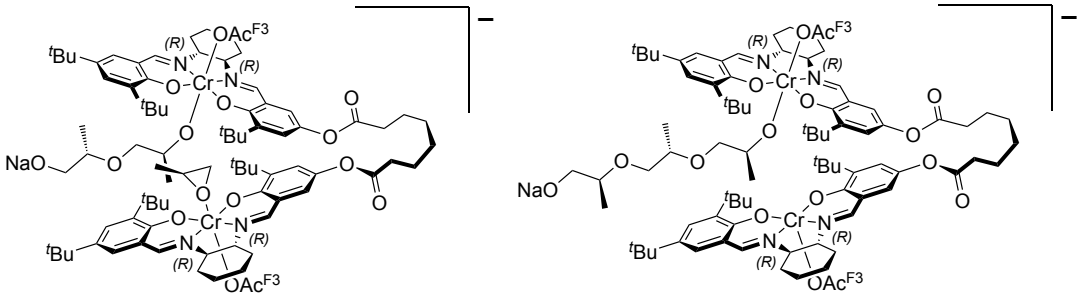
Experimental Mass	Experimental Relative Area	Simulated Mass	Simulated Relative Area	Δ ppm	Total Area
1607.6801	8.0	1607.6820	9.2	-1.16	1349
1608.6850	7.3	1608.6851	9.3	-0.07	1272
1609.6725	91.8	1609.6767	90.1	-2.65	16352
1610.6792	100.0	1610.6795	100.0	-0.18	18535
1611.6807	60.7	1611.6816	60.4	-0.55	11147
1612.6832	22.2	1612.6836	25.9	-0.22	4047
1613.6866	5.6	1613.6858	8.8	0.54	1123
1614.6849	1.4	1614.6878	2.5	-1.79	298

Proposed Structure:



Experimental Mass	Experimental Relative Area	Simulated Mass	Simulated Relative Area	Δ ppm	Total Area
1629.6634	7.7	1629.6628	9.2	0.38	255
1630.6640	7.6	1630.6662	9.3	-1.31	255
1631.6594	87.4	1631.6575	90.1	1.14	2984
1632.6618	100.0	1632.6601	100.0	1.08	3424
1633.6590	56.3	1633.6624	60.5	-2.11	1916
1634.6633	19.5	1634.6646	26.0	-0.79	673
1635.6685	5.5	1635.6665	8.8	1.22	201
1636.6684	1.4	1636.6687	2.5	-0.15	54

Proposed Structure:



Experimental Mass	Experimental Relative Area	Simulated Mass	Simulated Relative Area	Δ ppm	Total Area
1687.7064	7.2	1687.7049	8.9	0.90	413
1688.7086	7.4	1688.7077	9.4	0.51	426
1689.6985	87.3	1689.6997	87.5	-0.72	4948
1690.7024	100.0	1690.7020	100.0	0.24	5736
1691.7006	59.6	1691.7044	62.3	-2.25	3456
1692.7063	22.6	1692.7066	27.5	-0.19	1304
1693.7063	6.1	1693.7086	9.6	-1.33	383
1694.7138	1.5	1694.7107	2.8	1.83	95

VI. Computational Analysis and Coordinates

Quantum chemical calculations were conducted utilizing Density Functional Theory (DFT) with the Q-Chem 4.3 ab initio quantum chemistry package. Consistent with previous work,[6] gas phase geometry optimizations were performed with the B3LYP density functional[7] with spin unrestricted formalism and a mixed 6-31G/6-31G* basis set.[8] The 6-31G* basis set was applied to all heavy atoms and reactive carbons, while hydrogens and non-reactive carbons were treated with 6-31G basis set (Figure S16). Previous literature[9] work has found that the heptet state corresponding to two chromium (III) of spin 3/2 was the preferred electronic state. As such all calculations were performed using this charge and spin for chromium. Frequency calculations were conducted at the same level of theory with the same basis set, ensuring that all optimized structures were stable minima or transitions states. Single point energies calculated with the Solvent Model based on Density (SMD) solvation model were performed at B3LYP level of theory with def2-TZVP basis set and def2/J auxiliary set with RIJCOSX integration method.[10–13] Transition state (TS) structures were determined using the double-ended variant of the Growing String Method (GSM).[14–16] GSM was used to find the exact transition state between an optimized reactant and product by finding the minimum energy pathway and TS saddle point between the two structures on the potential energy surface (PES). GSM calculations were considered converged when the transition state node has a RMS gradient less than 0.0005 HT/ Å. The EMSL Basis Set Library was the source of all basis sets used.[17]

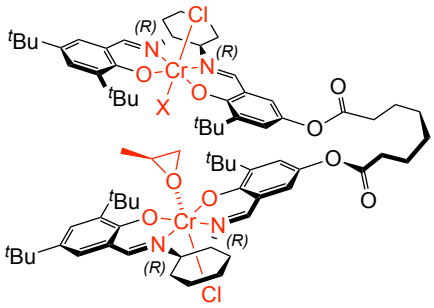


Figure S16. Visual representation of mixed basis set application. Atoms in red were modeled with the 6-31G* basis set and atoms in black were modeled with the 6-31G basis set. "X" is $[OH]^-$, $[1,2\text{-HP}]^-$, or oligomer.

Truncation of this bimetallic chromium catalyst was implement to aid in reducing computation time. This truncation consisted of removing the *para*-^{t}Bu groups. In all calculations, $[Cl]^-$ anions were used rather than $[OAc^{F3}]^-$. Consistent activation energies and relative resting state energies provided quantitative agreement between models (Figure S17).

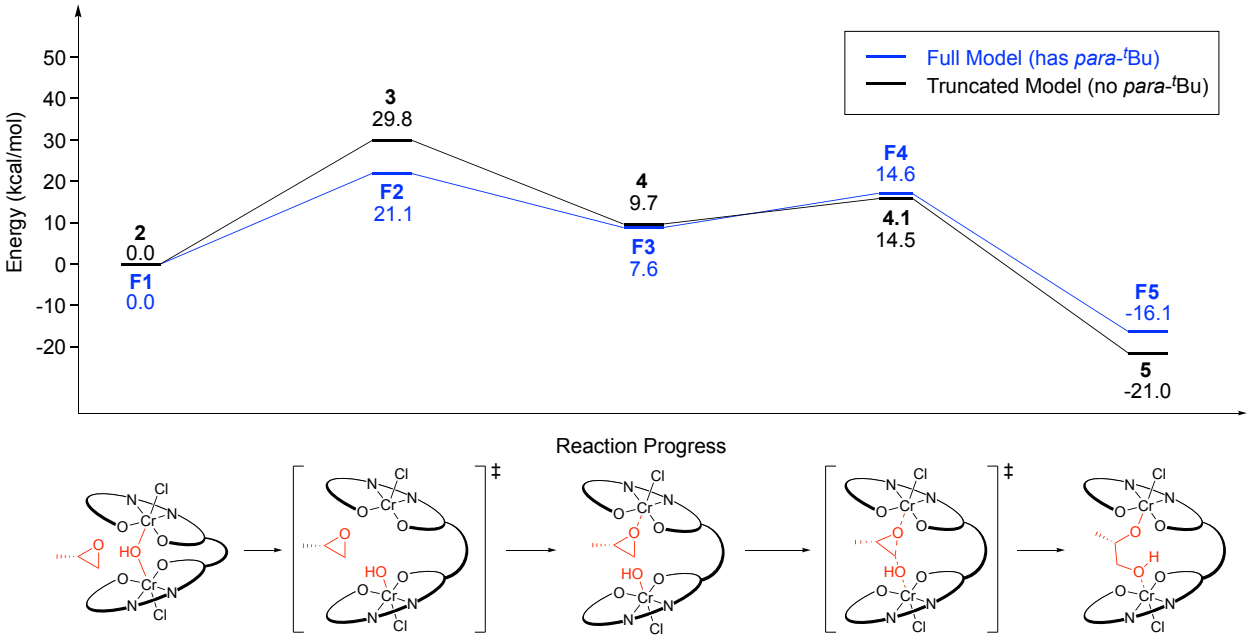


Figure S17. Electronic PES comparison for full catalyst and truncated models.

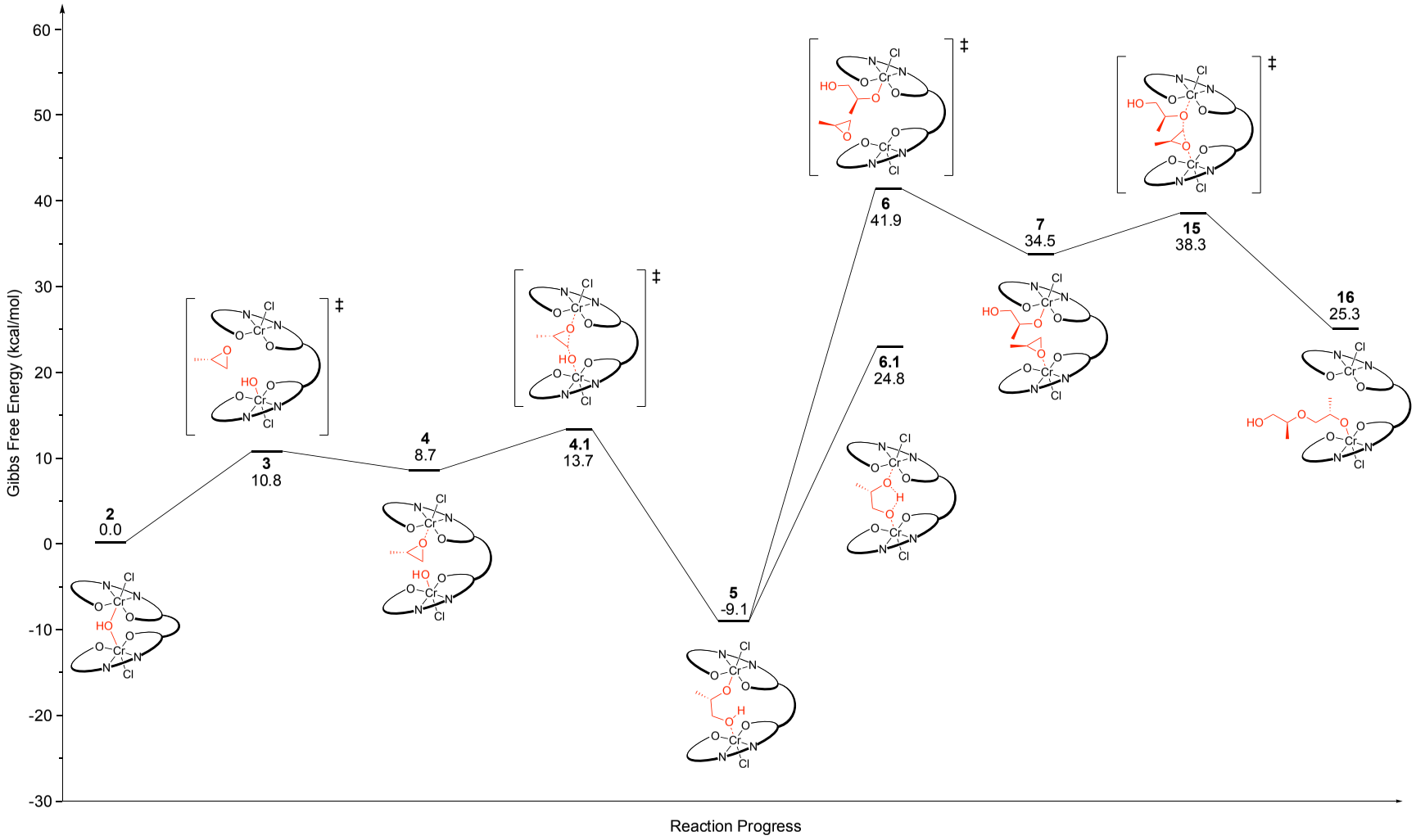


Figure S18. Gibbs free energy PES of ring opening epoxide polymerization starting from hydroxide.

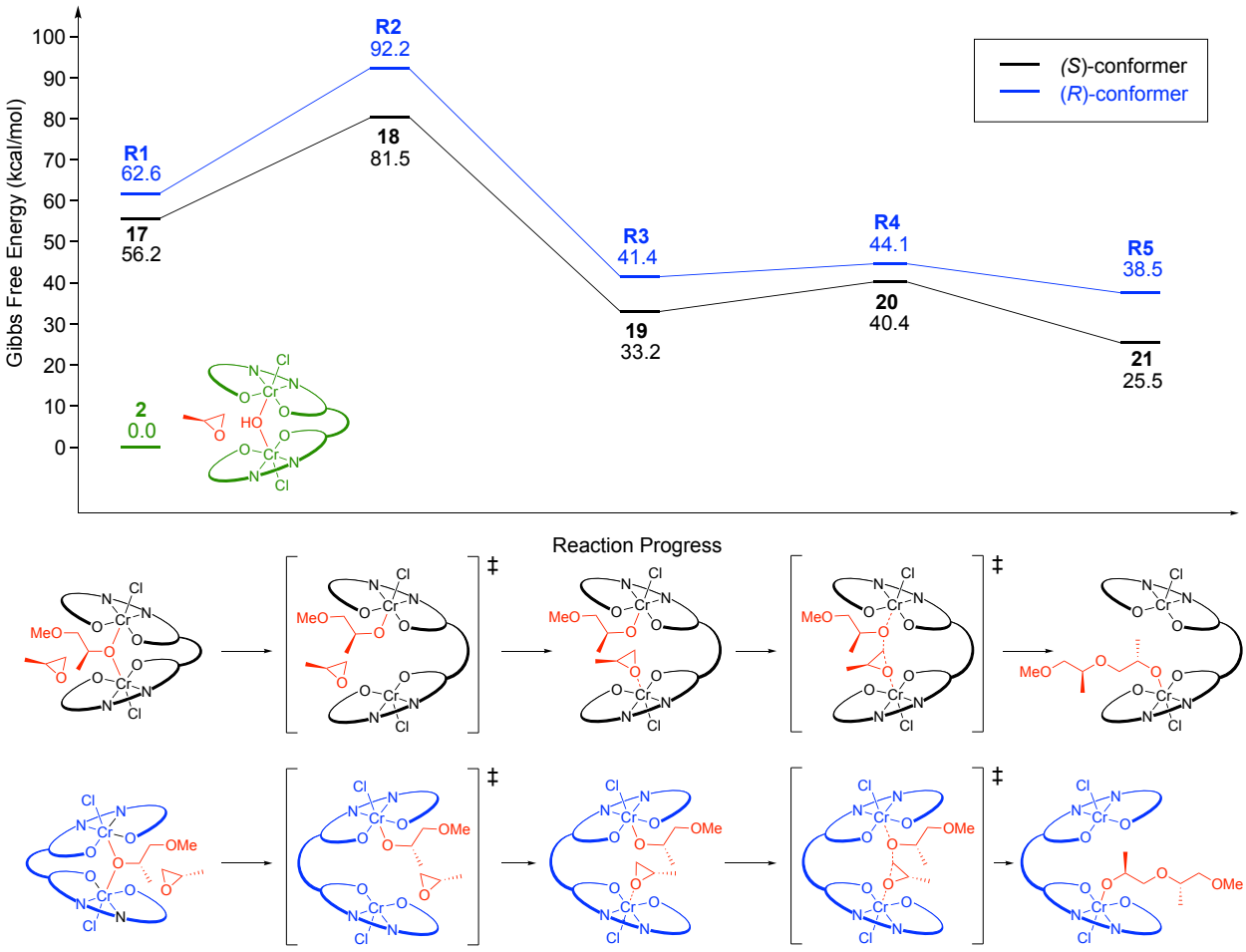


Figure S19. Gibbs free energy PES for (*S*)- and (*R*)-conformers of short chain ring-opening epoxide polymerization. Energies are referenced to **2.**

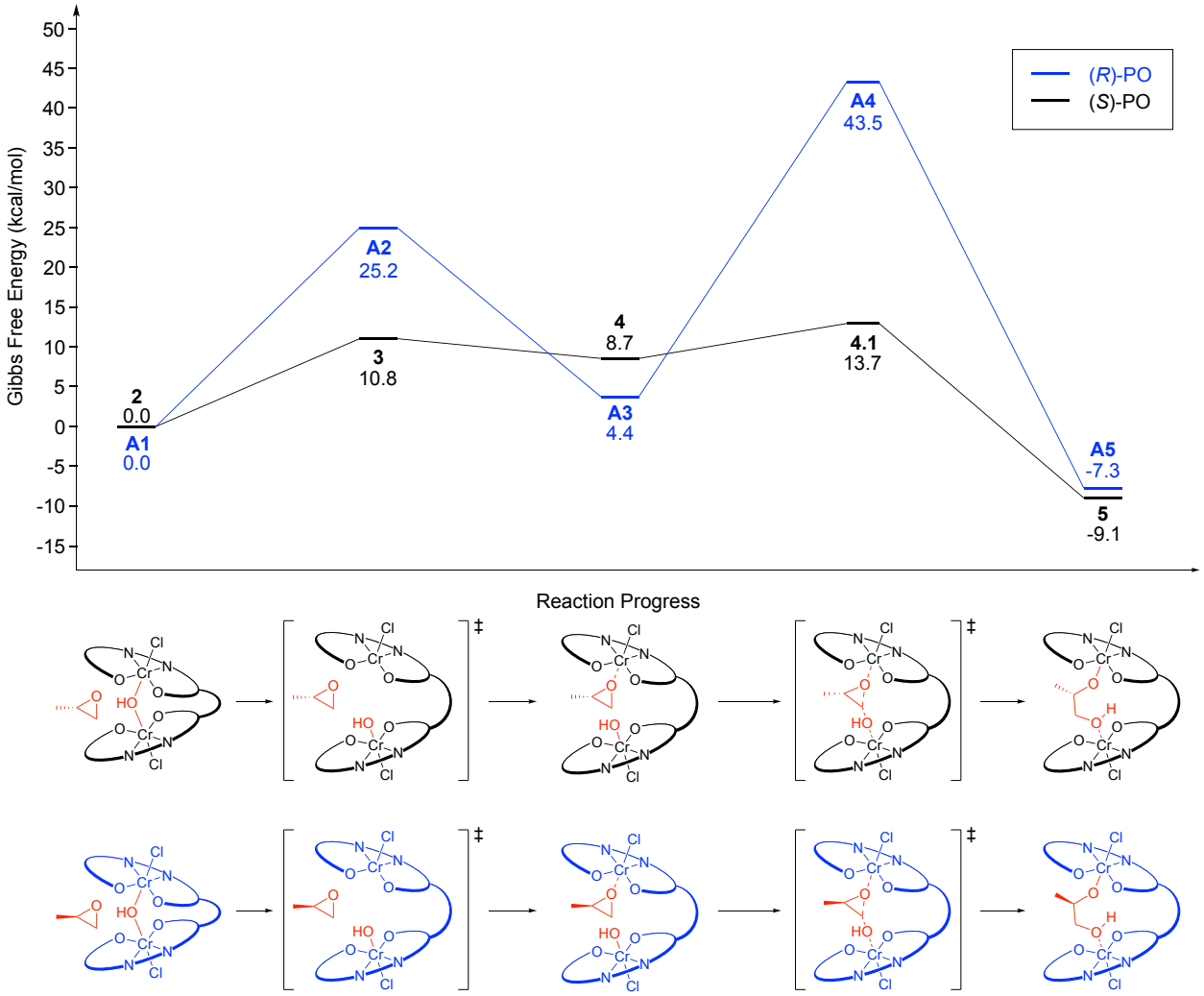


Figure S20. Gibbs free energy PES of short chain ring-opening epoxide polymerization with (*R*)- and (*S*)-PO.

Table S2. Total Electronic Energies and Free Energy Corrections

species	SMD/B3LYP/def2-TZVP Energy (Hartree)	Gibbs Free Energy Correction at 298.15 K (Hartree)
2	-6393.732	1.291
3	-6393.704	1.289
4	-6586.806	1.376
4.1	-6586.798	1.354
5	-6586.835	1.375
6	-6586.824	1.371
6.1	-6586.824	1.371
7	-6779.897	1.463
15	-6779.890	1.435
16	-6779.911	1.466
17	-6626.061	0.841
18	-6626.076	0.858
19	-6819.169	0.938
20	-6819.152	0.927
21	-6819.175	0.918
F1	-6708.327	-
F2	-6708.294	-
F3	-6901.415	-
F4	-6901.426	-
F5	-6901.464	-
R1	-6626.631	0.570
R2	-6626.609	0.529
R3	-6819.721	0.574
R4	-6819.701	0.532

R5	-6819.747	0.571
A1	-6394.244	0.512
A2	-6587.287	0.476
A3	-6587.320	0.518
A4	-6587.258	0.488
A5	-6587.339	0.509

Table S3. XYZ coordinates and Gibbs Free Energy or Electronic Energy (Hartree) for all reported structures

2:
-6393.7323

Cr	-1.8110	-1.4892	1.1730
Cr	0.3640	-0.9169	-1.9613
Cl	-3.4994	-1.5725	2.8336
Cl	1.5905	-0.0610	-3.7990
N	-2.0714	-3.4752	0.7874
N	-3.2645	-1.2770	-0.2169
N	0.8995	0.6916	-0.8677
N	2.0798	-1.6946	-1.1703
O	-1.2722	-0.0697	-2.5193
O	-2.2935	5.8489	-0.3159
O	-0.4245	-1.9546	2.4583
O	-2.8112	5.2543	-2.4747
O	-1.6105	0.4247	1.3015
O	-5.5050	4.5039	-1.6592
O	-5.5746	4.2457	0.6214
O	0.0375	-2.6075	-2.8677
O	-0.4578	-1.6483	-0.2898
C	-1.2976	3.4967	-1.6069
C	0.9552	-5.2939	1.7625
C	-0.9054	-4.6742	-4.5721
C	1.4701	-3.0267	3.3898
C	1.6664	-1.8576	4.3715
C	-2.2148	-3.9626	-4.1552
C	-1.5429	1.2187	-2.5384
C	-0.1540	-3.7938	-5.6071
C	0.0506	-4.2050	1.7299
C	-1.3037	-5.9912	-5.2746
C	0.4416	-1.7670	5.3203
C	0.3269	-3.0227	2.5068
C	1.8210	-0.5150	3.6152
C	-2.3399	3.9218	-2.4020
C	-1.1733	-4.3863	0.9742
C	-2.5687	1.7112	-3.4210
C	-2.8144	6.0787	-1.3940
C	-2.9527	3.0443	-3.3111
C	-3.5494	7.3654	-1.7433
C	-1.6149	4.1464	3.6282
C	-0.0250	2.7050	2.3717
C	-2.0238	0.2353	-5.3991
C	-3.9235	-0.3978	-3.8692
C	-3.5186	-5.0679	-0.5968
C	-3.7675	8.2421	-0.5002
C	-3.1625	0.7915	-4.5021
C	-3.3483	-3.7099	0.0951
C	-4.9481	-5.1809	-1.1655
C	-3.5841	-2.5446	-0.9146
C	-1.4605	2.7693	2.9474
C	-2.5624	1.3168	1.1210
C	-2.5171	2.5567	1.8470
C	-4.8009	7.6168	0.4570
C	-3.6351	1.0969	0.1935
C	-4.1593	1.5410	-5.4129
C	-5.0222	-2.6426	-1.4569
C	-3.8606	-0.1624	-0.4814
C	-5.2871	-4.0124	-2.1112
C	-1.6192	1.6731	4.0353
C	-3.4983	3.5137	1.5922
C	-4.5916	2.1063	-0.0441
C	-4.5207	3.2876	0.6625
C	-6.2524	7.7851	-0.0424
C	-6.0337	4.7071	-0.5827
C	-7.2183	6.7214	0.5261
C	-7.3293	5.4743	-0.3816
C	-0.8717	2.1525	-1.6853
C	2.3290	-4.1219	3.3595
C	2.1000	-5.2483	2.5369
C	2.9287	-2.0437	5.2414
C	0.0077	-4.9234	-3.3586
C	0.2656	1.8158	-0.8658
C	0.5179	-3.7943	-2.6127
C	0.4213	-6.2010	-2.9927
C	1.3641	-6.4337	-1.9651
C	1.5577	-4.0260	-1.6410
C	2.0281	0.4260	0.0509
C	1.9484	-5.3514	-1.3330
C	2.3207	-2.9577	-1.0280
C	2.9435	-0.6275	-0.6345
C	2.8576	1.6686	0.4215
C	4.0788	-1.0511	0.3029
C	4.0801	1.3072	1.2887

C	4.9306	0.1851	0.6603
H	-2.7562	-4.5860	-3.4365
H	0.7392	-6.1615	1.1448
H	0.3542	-2.6857	5.9153
H	-2.0033	-2.9908	-3.7075
H	0.7634	-4.2998	-5.9361
H	2.6629	-0.5860	2.9205
H	0.1102	-2.8247	-5.1767
H	-0.4217	-6.5312	-5.6425
H	-1.8636	-6.6532	-4.5998
H	0.5769	-0.9181	6.0046
H	2.0247	0.2916	4.3335
H	-2.8535	-3.8169	-5.0377
H	-1.3100	-5.3840	0.5525
H	-1.3130	-0.3508	-4.8146
H	-2.7680	-5.1717	-1.3919
H	0.1222	3.5167	1.6471
H	-2.9628	7.8959	-2.5065
H	-1.5045	4.9626	2.9019
H	-2.8080	8.3553	0.0175
H	-3.2818	-0.9238	-3.1612
H	-0.7980	-3.6339	-6.4835
H	-0.4785	-1.6211	4.7493
H	-0.8364	4.2519	4.3940
H	-1.9449	-5.7524	-6.1319
H	-2.8555	-2.6490	-1.7291
H	0.7011	2.8335	3.1869
H	0.9152	-0.2748	3.0574
H	-1.4817	1.0587	-5.8808
H	-5.6561	-5.1742	-0.3229
H	-4.8228	-0.0332	-3.3550
H	-4.1042	9.2424	-0.8087
H	-3.3497	-5.8789	0.1235
H	-2.5924	4.2397	4.1179
H	-5.0696	-6.1383	-1.6892
H	0.1487	1.7434	1.8872
H	-2.4632	-0.4015	-6.1801
H	-3.7395	3.4519	-3.9306
H	-4.4993	7.0878	-2.2164
H	-4.2375	-1.0971	-4.6562
H	-4.5597	6.5565	0.5867
H	-4.7148	8.0722	1.4535
H	-0.8795	1.8416	4.8311
H	-4.1133	-3.6032	0.8777
H	-3.6760	2.3806	-5.9282
H	-5.2050	-1.8598	-2.1962
H	-5.0126	1.9254	-4.8390
H	-4.6846	-4.0922	-3.0228
H	-4.6436	-0.1353	-1.2365
H	-3.5031	4.4568	2.1204
H	-4.5395	0.8434	-6.1698
H	-2.6236	1.7176	4.4732
H	-6.3410	-4.0733	-2.4138
H	-1.4741	0.6765	3.6150
H	-6.6020	8.7934	0.2225
H	-6.2766	7.7293	-1.1414
H	-5.7125	-2.4815	-0.6159
H	-5.3844	1.9372	-0.7635
H	-6.8892	6.4123	1.5267
H	-7.6795	5.7723	-1.3751
H	-8.2276	7.1412	0.6301
H	-8.0596	4.7779	0.0522
H	-0.8066	4.1728	-0.9233
H	3.2023	-4.1257	4.0015
H	0.0303	-2.4604	-0.0921
H	2.8003	-6.0775	2.5431
H	3.0147	-1.1931	5.9286
H	0.0289	-7.0588	-3.5271
H	3.8363	-2.0824	4.6240
H	2.8708	-2.9629	5.8382
H	0.6007	2.6189	-0.2150
H	1.6552	-7.4488	-1.7143
H	1.6013	-0.0342	0.9510
H	3.3708	-0.1429	-1.5248
H	2.2397	2.3887	0.9674
H	3.1852	2.1454	-0.5135
H	2.7130	-5.4989	-0.5750
H	3.1702	-3.2826	-0.4228
H	3.6603	-1.5115	1.2092
H	3.7347	0.9917	2.2794
H	4.7094	-1.8031	-0.1885
H	5.3977	0.5623	-0.2623
H	4.6976	2.2036	1.4359
H	5.7403	-0.1030	1.3436

3:
-6393.7045

Cr	-5.1454	-1.9238	1.2169
Cr	-4.1709	1.1129	-3.2460
Cl	-7.1731	-2.1874	2.4798

Cl	-2.6675	1.8436	-4.7705	C	-6.0136	2.2634	1.3158
O	-5.6416	2.2139	-3.7517	C	-9.0557	9.6037	-2.8309
O	-5.5528	8.2495	-1.3744	C	-6.5777	0.6395	-0.4644
O	-3.9599	-2.3663	2.7074	C	-8.5617	4.3671	-6.2086
O	-6.2117	7.7244	-3.5136	C	-7.7850	-3.2454	-1.9382
O	-5.1687	0.0425	1.4019	C	-6.6818	-0.6844	-1.0427
O	-8.9955	5.0134	0.2783	C	-7.8462	-4.6202	-2.6315
O	-7.9487	3.9082	-1.4495	C	-6.1920	1.5941	3.7350
O	-4.9859	-0.4312	-3.9736	C	-6.6854	3.2414	0.5856
O	-3.5924	-1.7118	0.1166	C	-7.2638	1.6639	-1.1547
N	-5.1572	-3.8874	0.7064	C	-7.3029	2.9397	-0.6408
N	-6.2764	-1.7820	-0.4997	C	-9.3757	8.0906	-2.9715
N	-3.6989	2.4189	-1.7744	C	-8.7669	4.8647	-0.9067
N	-2.8454	-0.0377	-2.2760	C	-8.9639	7.2244	-1.7700
C	-5.1595	5.6705	-2.5648	C	-9.3222	5.7432	-2.0098
C	-2.0374	-5.3895	1.8658	C	-5.0173	4.2664	-2.6691
C	-6.3051	-2.0804	-5.8974	C	-0.7785	-3.9901	3.3672
C	-1.7714	-3.0125	3.3899	C	-0.8989	-5.1849	2.6251
C	-1.5928	-1.6882	4.1502	C	-0.2308	-1.6084	4.8736
C	-7.5114	-1.3753	-5.2246	C	-5.3040	-2.6175	-4.8575
C	-5.7594	3.5236	-3.6405	C	-4.1245	3.6429	-1.7221
C	-5.5791	-1.0713	-6.8289	C	-4.6198	-1.7088	-3.9839
C	-3.0737	-4.4285	1.8319	C	-4.9791	-3.9739	-4.7714
C	-6.8781	-3.2100	-6.7814	C	-4.0099	-4.4681	-3.8760
C	-2.7013	-1.5107	5.2205	C	-3.5809	-2.1959	-3.1321
C	-2.9800	-3.2333	2.6309	C	-2.7715	1.8638	-0.7465
C	-1.6571	-0.5112	3.1408	C	-3.3079	-3.5800	-3.0766
C	-6.0139	6.3233	-3.4316	C	-2.7617	-1.3332	-2.3094
C	-4.2082	-4.7176	0.9859	C	-1.9127	0.7954	-1.4740
C	-6.6906	4.2176	-4.4846	C	-1.8478	2.8844	-0.0654
C	-6.0253	8.5654	-2.4504	C	-0.9819	0.0614	-0.4979
C	-6.7685	5.6007	-4.3739	C	-0.9269	2.1596	0.9357
C	-6.4643	9.9727	-2.8098	C	-0.0835	1.0806	0.2318
C	-5.7943	3.9988	3.1766	H	-8.1264	-2.1097	-4.6908
C	-3.9569	2.3546	2.8185	H	-2.1500	-6.2943	1.2703
C	-6.6960	2.7256	-6.5315	H	-2.6524	-2.3264	5.9545
C	-8.4195	2.3774	-4.7084	H	-7.1792	-0.5982	-4.5338
C	-6.2943	-5.5766	-0.8496	H	-4.7531	-1.5677	-7.3548
C	-7.7943	10.0928	-3.5841	H	-0.8098	-0.5662	2.4453
C	-7.5752	3.4365	-5.4697	H	-5.1824	-0.2304	-6.2563
C	-6.3087	-4.2137	-0.1447	H	-6.0845	-3.7292	-7.3339
C	-7.6059	-5.7724	-1.6370	H	-7.4285	-3.9444	-6.1783
C	-6.4474	-3.0792	-1.1970	H	-2.5498	-0.5579	5.7486
C	-5.4894	2.5514	2.7332	H	-1.6044	0.4435	3.6824
C	-5.8993	0.9304	0.7708	H	-8.1328	-0.9070	-5.9997

H	-4.2293	-5.7229	0.5556
H	-5.9841	2.0523	-6.0505
H	-5.4354	-5.6191	-1.5354
H	-3.4454	3.0962	2.1929
H	-6.5144	10.5324	-1.8700
H	-5.3087	4.7319	2.5181
H	-7.9198	11.1563	-3.8307
H	-9.1417	1.9253	-5.4013
H	-6.2896	-0.6891	-7.5752
H	-3.6867	-1.5126	4.7519
H	-5.4104	4.1436	4.1939
H	-7.5715	-2.7702	-7.5082
H	-5.6165	-3.1829	-1.9038
H	-3.6299	2.5003	3.8574
H	-2.5863	-0.5480	2.5683
H	-6.1426	3.4667	-7.1224
H	-8.4423	-5.8173	-0.9238
H	-8.9660	2.8423	-3.8787
H	-7.7041	9.5520	-4.5342
H	-6.1797	-6.3819	-0.1124
H	-6.8736	4.1943	3.1803
H	-7.5806	-6.7323	-2.1699
H	-3.6771	1.3507	2.5006
H	-7.3388	2.1445	-7.2077
H	-7.4333	6.1677	-5.0123
H	-5.6630	10.4189	-3.4180
H	-7.7742	1.5930	-4.3112
H	-9.9101	10.1753	-3.2184
H	-8.9695	9.8655	-1.7649
H	-5.8148	1.7942	4.7478
H	-7.1828	-4.1442	0.5177
H	-8.0331	5.1097	-6.8201
H	-7.9086	-2.4616	-2.6887
H	-9.2191	4.8917	-5.5026
H	-7.0741	-4.6479	-3.4119
H	-7.1814	-0.7112	-2.0132
H	-6.7874	4.2417	0.9754
H	-9.1856	3.7601	-6.8752
H	-7.2748	1.7717	3.7238
H	-8.8196	-4.7449	-3.1253
H	-6.0091	0.5473	3.4821
H	-10.4587	7.9646	-3.1193
H	-8.8883	7.6995	-3.8754
H	-8.5993	-3.1421	-1.2075
H	-7.7580	1.4479	-2.0944
H	-7.8907	7.3014	-1.5816
H	-8.9288	5.4123	-2.9743
H	-9.4661	7.5755	-0.8591
H	-10.4155	5.6323	-2.0226
H	-4.6020	6.2109	-1.8143
H	0.1342	-3.8356	3.9324
H	-3.6337	-0.7673	-0.0852
H	-0.1019	-5.9223	2.6463
H	-0.1607	-0.6445	5.3931
H	-5.4883	-4.6819	-5.4138
H	0.6052	-1.6787	4.1651
H	-0.1285	-2.4087	5.6179
H	-3.7882	4.2901	-0.9120
H	-3.8063	-5.5329	-3.8312
H	-3.3867	1.3642	0.0158
H	-1.3042	1.3368	-2.2129
H	-2.4303	3.6475	0.4602
H	-1.2520	3.3878	-0.8413
H	-2.5517	-3.9328	-2.3813
H	-2.0142	-1.8388	-1.7078
H	-1.5739	-0.5179	0.2201
H	-1.5465	1.6858	1.7048
H	-0.3532	-0.6476	-1.0524
H	0.5876	1.5628	-0.4954
H	-0.2757	2.8881	1.4354
H	0.5418	0.5562	0.9646

4:
-6586.8065

Cr	-3.0288	-1.5213	1.9789
Cr	1.5815	-0.9559	-3.3134
Cl	-4.9830	-1.9593	3.1489
Cl	2.1697	0.2157	-5.3448
N	-2.8387	-3.4433	1.3654
N	-4.0646	-1.3797	0.2272
N	2.4134	0.5422	-2.2109
N	3.4913	-1.6782	-3.2857
O	-0.1460	-0.0417	-3.2844
O	-1.2801	-1.2543	0.8746
O	-2.1417	4.5915	0.4984
O	-1.8321	-1.8871	3.4434
O	-1.5979	5.0590	-1.6802
O	-3.1254	0.3926	2.2082
O	-4.9891	4.6423	-1.7153
O	-6.4952	4.1870	-0.0379

O	1.0028	-2.5901	-4.2044	C	-5.3561	7.7082	-0.0826
O	1.2623	-1.7895	-1.6129	C	-6.0090	4.9022	-1.1095
C	0.0475	3.2851	-1.7236	C	-6.7931	7.1682	-0.2656
C	0.3905	-4.6862	2.5458	C	-6.9109	6.0885	-1.3742
C	-0.8844	-4.7073	-3.9696	C	-0.3578	-0.1371	1.1135
C	0.2658	-2.5122	4.3675	C	0.4565	2.0005	-2.1547
C	-1.0679	-0.2454	-0.1670	C	1.3620	-3.3730	4.3154
C	0.1730	-1.3697	5.3959	C	1.4442	-4.4518	3.4103
C	-1.2375	-3.8508	-2.7250	C	1.4170	-1.3090	6.3089
C	-0.4670	1.1511	-2.8623	C	0.6354	-4.9306	-3.9968
C	-1.3810	-3.9778	-5.2441	C	1.0869	-0.5256	1.2569
C	-0.7433	-3.8405	2.5354	C	1.8150	1.6252	-1.8389
C	-1.6680	-6.0332	-3.8514	C	1.5082	-3.7825	-3.9974
C	-1.0671	-1.5916	6.3033	C	1.2022	-6.2018	-3.9277
C	-0.8104	-2.7198	3.4332	C	2.5933	-6.4071	-3.8110
C	0.0457	0.0069	4.6934	C	2.9110	-3.9915	-3.7534
C	-1.2361	3.7137	-1.9632	C	3.7760	0.1852	-1.7582
C	-1.8051	-4.1795	1.6163	C	3.4274	-5.3067	-3.6997
C	-1.8202	1.6195	-3.0627	C	3.8321	-2.9073	-3.4821
C	-2.0262	5.3768	-0.4205	C	4.4448	-0.6156	-2.9185
C	-2.1726	2.8853	-2.6035	C	4.6602	1.3622	-1.3181
C	-2.2738	6.8775	-0.3516	C	5.8577	-1.0767	-2.5363
C	-3.8238	4.2704	4.1535	C	6.0793	0.8869	-0.9507
C	-1.9110	2.8527	3.4318	C	6.7270	0.1234	-2.1197
C	-2.3359	0.6209	-5.3116	H	-0.9834	-4.3939	-1.8042
C	-2.9332	-0.6768	-3.2366	H	0.4236	-5.5202	1.8482
C	-3.7468	-5.1416	-0.3281	H	-0.7709	0.5547	1.8395
C	-3.0250	7.2956	0.9199	H	-0.9751	-2.5433	6.8440
C	-2.8180	0.7462	-3.8424	H	-0.7081	-2.8975	-2.7273
C	-3.9056	-3.8115	0.4175	H	-1.1527	-4.5747	-6.1372
C	-4.9591	-5.3674	-1.2541	H	0.9363	0.2150	4.0873
C	-4.0332	-2.6249	-0.5781	H	-0.9020	-3.0019	-5.3346
C	-3.4474	2.8631	3.6398	H	-1.5025	-6.6755	-4.7262
C	-3.9809	1.2502	1.6896	H	-1.3794	-6.5892	-2.9496
C	-4.1662	2.5289	2.3232	H	-1.1318	-0.7775	7.0390
C	-4.5027	6.8661	0.8864	H	-0.0499	0.7935	5.4540
C	-4.7178	0.9574	0.4909	H	-1.9299	0.3906	-0.3460
C	-4.2328	1.3660	-3.8380	H	-2.3127	-3.6517	-2.7282
C	-5.2315	-2.8392	-1.5174	H	-1.6926	-5.1402	1.1082
C	-4.6740	-0.3141	-0.1863	H	-1.3252	0.2040	-5.3474
C	-5.1367	-4.1987	-2.2409	H	-2.8265	-5.1279	-0.9244
C	-3.8365	1.8334	4.7331	H	-1.6336	3.5407	2.6270
C	-5.0076	3.4508	1.7118	H	-1.2914	7.3687	-0.4053
C	-5.5347	1.9479	-0.1062	H	-3.5167	5.0454	3.4389
C	-5.6610	3.1718	0.5028	H	-2.5334	6.8265	1.7806

H	-2.0115	-1.2377	-3.3818
H	-2.4711	-3.8431	-5.1840
H	-1.9811	-1.6057	5.7052
H	-3.3035	4.4467	5.1026
H	-2.7403	-5.8071	-3.7886
H	-3.1063	-2.5896	-1.1645
H	-1.4203	3.1641	4.3644
H	-0.8380	0.0310	4.0566
H	-2.3300	1.6077	-5.7923
H	-5.8657	-5.4615	-0.6375
H	-3.1367	-0.6199	-2.1640
H	-2.9566	8.3855	1.0462
H	-3.6671	-5.9633	0.3955
H	-4.9036	4.3581	4.3323
H	-4.8364	-6.3091	-1.8043
H	-1.5687	1.8500	3.1831
H	-3.0189	-0.0371	-5.8684
H	-3.1747	3.2725	-2.7256
H	-2.8141	7.1739	-1.2577
H	-3.7603	-1.2104	-3.7270
H	-4.5319	5.8093	0.6140
H	-4.9383	6.9422	1.8935
H	-3.2717	2.0499	5.6506
H	-4.8291	-3.8328	1.0125
H	-4.2491	2.3398	-4.3420
H	-5.2740	-2.0423	-2.2673
H	-4.5981	1.5067	-2.8124
H	-4.2863	-4.1788	-2.9348
H	-5.2202	-0.3415	-1.1294
H	-5.1707	4.4225	2.1531
H	-4.9166	0.6933	-4.3704
H	-4.9089	1.9039	4.9565
H	-6.0395	-4.3507	-2.8469
H	-3.6163	0.8142	4.4093
H	-5.3947	8.7392	0.2986
H	-4.8677	7.7539	-1.0668
H	-6.1521	-2.7939	-0.9174
H	-6.0497	1.7364	-1.0374
H	-7.1522	6.7446	0.6816
H	-6.6222	6.5136	-2.3404
H	-7.4702	7.9891	-0.5354
H	-7.9500	5.7424	-1.4299
H	-0.5317	-0.6605	-1.0168
H	0.7565	3.9345	-1.2185
H	2.1912	-3.2146	4.9950
H	1.1427	-2.7468	-1.6999
H	2.3226	-5.0885	3.4021
H	1.2905	-0.4819	7.0178
H	0.5545	-7.0716	-3.9425
H	2.3316	-1.1286	5.7286
H	1.5422	-2.2374	6.8814
H	1.2528	-1.0327	2.2142
H	1.3804	-1.1645	0.4162
H	2.3508	2.3530	-1.2245
H	1.6934	0.3921	1.2411
H	2.9937	-7.4151	-3.7720
H	3.6429	-0.5159	-0.9211
H	4.4874	0.0550	-3.7880
H	4.2129	1.8680	-0.4539
H	4.7125	2.0909	-2.1401
H	4.4969	-5.4374	-3.5439
H	4.8805	-3.2044	-3.3911
H	5.7899	-1.7917	-1.7021
H	6.0251	0.2243	-0.0735
H	6.3208	-1.5995	-3.3828
H	6.8382	0.8037	-2.9773
H	6.6974	1.7495	-0.6685
H	7.7325	-0.2202	-1.8428

4.1:
-6586.7986

Cr	1.3919	-0.4314	-3.1091
Cr	-2.8141	-1.7512	2.2813
Cl	1.9754	0.8775	-5.0197
Cl	-4.7652	-1.3594	3.7150
O	1.0913	-1.5726	-1.4270
O	0.9463	-2.0181	-4.1450
O	-6.1917	3.9206	0.1854
O	-5.1764	4.4218	-1.8313
O	-2.4762	0.1510	1.9448
O	-1.9552	5.6012	-2.2503
O	-1.6384	-1.9995	3.8159
O	-1.8889	5.6105	0.0549
O	-1.4155	-2.3231	1.1011
O	-0.3665	0.3235	-2.9890
N	3.3290	-1.0743	-3.0265
N	2.0745	1.0386	-1.9096
N	-4.0517	-1.7430	0.6692
N	-3.2571	-3.7491	2.2874
C	6.3591	0.6927	-1.3310

C	5.5552	1.3541	-0.1972	C	-2.1476	4.3583	3.1833
C	5.5777	-0.4789	-1.9589	C	-2.7683	7.5467	-1.1532
C	4.1795	1.8359	-0.6972	C	-2.3779	3.3563	-3.0073
C	4.2035	-0.0123	-2.4641	C	-2.1759	6.1627	-1.0090
C	3.7695	-2.2260	-3.4437	C	-2.0214	2.0330	-3.2504
C	3.6513	-4.5210	-4.2642	C	-2.5838	-4.6438	2.9405
C	3.3910	0.6791	-1.3317	C	-1.5045	4.2499	-2.3710
C	2.9853	-3.2949	-4.0140	C	0.8955	-0.7302	4.6153
C	2.9671	-5.6042	-4.7768	C	-1.0980	-3.0990	4.3037
C	1.5875	-5.4819	-5.0501	C	-0.8570	-0.8902	6.4517
C	1.5881	-3.1643	-4.3241	C	-1.2196	-5.5444	-5.6406
C	1.4527	2.1564	-1.6724	C	-1.5165	-4.4095	3.8847
C	0.9111	-2.9815	1.1859	C	-0.8905	-3.1311	-6.2394
C	0.8731	-4.3035	-4.8418	C	-0.7244	1.5984	-2.8182
C	1.4906	-1.6744	6.8587	C	-1.4146	-3.8098	-3.8502
C	0.1358	-5.4417	5.3480	C	0.3675	-1.5910	5.7980
C	0.5316	-4.1562	5.7738	C	-0.2985	-1.7050	-0.6720
C	0.1512	2.5241	-2.1616	C	-0.0541	-2.9870	5.2941
C	-0.0780	-1.8785	0.8203	C	-0.6387	-4.2009	-5.1407
C	-7.2564	5.5308	-1.1925	C	-0.8843	-5.5558	4.4234
C	-7.1971	6.7621	-0.2532	C	-0.2599	3.8596	-1.9397
C	-6.0951	4.5799	-1.0221	H	7.3261	0.3343	-0.9563
C	-5.9460	7.6506	-0.4501	H	6.1129	2.1993	0.2247
C	-5.2087	2.9444	0.5802	H	6.5743	1.4402	-2.1086
C	-5.3624	1.6349	0.1902	H	6.1614	-0.9067	-2.7829
C	-4.1628	3.3393	1.4258	H	5.4121	0.6298	0.6180
C	-2.1037	2.0492	4.1518	H	5.4361	-1.2732	-1.2109
C	-5.4134	-4.7729	-1.3498	H	4.8347	-2.4491	-3.3535
C	-4.6672	-0.6955	0.2178	H	4.7124	-4.5961	-4.0365
C	-5.3520	-3.3060	-0.8818	H	4.3143	2.6327	-1.4430
C	-4.3316	1.7466	-4.3039	H	3.6133	2.2623	0.1394
C	-4.4575	0.6606	0.6680	H	4.3289	0.7235	-3.2706
C	-4.7579	7.2548	0.4496	H	3.1860	-0.0845	-0.5672
C	-3.2312	2.4225	1.9073	H	3.4746	-6.5446	-4.9645
C	-3.3689	1.0407	1.5256	H	1.9424	-2.7102	0.9186
C	-2.0713	2.8554	2.8237	H	1.9377	2.9085	-1.0492
C	-4.2146	-3.1082	0.1327	H	0.6350	-3.9044	0.6597
C	-5.5654	-5.7299	-0.1547	H	0.8639	-3.1794	2.2598
C	-4.3613	-4.0681	1.3500	H	1.1720	-2.2380	7.7443
C	-2.9748	1.0707	-3.9899	H	2.3993	-2.1409	6.4578
C	-3.4551	8.0197	0.1397	H	1.0721	-6.3527	-5.4374
C	-4.4360	-5.5313	0.8774	H	1.7501	-0.6600	7.1838
C	-3.2733	-0.1818	-3.1206	H	0.6225	-6.3235	5.7525
C	-2.3264	0.6296	-5.3307	H	1.4011	-2.4839	-1.5910
C	-0.7313	2.6065	2.0741	H	1.3240	-4.0884	6.5098

H	0.3993	4.5550	-1.4333
H	-0.6590	-2.6313	-1.1146
H	-8.1807	4.9755	-0.9955
H	-8.1035	7.3531	-0.4399
H	-7.2588	5.8557	-2.2376
H	-7.2518	6.4171	0.7870
H	-6.1823	1.3457	-0.4599
H	-6.3105	-3.0283	-0.4182
H	-5.6470	7.6159	-1.5074
H	-6.2053	8.6985	-0.2398
H	-2.0220	0.9786	3.9699
H	-6.2464	-4.9060	-2.0522
H	-3.0413	2.2324	4.6911
H	-4.9846	1.0191	-4.8009
H	-4.0973	4.3821	1.7000
H	-5.4100	-0.8105	-0.5748
H	-4.4928	-5.0165	-1.9013
H	-4.8326	2.0933	-3.3930
H	-5.2021	-2.6475	-1.7465
H	-4.2167	2.6040	-4.9779
H	-5.2909	-3.7961	1.8703
H	-1.2700	2.3664	4.7931
H	-5.0417	7.4288	1.4969
H	-4.5582	6.1816	0.3664
H	-4.0012	-0.8220	-3.6379
H	-3.4538	7.5337	-2.0063
H	-3.3517	3.7356	-3.2772
H	-2.9897	-0.0768	-5.8474
H	-0.6314	1.5475	1.8270
H	-5.5712	-6.7724	-0.4994
H	-3.0771	4.5947	3.7174
H	-4.5995	-6.1995	1.7320
H	-3.6639	9.0961	0.0643
H	-3.6957	0.1158	-2.1560
H	-6.5363	-5.5519	0.3318
H	-2.1669	1.4939	-5.9868
H	0.1221	-0.6166	3.8556
H	0.1145	2.9045	2.7087
H	-3.2529	-3.3459	-0.3438
H	-2.2919	-5.4197	-5.8295
H	-1.3126	4.6046	3.8505
H	-1.6784	-0.8090	5.7382
H	-1.9675	-3.0449	-6.4345
H	-2.3655	-0.7565	-2.9397
H	-2.7539	7.8808	0.9704
H	-2.0713	4.9944	2.2969
H	-1.9493	8.2272	-1.4286
H	-0.7074	3.1990	1.1522
H	-3.4724	-5.8098	0.4252
H	-1.3630	0.1466	-5.1617
H	-2.8221	-5.7003	2.7911
H	-2.4897	-3.7529	-4.0646
H	-0.8055	-0.7964	-0.9711
H	1.1838	0.2663	4.9758
H	-0.5771	0.1164	6.7894
H	-1.1007	-6.3426	-4.8976
H	-0.7526	-5.8684	-6.5786
H	-0.5117	-2.1578	-5.9259
H	1.7783	-1.1992	4.1604
H	-0.3947	-3.4188	-7.1748
H	-1.0879	-2.8368	-3.4834
H	-1.2005	-1.4632	7.3222
H	0.1303	-0.9208	1.3130
H	-1.2174	-6.5374	4.0906
H	-1.2638	-4.5618	-3.0641

5:
-6586.835

Cr	-2.8453	-1.7230	2.1963
Cr	1.4379	-0.3409	-2.7524
Cl	-4.2876	-0.7997	3.9056
Cl	2.3891	1.1003	-4.2885
N	-3.4967	-3.5682	2.7647
N	-4.4793	-1.7861	0.9922
N	1.7109	0.9683	-1.2581
N	3.2719	-1.0125	-2.1443
O	-0.3633	0.2882	-2.9253
O	-1.9791	-2.7466	0.8139
O	-2.1096	5.6527	-0.1992
O	-1.3319	-1.8596	3.3928
O	-2.1374	5.5207	-2.4857
O	-2.3828	0.0306	1.4761
O	-4.9908	4.5306	-1.8343
O	-6.0827	3.9368	0.0964
O	1.2598	-1.8340	-3.9507
O	0.8094	-1.6909	-1.2740
C	-0.4790	3.8225	-1.8794
C	-0.5751	-5.4096	3.9675
C	0.2624	-3.6526	-5.8652
C	0.6857	-2.8715	4.0961

C	-0.5653	-1.7749	-0.7866	C	1.3694	-4.0485	4.3954
C	1.3453	-1.4830	4.2269	C	0.7584	-5.3191	4.3323
C	-0.9251	-3.5767	-4.8655	C	2.8305	-1.5866	4.6374
C	-0.7898	1.5258	-2.7439	C	1.5871	-3.8662	-5.1110
C	0.3145	-2.3407	-6.6959	C	-0.0725	-4.0588	0.2078
C	-1.3236	-4.2587	3.6297	C	1.1069	2.1123	-1.1901
C	-0.0298	-4.8084	-6.8480	C	2.0253	-2.8785	-4.1580
C	0.6096	-0.6598	5.3185	C	2.3871	-4.9881	-5.3107
C	-0.6936	-2.9640	3.6855	C	3.6045	-5.1908	-4.6218
C	1.2963	-0.6910	2.8927	C	3.2696	-3.0746	-3.4608
C	-1.6595	4.1859	-2.4826	C	2.7574	0.5292	-0.3211
C	-2.7082	-4.4689	3.2434	C	4.0339	-4.2422	-3.7134
C	-2.0740	1.9102	-3.2632	C	3.8148	-2.1302	-2.5095
C	-2.3990	6.1182	-1.2839	C	3.9059	-0.0840	-1.1742
C	-2.4612	3.2400	-3.1387	C	3.2736	1.5824	0.6650
C	-3.0606	7.4665	-1.5114	C	4.9820	-0.6895	-0.2575
C	-1.8312	4.1773	2.8275	C	4.3532	0.9633	1.5747
C	-0.5230	2.4738	1.5479	C	5.5010	0.3683	0.7385
C	-2.3509	0.2602	-5.1753	H	-0.9775	-4.4950	-4.2647
C	-3.3037	-0.2628	-2.8854	H	-1.0681	-6.3794	3.9243
C	-5.3109	-5.2893	2.2459	H	-0.0381	-2.1795	1.2410
C	-3.5778	8.0739	-0.1978	H	0.6989	-1.1583	6.2930
C	-3.0033	0.8666	-3.9058	H	-0.8184	-2.7158	-4.2032
C	-4.8685	-3.8200	2.2907	H	1.0962	-2.4082	-7.4643
C	-6.7413	-5.4082	1.6850	H	1.8140	-1.2518	2.1031
C	-4.9790	-3.1652	0.8696	H	0.5177	-1.4786	-6.0576
C	-1.8028	2.6947	2.3895	H	0.7616	-4.8974	-7.6036
C	-3.2945	0.9455	1.2170	H	-0.1273	-5.7688	-6.3250
C	-3.0395	2.3236	1.5488	H	1.0643	0.3386	5.3904
C	-4.8208	7.3267	0.3257	H	1.8035	0.2749	3.0262
C	-4.5428	0.6047	0.5859	H	-0.8726	-0.7539	-0.5680
C	-4.3609	1.4866	-4.3072	H	-1.8639	-3.4760	-5.4271
C	-6.3970	-3.3074	0.3028	H	-3.0659	-5.4959	3.3629
C	-5.0072	-0.7588	0.4181	H	-1.4104	-0.2363	-4.9285
C	-6.8305	-4.7851	0.2797	H	-4.6155	-5.8520	1.6048
C	-1.7245	1.8374	3.6815	H	-0.5433	3.1391	0.6803
C	-3.9494	3.2921	1.1254	H	-2.3238	8.1256	-1.9923
C	-5.4238	1.6248	0.1669	H	-1.7956	4.8555	1.9702
C	-5.1135	2.9409	0.4274	H	-2.7760	8.0254	0.5481
C	-6.0943	7.6952	-0.4627	H	-2.3866	-0.7774	-2.6020
C	-5.9425	4.6170	-1.0814	H	-0.6531	-2.1940	-7.1957
C	-7.2481	6.6824	-0.3018	H	-0.4462	-0.5486	5.0645
C	-7.1530	5.5044	-1.3019	H	-0.9549	4.3679	3.4606
C	-0.6457	-2.6542	0.4592	H	-0.9748	-4.6002	-7.3646
C	-0.0317	2.4855	-1.9895	H	-4.2585	-3.6905	0.2281

H	0.3629	2.7038	2.1593
H	0.2668	-0.5061	2.5839
H	-2.1556	1.0497	-5.9127
H	-7.4380	-4.8851	2.3571
H	-3.7704	0.1488	-1.9829
H	-3.8260	9.1330	-0.3568
H	-5.2586	-5.7247	3.2523
H	-2.7323	4.3919	3.4175
H	-7.0453	-6.4629	1.6556
H	-0.4650	1.4349	1.2120
H	-3.0387	-0.4722	-5.6216
H	-3.4142	3.5816	-3.5114
H	-3.8707	7.3221	-2.2360
H	-3.9930	-0.9872	-3.3424
H	-4.6244	6.2513	0.2756
H	-4.9823	7.5601	1.3870
H	-0.8880	2.2047	4.2939
H	-5.5266	-3.2464	2.9579
H	-4.2393	2.2594	-5.0773
H	-6.4381	-2.8933	-0.7128
H	-4.8611	1.9326	-3.4382
H	-6.1690	-5.3419	-0.4008
H	-5.8999	-0.8747	-0.2021
H	-3.7758	4.3371	1.3396
H	-5.0006	0.6932	-4.7140
H	-2.6523	1.9199	4.2586
H	-7.8522	-4.8711	-0.1128
H	-1.5649	0.7833	3.4602
H	-6.4260	8.6922	-0.1377
H	-5.8546	7.7820	-1.5332
H	-7.0896	-2.7247	0.9277
H	-6.3616	1.3698	-0.3182
H	-7.2619	6.2850	0.7214
H	-7.0933	5.8938	-2.3233
H	-8.2101	7.1845	-0.4718
H	-8.0521	4.8830	-1.2094
H	-1.1959	-2.1860	-1.5819
H	0.0909	4.5368	-1.2974
H	2.4110	-3.9975	4.6920
H	1.0652	-2.5808	-1.5661
H	1.3299	-6.2100	4.5739
H	3.2423	-0.5732	4.7219
H	2.0743	-5.7432	-6.0227
H	3.4157	-2.1366	3.8878
H	2.9475	-2.0854	5.6082
H	-0.1984	-4.6569	1.1160
H	-0.6178	-4.5457	-0.6137
H	1.4240	2.8479	-0.4507
H	1.0019	-4.0405	-0.0342
H	4.1928	-6.0827	-4.8132
H	2.3163	-0.2955	0.2535
H	4.3394	0.7296	-1.7732
H	2.4366	1.9501	1.2709
H	3.6921	2.4345	0.1099
H	4.9726	-4.3750	-3.1787
H	4.7748	-2.4216	-2.0772
H	4.5434	-1.5356	0.2911
H	3.8927	0.1708	2.1794
H	5.8201	-1.0741	-0.8517
H	5.9930	1.1755	0.1752
H	4.7390	1.7210	2.2687
H	6.2569	-0.0841	1.3929

6.1:
-6586.824

Cr	-2.1507	-1.3470	2.0775
Cr	0.5831	-1.0132	-2.5670
Cl	-4.0999	-1.0815	3.3264
Cl	1.4506	0.6461	-4.0524
O	-1.1988	-0.2372	-2.7144
O	-1.5354	5.7141	0.0290
O	-1.0064	-1.6012	3.6105
O	-2.7021	5.0386	-1.8396
O	-1.8610	0.5421	1.8342
O	-5.8231	3.7911	-2.0432
O	-5.7388	4.1694	0.2223
O	0.4273	-2.3189	-3.9865
O	-0.2261	-2.3289	-1.3252
O	-0.4216	-1.6208	0.9766
N	-2.5354	-3.3543	1.9955
N	-3.2164	-1.3493	0.3513
N	0.9777	0.2449	-1.0185
N	2.5397	-1.5262	-2.2708
C	-1.2136	3.1332	-1.2105
C	-0.7551	-5.1149	4.6693
C	-0.7759	-4.3847	-5.4950
C	0.5492	-2.6250	5.0699
C	1.3233	-1.3005	5.1926
C	-1.6200	-4.4293	-4.1901
C	-1.5060	1.0231	-2.4853

C	-1.1701	-3.1281	-6.3163	C	1.2337	-3.2840	-4.3279
C	-1.1866	-3.9837	3.9314	C	1.6043	-5.3478	-5.5719
C	-1.1544	-5.6244	-6.3333	C	2.9750	-5.3508	-5.2250
C	0.4301	-0.1865	5.7966	C	2.6146	-3.3249	-3.9189
C	-0.5823	-2.6995	4.1784	C	2.1964	-0.1405	-0.2897
C	1.8259	-0.8602	3.7889	C	3.4623	-4.3512	-4.4041
C	-2.2479	3.6952	-1.9270	C	3.1902	-2.3902	-2.9848
C	-2.1596	-4.2139	2.8904	C	3.2335	-0.5747	-1.3645
C	-2.5786	1.6439	-3.2192	C	2.7767	0.9014	0.6755
C	-2.2703	5.9382	-0.9203	C	4.5054	-1.1116	-0.6875
C	-2.9163	2.9579	-2.9195	C	4.0604	0.3605	1.3328
C	-2.8217	7.3199	-1.2456	C	5.0932	-0.0556	0.2705
C	-1.9574	4.6504	3.3885	C	0.1336	-3.4254	-0.5075
C	-0.3274	3.0050	2.4662	C	1.3426	-4.2527	-0.9403
C	-2.2018	0.5630	-5.4590	C	0.3300	-2.8600	0.9352
C	-3.9056	-0.4235	-3.8776	H	-1.4308	-5.3667	-3.6472
C	-3.5067	-5.1374	0.4425	H	-1.2412	-6.0709	4.4839
C	-3.4331	7.9805	0.0059	H	0.0965	-0.4738	6.8026
C	-3.2607	0.8931	-4.3740	H	-1.3815	-3.5854	-3.5377
C	-3.5386	-3.6867	0.9523	H	-0.6182	-3.1110	-7.2655
C	-4.5832	-5.3546	-0.6411	H	2.4866	-1.6330	3.3729
C	-3.3401	-2.6995	-0.2336	H	-0.9505	-2.2162	-5.7600
C	-1.7791	3.1687	2.9910	H	-0.6292	-5.6273	-7.2974
C	-2.7819	1.3936	1.4147	H	-0.9182	-6.5553	-5.8014
C	-2.7952	2.7348	1.9227	H	1.0127	0.7425	5.8750
C	-4.7143	7.2641	0.4686	H	2.4008	0.0712	3.8829
C	-3.7449	1.0192	0.4218	H	-2.6866	-4.3912	-4.4521
C	-4.3783	1.7349	-5.0275	H	-2.5496	-5.2339	2.8510
C	-4.4523	-2.8986	-1.2719	H	-1.3742	-0.0115	-5.0378
C	-3.8125	-0.3103	-0.1375	H	-2.5093	-5.3371	0.0253
C	-4.4250	-4.3478	-1.7928	H	-0.1565	3.6750	1.6150
C	-1.9652	2.3025	4.2643	H	-1.9802	7.9270	-1.6076
C	-3.7794	3.6047	1.4602	H	-1.8315	5.3081	2.5203
C	-4.7024	1.9454	-0.0422	H	-2.6814	7.9525	0.8043
C	-4.7210	3.2153	0.4960	H	-3.1489	-1.0508	-3.4030
C	-5.9077	7.4801	-0.4827	H	-2.2461	-3.1640	-6.5388
C	-6.2024	4.3772	-1.0478	H	-0.4446	-0.0019	5.1726
C	-7.1460	6.6198	-0.1183	H	-1.1983	4.9059	4.1386
C	-7.3335	5.3955	-1.0380	H	-2.2335	-5.6009	-6.5291
C	-0.8233	1.8036	-1.4943	H	-2.3788	-2.9017	-0.7203
C	0.9289	-3.7753	5.7550	H	0.3762	3.2760	3.2657
C	0.2741	-5.0167	5.5865	H	0.9935	-0.6966	3.1012
C	2.5673	-1.4414	6.0968	H	-1.7955	1.4896	-5.8827
C	0.7221	-4.3584	-5.1482	H	-5.5777	-5.2314	-0.1852
C	0.3186	1.3270	-0.7572	H	-4.7092	-0.2041	-3.1607

H	-3.6516	9.0367	-0.2092
H	-3.6745	-5.8441	1.2638
H	-2.9463	4.8261	3.8329
H	-4.5226	-6.3836	-1.0194
H	-0.1459	1.9705	2.1681
H	-2.6717	-0.0187	-6.2649
H	-3.7185	3.4565	-3.4432
H	-3.5512	7.2455	-2.0561
H	-4.3429	-0.9632	-4.7294
H	-4.5129	6.1923	0.5613
H	-4.9979	7.6165	1.4711
H	-1.2211	2.5978	5.0176
H	-4.5236	-3.4667	1.3894
H	-3.9711	2.6461	-5.4839
H	-4.3116	-2.2107	-2.1073
H	-5.1423	2.0257	-4.2947
H	-3.4683	-4.5216	-2.3025
H	-4.4432	-0.4142	-1.0195
H	-3.8376	4.6132	1.8443
H	-4.8553	1.1404	-5.8171
H	-2.9690	2.4542	4.6805
H	-5.2193	-4.4908	-2.5366
H	-1.8425	1.2429	4.0360
H	-6.1730	8.5474	-0.4668
H	-5.6033	7.2523	-1.5143
H	-5.4267	-2.6800	-0.8096
H	-5.4119	1.6505	-0.8037
H	-7.0668	6.2803	0.9217
H	-7.4699	5.7163	-2.0763
H	-8.0593	7.2248	-0.1933
H	-8.2443	4.8550	-0.7387
H	-0.6925	3.6898	-0.4487
H	1.7683	-3.7301	6.4389
H	0.6004	-5.8837	6.1515
H	3.0984	-0.4819	6.1163
H	1.2352	-6.1581	-6.1914
H	3.2548	-2.2083	5.7164
H	2.2883	-1.6993	7.1267
H	0.6424	1.9763	0.0549
H	3.6258	-6.1387	-5.5909
H	1.9464	-1.0306	0.2924
H	3.4688	0.3123	-1.9690
H	2.0367	1.1381	1.4487
H	2.9994	1.8260	0.1232
H	4.5070	-4.3469	-4.0987
H	4.2727	-2.4808	-2.8607
H	4.2458	-2.0213	-0.1255
H	3.8064	-0.5109	1.9505
H	5.2592	-1.3863	-1.4347
H	5.3905	0.8289	-0.3121
H	4.4836	1.1188	2.0043
H	5.9981	-0.4518	0.7500
H	-0.7358	-4.1080	-0.4743
H	1.2225	-4.6052	-1.9681
H	1.4479	-5.1241	-0.2774
H	2.2580	-3.6576	-0.8829
H	1.3853	-2.6350	1.1351
H	-0.0303	-3.5406	1.7022
H	-0.5498	-1.4805	-0.0339

6:
-6586.7947

Cr	1.1198	-0.8014	-2.6614
Cr	-2.5076	-1.5441	1.7741
Cl	2.3726	-0.1629	-4.6252
Cl	-4.3523	-1.5031	3.1043
O	0.9955	-0.1303	1.1588
O	-0.0019	-1.1498	-1.1009
O	0.6040	-2.5145	-3.4321
O	-5.8708	4.2035	0.3314
O	-5.8966	4.0643	-1.9622
O	-2.1580	0.3180	1.6620
O	-2.7210	4.9379	-1.6863
O	-1.1945	-1.9076	3.1044
O	-1.5546	5.6430	0.1679
O	-0.3933	0.2112	-3.3243
N	2.8908	-1.6120	-2.0258
N	1.8249	0.8400	-1.6798
N	-3.5816	-1.4075	0.0596
N	-2.6661	-3.5268	1.3724
C	1.1995	-1.5348	0.9361
C	0.3408	-3.5102	-0.4107
C	0.1244	-2.0423	-0.0385
C	5.9594	0.1907	-0.4437
C	5.2254	1.4470	0.0700
C	4.9907	-0.9932	-0.6634
C	4.0381	1.8196	-0.8420
C	3.8562	-0.5579	-1.6094
C	3.3327	-2.7780	-2.3840
C	3.2496	-5.0604	-3.2299

C	3.0913	0.6119	-0.9508	C	-0.6130	-3.0219	3.4914
C	2.5932	-3.8165	-3.0549	C	-0.6650	-1.1323	5.9405
C	2.6243	-6.1163	-3.8640	C	-1.3437	-5.8460	-5.4420
C	1.3090	-5.9412	-4.3515	C	-0.9153	-4.2907	2.8892
C	1.2578	-3.6330	-3.5625	C	-0.8677	-3.4217	-5.8086
C	1.1122	1.8930	-1.4331	C	-0.9395	1.2642	-2.7857
C	0.6113	-4.7443	-4.2228	C	-1.7866	-4.2208	-3.5962
C	1.7064	-1.7885	6.3748	C	0.6424	-1.6293	5.2647
C	0.7678	-5.3797	4.2675	C	0.3718	-2.9611	4.5402
C	1.0350	-4.1378	4.8844	C	-0.8177	-4.5650	-4.7589
C	-0.2234	2.1503	-1.9076	C	-0.2075	-5.4504	3.2923
C	-7.4131	5.5793	-0.8320	C	-0.8074	3.3668	-1.4801
C	-7.2170	6.7135	0.1979	H	0.4992	0.1388	0.3556
C	-6.2967	4.5514	-0.9235	H	1.1584	-2.0461	1.9004
C	-5.9833	7.6036	-0.0955	H	2.1842	-1.7142	0.4746
C	-4.8812	3.2038	0.5150	H	1.2972	-3.6340	-0.9207
C	-4.9418	1.9702	-0.0922	H	0.3420	-4.1305	0.4935
C	-3.8852	3.5013	1.4586	H	-0.4487	-3.8503	-1.0873
C	-1.9137	1.9690	4.0973	H	-0.8441	-2.0012	0.5283
C	-5.2045	-4.2078	-2.1036	H	6.7523	-0.0995	0.2586
C	-4.1516	-0.3115	-0.3390	H	5.9278	2.2878	0.1436
C	-5.0508	-2.7969	-1.5023	H	6.4418	0.4268	-1.4041
C	-4.6086	0.9896	-4.0282	H	5.5497	-1.8419	-1.0733
C	-4.0164	0.9743	0.2923	H	4.8415	1.2494	1.0817
C	-4.7435	7.2364	0.7462	H	4.5519	-1.3120	0.2932
C	-2.9327	2.5641	1.8466	H	4.3784	-3.0318	-2.1890
C	-3.0163	1.2485	1.2798	H	4.2627	-5.1686	-2.8473
C	-1.8336	2.9074	2.8637	H	4.3913	2.0878	-1.8475
C	-3.7771	-2.6981	-0.6442	H	3.5180	2.6888	-0.4249
C	-5.1616	-5.3003	-1.0202	H	4.2860	-0.1822	-2.5486
C	-3.7940	-3.7970	0.4520	H	2.7971	0.3151	0.0640
C	-3.1045	0.6340	-4.0259	H	3.1302	-7.0675	-3.9950
C	-3.4532	7.8932	0.2235	H	1.5115	2.6629	-0.7677
C	-3.8712	-5.1930	-0.1807	H	1.3875	-2.5081	7.1409
C	-2.9549	-0.8566	-3.6061	H	2.6707	-2.1150	5.9625
C	-2.5613	0.7814	-5.4726	H	0.8372	-6.7812	-4.8490
C	-0.4458	2.7607	2.1870	H	1.8543	-0.8144	6.8566
C	-1.9597	4.3619	3.3684	H	1.3173	-6.2650	4.5698
C	-2.9562	7.1984	-1.0572	H	1.7872	-4.1100	5.6631
C	-2.8459	2.7780	-2.6539	H	-0.2373	4.0397	-0.8563
C	-2.3280	5.8434	-0.7553	H	-8.3325	5.0262	-0.5872
C	-2.3102	1.5798	-3.1091	H	-8.1309	7.3225	0.1885
C	-1.9394	-4.4667	1.8909	H	-7.5377	5.9952	-1.8375
C	-2.0914	3.6755	-1.8731	H	-7.1301	6.2780	1.2012
C	1.1564	-0.5461	4.2819	H	-5.6898	1.7552	-0.8443

H	-5.9160	-2.5607	-0.8653
H	-5.7395	7.5330	-1.1658
H	-6.2279	8.6588	0.0942
H	-1.7396	0.9301	3.8154
H	-6.1462	-4.2655	-2.6644
H	-2.8984	2.0468	4.5774
H	-5.1510	0.2564	-4.6381
H	-3.8780	4.4928	1.8881
H	-4.8086	-0.3333	-1.2073
H	-4.3899	-4.3838	-2.8139
H	-5.0239	0.9845	-3.0120
H	-5.0168	-2.0646	-2.3147
H	-4.7859	1.9840	-4.4544
H	-4.6981	-3.6255	1.0550
H	-1.1454	2.2711	4.8226
H	-4.9259	7.5337	1.7887
H	-4.6114	6.1503	0.7491
H	-3.7484	-1.4500	-4.0834
H	-3.7630	7.0701	-1.7850
H	-3.8645	3.0649	-2.8775
H	-3.0853	0.0817	-6.1399
H	-0.2747	1.7307	1.8716
H	-5.2254	-6.2945	-1.4807
H	-2.9185	4.5250	3.8798
H	-3.8712	-5.9676	0.5964
H	-3.6321	8.9588	0.0208
H	-3.0185	-0.9676	-2.5219
H	-6.0298	-5.1894	-0.3534
H	-2.7195	1.8043	-5.8386
H	0.4535	-0.3596	3.4712
H	0.3368	3.0372	2.9071
H	-2.8931	-2.8567	-1.2789
H	-2.3680	-5.6681	-5.7935
H	-1.1535	4.5494	4.0881
H	-1.4475	-0.9651	5.1982
H	-1.8948	-3.3257	-6.1883
H	-1.9863	-1.2519	-3.9067
H	-2.6602	7.8269	0.9783
H	-1.8623	5.0768	2.5435
H	-2.1754	7.8055	-1.5386
H	-0.3881	3.4321	1.3237
H	-2.9926	-5.3539	-0.8216
H	-1.4913	0.5527	-5.4868
H	-2.0929	-5.4984	1.5689
H	-2.7819	-4.0242	-4.0148
H	1.3123	0.3900	4.8361
H	-0.4639	-0.1864	6.4615
H	-1.3602	-6.6958	-4.7465
H	-0.7245	-6.1145	-6.3078
H	-0.5578	-2.4747	-5.3645
H	2.1152	-0.8496	3.8418
H	-0.2034	-3.6541	-6.6507
H	-1.4464	-3.3293	-3.0654
H	-1.0176	-1.8688	6.6751
H	-0.4498	-6.3981	2.8165
H	-1.8579	-5.0636	-2.8936

7:
-6779.897

Cr	1.4814	-1.3681	-3.1245
Cr	-3.1954	-1.2780	2.4463
Cl	1.9863	-0.3450	-5.2639
Cl	-4.9884	-2.2445	3.5536
O	3.0797	-2.2552	0.5231
O	1.1380	-1.9566	-1.3170
O	0.7193	-2.9143	-3.9985
O	-6.8181	4.1192	-0.1291
O	-5.1467	4.1787	-1.7104
O	-3.7565	0.5336	2.7773
O	-1.3105	4.7915	-1.3813
O	-1.9388	-1.3735	3.9022
O	-2.3429	4.0795	0.5368
O	-0.1885	-0.3618	-3.0916
O	-1.6486	-0.5299	1.2408
N	3.3445	-2.1805	-3.2423
N	2.5004	0.1633	-2.2337
N	-4.2011	-1.3176	0.6774
N	-2.5316	-3.0684	1.7785
C	2.5655	-3.4284	-0.1029
C	0.5534	-4.3759	-1.3003
C	1.1355	-3.1496	-0.5945
C	6.7853	-0.5138	-2.5134
C	6.2930	0.5026	-1.4686
C	5.7986	-1.6920	-2.6532
C	4.8754	1.0062	-1.8037
C	4.4019	-1.1642	-3.0183
C	3.6143	-3.3618	-3.6990
C	3.1720	-5.5913	-4.5793
C	3.9063	-0.1822	-1.9256
C	2.6628	-4.3233	-4.2039

C	2.3562	-6.5459	-5.1563	C	-1.7150	-5.7772	-6.2074
C	1.0050	-6.2253	-5.4184	C	-0.4162	-3.0007	2.9719
C	1.2694	-4.0224	-4.4119	C	-1.0167	-3.3797	-6.3676
C	1.9661	1.2841	-1.8783	C	-0.4129	0.8608	-2.7081
C	0.4443	-4.9958	-5.0868	C	-1.8458	-4.3262	-4.1832
C	1.0124	-0.2961	6.9553	C	-0.1609	-0.5630	5.9872
C	1.8414	-3.1207	3.8678	C	0.2202	-1.5677	4.8841
C	1.4914	-2.1406	4.8183	C	-1.0058	-4.6331	-5.4498
C	0.5932	1.6843	-2.0821	C	0.8817	-3.5607	2.9759
C	-6.8007	5.9522	-1.6288	C	0.2541	2.9782	-1.6183
C	-6.6003	7.0740	-0.5751	C	-1.5513	0.8595	0.7138
C	-6.1442	4.6561	-1.2092	C	-0.5763	0.3854	1.7161
C	-5.1179	7.3785	-0.2526	C	0.8083	-0.0354	1.3158
C	-6.1354	3.1142	0.6070	H	-0.7361	0.6843	2.7471
C	-5.9028	1.8619	0.0939	H	2.5356	-1.5617	0.1004
C	-5.6567	3.4775	1.8748	H	2.5880	-4.2472	0.6295
C	-4.5874	2.1178	5.1159	H	3.1854	-3.7139	-0.9668
C	-4.5822	-4.2259	-1.8617	H	1.2478	-4.7880	-2.0376
C	-4.9013	-0.3384	0.2038	H	0.3338	-5.1616	-0.5609
C	-5.0462	-3.0012	-1.0515	H	-0.3683	-4.1035	-1.8200
C	-4.1576	1.3449	-3.7079	H	0.5261	-2.9638	0.3068
C	-5.1390	0.9345	0.8417	H	7.7804	-0.8890	-2.2407
C	-4.5353	6.4685	0.8457	H	6.9873	1.3508	-1.4041
C	-4.8726	2.6212	2.6370	H	6.8779	-0.0125	-3.4884
C	-4.5782	1.3136	2.1093	H	6.1686	-2.3782	-3.4237
C	-4.2363	3.0856	3.9570	H	6.2714	0.0185	-0.4812
C	-3.9062	-2.5202	-0.1427	H	5.7331	-2.2476	-1.7065
C	-4.0796	-5.3582	-0.9469	H	4.6560	-3.6876	-3.7597
C	-3.4725	-3.6620	0.8124	H	4.2270	-5.7969	-4.4068
C	-2.8124	0.5895	-3.6228	H	4.8771	1.5610	-2.7524
C	-3.0761	6.7869	1.2127	H	4.5470	1.6940	-1.0154
C	-2.9681	-4.8615	-0.0005	H	4.4518	-0.6007	-3.9609
C	-3.0762	-0.7350	-2.8658	H	3.9152	-0.7389	-0.9814
C	-2.3375	0.2737	-5.0651	H	2.7468	-7.5204	-5.4317
C	-2.6968	3.1629	3.7732	H	2.5776	2.0346	-1.3711
C	-4.7141	4.4977	4.3637	H	1.3449	-1.2208	7.4440
C	-2.0939	6.4659	0.0783	H	1.8685	0.1522	6.4338
C	-2.0176	2.6903	-2.4093	H	0.3914	-6.9713	-5.9101
C	-1.9657	4.9748	-0.1937	H	0.6766	0.4031	7.7313
C	-1.7419	1.4152	-2.8899	H	2.8495	-3.5178	3.8364
C	-1.3548	-3.5456	2.0186	H	2.2491	-1.8294	5.5277
C	-1.0242	3.4553	-1.7761	H	1.0104	3.5970	-1.1444
C	-0.5901	0.7987	5.3859	H	-7.8751	5.7822	-1.7700
C	-0.7566	-1.9636	3.9046	H	-7.0899	7.9769	-0.9636
C	-1.3376	-1.1376	6.8213	H	-6.3579	6.2527	-2.5835

H	-7.1224	6.7885	0.3475
H	-6.2618	1.5957	-0.8939
H	-5.9128	-3.2534	-0.4237
H	-4.5245	7.2889	-1.1741
H	-5.0275	8.4233	0.0806
H	-4.2601	1.1017	4.8910
H	-5.4025	-4.5865	-2.4957
H	-5.6720	2.1090	5.2865
H	-4.8835	0.7112	-4.2332
H	-5.8806	4.4740	2.2250
H	-5.3547	-0.4384	-0.7834
H	-3.7690	-3.9155	-2.5276
H	-4.5533	1.5849	-2.7124
H	-5.3456	-2.2099	-1.7460
H	-4.0545	2.2835	-4.2664
H	-4.3529	-3.9515	1.4021
H	-4.0920	2.4627	6.0343
H	-5.1606	6.5683	1.7445
H	-4.5784	5.4189	0.5485
H	-3.8830	-1.2918	-3.3639
H	-2.3810	6.9606	-0.8566
H	-3.0032	3.1258	-2.5034
H	-3.0895	-0.3532	-5.5654
H	-2.2957	2.1895	3.4916
H	-3.7033	-6.1909	-1.5543
H	-5.8048	4.5355	4.4844
H	-2.6578	-5.6707	0.6732
H	-2.9818	7.8492	1.4799
H	-3.3866	-0.5039	-1.8429
H	-4.9177	-5.7394	-0.3444
H	-2.2209	1.2033	-5.6367
H	-1.4968	0.6841	4.7924
H	-2.2310	3.4734	4.7183
H	-3.0315	-2.2718	-0.7587
H	-2.7318	-5.4530	-6.4607
H	-4.2511	4.7597	5.3225
H	-2.2040	-1.3282	6.1834
H	-2.0564	-3.1126	-6.6047
H	-2.1764	-1.3512	-2.8392
H	-2.7981	6.1938	2.0929
H	-4.4134	5.2497	3.6221
H	-1.0875	6.8354	0.3231
H	-2.4476	3.8839	2.9874
H	-2.0889	-4.5613	-0.5841
H	-1.3822	-0.2560	-5.0500
H	-1.0113	-4.4277	1.4759
H	-2.8777	-4.1076	-4.4895
H	-0.7917	1.5108	6.1979
H	-1.6185	-0.4174	7.6027
H	-1.7845	-6.6851	-5.5931
H	-1.1889	-6.0227	-7.1387
H	-0.5348	-2.5325	-5.8751
H	0.2091	1.2120	4.7555
H	-0.4882	-3.5929	-7.3058
H	-1.4377	-3.4611	-3.6585
H	-1.0342	-2.0754	7.3050
H	1.1167	-4.3242	2.2403
H	-1.8576	-5.1912	-3.5063
H	-2.3513	1.5251	1.0076
H	-1.2596	0.8784	-0.3284
H	0.7906	-0.4186	0.2883
H	1.1927	-0.8187	1.9768
H	1.4827	0.8310	1.3662

15:
-6779.8909

Cr	-3.2005	-1.4770	2.4133
Cr	1.5685	-0.9754	-2.9794
Cl	-5.1940	-1.5788	3.7662
Cl	1.6011	0.1085	-5.1868
O	-1.6289	-1.6201	1.1691
O	-0.1548	-0.1379	-2.6726
O	-1.8778	5.1357	0.3846
O	-2.0330	-1.7773	3.9263
O	-1.6387	5.1653	-1.9147
O	-3.1901	0.4595	2.4706
O	-5.2001	4.3860	-1.8726
O	-6.4645	4.2656	0.0610
O	0.9062	-2.6284	-3.7486
O	1.5268	-1.7978	-1.1220
O	3.3325	-1.0170	0.6296
N	-3.3373	-3.4918	2.1322
N	-4.3578	-1.4166	0.7502
N	2.4784	0.6943	-2.2393
N	3.4741	-1.4959	-3.4799
C	0.2094	0.0306	1.6959
C	-0.1938	-1.3676	1.2977
C	-0.3848	-1.6651	-0.1375
C	0.0764	3.4428	-1.8419
C	-0.7433	-5.2250	4.0751

C	-0.8156	-4.7157	-4.6972	C	0.2134	-3.8943	5.8393
C	-0.5431	-2.7743	5.5000	C	0.1443	-5.1110	5.1274
C	-0.5469	-1.4946	6.3627	C	0.3965	-1.6193	7.5822
C	-1.1345	-4.6890	-3.1746	C	0.7094	-4.6852	-4.9372
C	-0.4876	1.1419	-2.5247	C	1.8797	1.8128	-1.9497
C	-1.4713	-3.4837	-5.3816	C	1.4967	-3.5824	-4.4435
C	-1.5330	-4.1219	3.6688	C	1.3622	-5.6853	-5.6519
C	-1.4700	-5.9891	-5.2854	C	2.7490	-5.6605	-5.9189
C	-1.9886	-1.2534	6.8958	C	2.9096	-3.5562	-4.7064
C	-1.3903	-2.8591	4.3385	C	3.9452	0.4960	-2.0973
C	-0.0925	-0.2615	5.5381	C	3.5050	-4.6036	-5.4547
C	-1.2378	3.7948	-2.0339	C	3.7773	-2.5004	-4.2553
C	-2.5248	-4.3632	2.6481	C	4.4206	-0.3543	-3.3003
C	-1.8430	1.5515	-2.7718	C	4.7932	1.7735	-1.9759
C	-1.9509	5.7282	-0.6930	C	5.8990	-0.7441	-3.1197
C	-2.1899	2.8718	-2.4920	C	6.2856	1.4128	-1.8234
C	-2.3376	7.1800	-0.8870	C	6.7733	0.5196	-2.9782
C	-3.2389	4.6592	3.8456	C	2.2146	-2.8954	-0.4565
C	-1.6041	2.8933	3.1725	C	2.4084	-4.1594	-1.2900
C	-2.3502	0.3296	-4.8990	C	3.5457	-2.3544	0.0943
C	-2.9486	-0.7707	-2.6999	H	-0.1135	0.2279	2.7182
C	-4.3388	-5.2311	0.5394	H	1.2993	0.1268	1.6580
C	-3.1239	7.7481	0.3062	H	-0.2511	0.7713	1.0366
C	-2.8426	0.5868	-3.4464	H	0.2997	-2.1359	1.8975
C	-4.4100	-3.8292	1.1661	H	-0.4932	-2.6878	-0.4610
C	-5.4880	-5.4409	-0.4682	H	-0.6514	-0.8828	-0.8281
C	-4.4000	-2.7318	0.0671	H	-0.7021	-5.5633	-2.6707
C	-3.0903	3.1494	3.5399	H	-0.8546	-6.1696	3.5467
C	-3.9988	1.3453	1.9115	H	-2.3099	-2.0934	7.5246
C	-3.9926	2.7123	2.3712	H	-0.7381	-3.7807	-2.7194
C	-4.5603	7.1980	0.4007	H	-1.2963	-3.5081	-6.4637
C	-4.8791	0.9775	0.8364	H	0.9086	-0.4208	5.1177
C	-4.2639	1.1979	-3.5120	H	-1.0614	-2.5559	-4.9845
C	-5.5569	-2.9397	-0.9249	H	-1.3416	-6.0501	-6.3731
C	-4.9594	-0.3564	0.2991	H	-1.0650	-6.9042	-4.8357
C	-5.4898	-4.3465	-1.5499	H	-2.0117	-0.3399	7.5046
C	-3.4702	2.3505	4.8174	H	-0.0568	0.6260	6.1834
C	-4.8175	3.6242	1.7249	H	-2.2228	-4.7151	-3.0247
C	-5.6890	1.9540	0.2083	H	-2.5942	-5.4053	2.3280
C	-5.6407	3.2508	0.6536	H	-1.3278	-0.0568	-4.9076
C	-5.5295	7.7973	-0.6380	H	-3.3732	-5.3522	0.0262
C	-6.1386	4.7851	-1.1799	H	-1.3418	3.4306	2.2552
C	-6.9369	7.1546	-0.6296	H	-1.4046	7.7427	-1.0386
C	-7.0788	5.9082	-1.5403	H	-2.9387	5.2681	2.9849
C	0.4773	2.1087	-2.0937	H	-2.5808	7.4982	1.2248

H	-2.0236	-1.3381	-2.7916
H	-2.5560	-3.4927	-5.2085
H	-2.6983	-1.1424	6.0739
H	-2.5827	4.9146	4.6860
H	-2.5463	-5.9643	-5.0804
H	-3.4460	-2.8184	-0.4742
H	-0.9540	3.2442	3.9848
H	-0.7940	-0.0741	4.7263
H	-2.3706	1.2609	-5.4782
H	-6.4478	-5.4217	0.0690
H	-3.1551	-0.6128	-1.6379
H	-3.1494	8.8448	0.2329
H	-4.3903	-5.9979	1.3222
H	-4.2646	4.9222	4.1345
H	-5.4009	-6.4332	-0.9289
H	-1.4381	1.8293	3.0217
H	-3.0096	-0.3972	-5.3942
H	-3.2018	3.2311	-2.6264
H	-2.8948	7.2575	-1.8260
H	-3.7676	-1.3594	-3.1364
H	-4.5144	6.1091	0.3057
H	-4.9610	7.3981	1.4042
H	-2.8010	2.6298	5.6420
H	-5.3496	-3.7199	1.7271
H	-4.2908	2.1138	-4.1116
H	-5.5139	-2.1896	-1.7223
H	-4.6515	1.4358	-2.5157
H	-4.5756	-4.4308	-2.1560
H	-5.5940	-0.4484	-0.5833
H	-4.8385	4.6581	2.0359
H	-4.9401	0.4740	-3.9833
H	-4.5008	2.5749	5.1202
H	-6.3361	-4.4895	-2.2339
H	-3.3866	1.2758	4.6470
H	-5.6247	8.8746	-0.4370
H	-5.1029	7.7124	-1.6480
H	-6.5140	-2.8079	-0.3985
H	-6.3344	1.6741	-0.6171
H	-7.2129	6.8779	0.3957
H	-6.8797	6.1749	-2.5825
H	-7.6783	7.8887	-0.9720
H	-8.1055	5.5300	-1.4677
H	0.8052	4.1814	-1.5239
H	0.8769	-3.8454	6.6954
H	0.7592	-5.9521	5.4291
H	0.3388	-0.6972	8.1719
H	0.7904	-6.5239	-6.0316
H	1.4420	-1.7558	7.2781
H	0.1137	-2.4525	8.2379
H	2.4805	2.6495	-1.5892
H	3.2049	-6.4639	-6.4879
H	4.0892	-0.0887	-1.1801
H	4.3074	0.2629	-4.2028
H	4.4774	2.3561	-1.1028
H	4.6421	2.4025	-2.8655
H	4.5740	-4.5615	-5.6530
H	4.7987	-2.5720	-4.6371
H	5.9988	-1.3758	-2.2251
H	6.4295	0.8848	-0.8699
H	6.2541	-1.3327	-3.9733
H	6.7344	1.0869	-3.9196
H	6.8853	2.3305	-1.7731
H	7.8214	0.2333	-2.8222
H	1.5884	-3.1626	0.4075
H	1.4529	-4.5111	-1.6837
H	2.8359	-4.9528	-0.6608
H	3.0800	-3.9919	-2.1331
H	4.2924	-2.3203	-0.7130
H	3.9290	-2.9852	0.9018
H	2.5420	-0.6932	0.1259

16:
-6779.8909

Cr	1.2073	-0.8101	-3.0945
Cr	-2.8068	-1.3983	2.5949
Cl	1.6822	0.6757	-4.8055
Cl	-4.8540	-0.8822	3.7639
O	3.4208	-2.8480	-0.2393
O	0.7859	-2.1183	-1.2795
O	0.8863	-2.3077	-4.2474
O	-6.1354	4.0874	0.1729
O	-5.8376	3.8073	-2.0876
O	-2.4423	0.4594	2.1471
O	-2.6607	4.7685	-1.7458
O	-1.8119	-1.4718	4.2599
O	-1.2988	5.6503	-0.1140
O	-0.6009	-0.2030	-3.0198
O	-1.2985	-2.0767	1.6258
N	3.1994	-1.2244	-3.0695
N	1.7293	0.5221	-1.6748

N	-3.9282	-1.5187	0.8975	C	-4.3904	-5.2610	1.4342
N	-3.2595	-3.3733	2.7308	C	-3.3439	-1.0684	-3.0325
C	2.6446	-3.7164	-1.0546	C	-2.7694	0.1843	-5.1502
C	0.4250	-4.4861	-1.9012	C	-0.7083	2.8614	2.3207
C	1.1410	-3.4921	-0.9869	C	-2.1781	4.7042	3.1417
C	6.0071	0.5183	-1.0209	C	-2.8190	7.0926	-1.3264
C	5.1187	0.9021	0.1751	C	-2.8920	2.5651	-2.5432
C	5.3606	-0.6089	-1.8508	C	-2.1605	5.7676	-0.9697
C	3.7184	1.3412	-0.2941	C	-2.4302	1.3088	-2.9211
C	3.9637	-0.1851	-2.3313	C	-2.5497	-4.2081	3.4149
C	3.7874	-2.0964	-3.8241	C	-2.0806	3.4795	-1.8476
C	3.9720	-3.9933	-5.3414	C	0.6230	0.0303	5.0006
C	3.0736	0.2338	-1.1335	C	-1.1759	-2.5098	4.7328
C	3.1354	-3.0613	-4.6785	C	-1.0741	-0.2449	6.8561
C	3.4419	-4.9428	-6.1939	C	-0.6982	-5.0949	-7.2196
C	2.0508	-4.9503	-6.4333	C	-1.4934	-3.8626	4.3431
C	1.7141	-3.0985	-4.8922	C	-0.6656	-2.6278	-6.7995
C	1.0233	1.5497	-1.3230	C	-1.0748	0.9625	-2.6067
C	1.1739	-4.0513	-5.8282	C	-1.2183	-4.2437	-4.9355
C	1.3236	-0.8416	7.2275	C	0.1818	-0.8667	6.1878
C	0.2454	-4.7285	5.8199	C	-0.1340	-2.2984	5.7128
C	0.5449	-3.4062	6.2146	C	-0.3250	-4.0123	-6.1829
C	-0.2993	1.8605	-1.8049	C	-0.7704	-4.9418	4.9052
C	-7.4253	5.4466	-1.2764	C	-0.8108	3.1294	-1.4388
C	-7.2587	6.6745	-0.3549	C	-0.4908	-1.7927	-0.5912
C	-6.3623	4.3681	-1.1445	C	-0.3968	-1.2945	0.8792
C	-5.9606	7.4780	-0.6081	C	0.9909	-1.3612	1.5360
C	-5.1517	3.1251	0.5431	H	-0.7026	-0.2376	0.8837
C	-5.2440	1.8014	0.1723	H	2.9267	-2.6859	0.5791
C	-4.1456	3.5679	1.4166	H	2.8135	-4.7683	-0.7692
C	-2.2622	2.4824	4.2941	H	2.9949	-3.5918	-2.0779
C	-5.2817	-4.6911	-0.8734	H	0.8385	-4.4645	-2.9109
C	-4.5195	-0.5173	0.3343	H	0.5296	-5.4999	-1.4937
C	-5.2193	-3.1896	-0.5388	H	-0.6407	-4.2506	-1.9674
C	-4.7768	0.8337	-3.7814	H	0.8188	-3.6661	0.0465
C	-4.3361	0.8663	0.7165	H	6.9975	0.1989	-0.6723
C	-4.7827	7.0406	0.2845	H	5.5850	1.7062	0.7583
C	-3.2048	2.6946	1.9503	H	6.1547	1.4023	-1.6602
C	-3.3063	1.2969	1.6242	H	6.0053	-0.8428	-2.7075
C	-2.1089	3.1772	2.9140	H	5.0150	0.0314	0.8388
C	-4.1052	-2.9181	0.4810	H	5.2554	-1.5156	-1.2414
C	-5.5042	-5.5260	0.4023	H	4.8782	-2.1424	-3.8350
C	-4.3149	-3.7670	1.7805	H	5.0441	-3.9464	-5.1623
C	-3.3185	0.3301	-3.7071	H	3.7923	2.2607	-0.8937
C	-3.4619	7.7415	-0.0826	H	3.0887	1.5633	0.5767

H	4.0410	0.6746	-3.0130
H	2.9730	-0.6710	-0.5277
H	4.0828	-5.6632	-6.6916
H	1.4313	2.2602	-0.6025
H	1.0572	-1.4138	8.1256
H	2.2526	-1.2535	6.8114
H	1.6591	-5.6820	-7.1291
H	1.5086	0.1981	7.5241
H	0.8011	-5.5611	6.2402
H	1.3349	-3.2590	6.9429
H	-0.2017	3.8052	-0.8575
H	-8.3938	4.9706	-1.0627
H	-8.1311	7.3216	-0.5174
H	-7.4312	5.7560	-2.3268
H	-7.2883	6.3430	0.6904
H	-6.0222	1.4692	-0.5061
H	-6.1802	-2.8644	-0.1133
H	-5.6787	7.3881	-1.6682
H	-6.1467	8.5468	-0.4256
H	-2.1994	1.3979	4.2012
H	-6.0815	-4.8823	-1.6005
H	-3.2319	2.7386	4.7387
H	-5.3820	0.0904	-4.3145
H	-4.1326	4.6132	1.6888
H	-5.2266	-0.6848	-0.4814
H	-4.3338	-4.9945	-1.3424
H	-5.1948	0.9811	-2.7780
H	-5.0428	-2.6090	-1.4507
H	-4.8510	1.7852	-4.3202
H	-5.2646	-3.4355	2.2231
H	-1.4634	2.8323	4.9633
H	-5.0451	7.2423	1.3327
H	-4.6412	5.9602	0.2020
H	-4.1073	-1.6909	-3.5201
H	-3.5631	6.9393	-2.1128
H	-3.8989	2.8842	-2.7667
H	-3.3768	-0.5460	-5.7042
H	-0.5982	1.7876	2.1517
H	-5.5434	-6.5961	0.1594
H	-3.1329	4.9917	3.6024
H	-4.5684	-5.8485	2.3439
H	-3.6460	8.8080	-0.2755
H	-3.5912	-0.9727	-1.9714
H	-6.4740	-5.2513	0.8431
H	-2.8189	1.1479	-5.6735
H	-0.1562	0.0760	4.2381
H	0.0645	3.1943	3.0282
H	-3.1369	-3.2292	0.0633
H	-1.7673	-5.0091	-7.4467
H	-1.3710	4.9943	3.8258
H	-1.9104	-0.2251	6.1545
H	-1.7392	-2.5841	-7.0289
H	-2.3752	-1.5615	-3.1179
H	-2.7466	7.6739	0.7463
H	-2.0475	5.2542	2.2023
H	-2.0281	7.7424	-1.7234
H	-0.5779	3.3999	1.3747
H	-3.4208	-5.5766	1.0206
H	-1.7310	-0.1558	-5.1343
H	-2.7298	-5.2824	3.3111
H	-2.2732	-4.2172	-5.2413
H	0.8194	1.0482	5.3661
H	-0.8482	0.7824	7.1766
H	-0.5091	-6.1036	-6.8288
H	-0.1370	-4.9692	-8.1542
H	-0.4230	-1.8202	-6.1058
H	1.5476	-0.3615	4.5553
H	-0.1031	-2.4776	-7.7301
H	-1.0444	-3.4678	-4.1900
H	-1.3573	-0.8330	7.7393
H	-1.0303	-5.9539	4.5984
H	-1.0088	-5.2249	-4.4897
H	-0.9691	-1.0609	-1.2270
H	-1.0977	-2.7010	-0.5810
H	1.2819	-2.4088	1.6980
H	0.9123	-0.9005	2.5227
H	1.7524	-0.8346	0.9526

17:
-6626.061

Cr	-1.6510	-1.5219	1.2819
Cr	0.4381	-1.1408	-1.9256
Cl	-3.4196	-1.2121	2.8966
Cl	1.3330	0.1098	-3.8131
O	-1.2581	-0.2779	-2.2860
O	-1.6387	5.8027	-0.1122
O	-0.3676	-1.7602	2.7388
O	-2.6704	5.0815	-2.0415
O	-1.5204	0.4115	1.1405
O	-5.7860	3.7743	-2.1134

O	-5.7443	3.9048	0.1814	C	-4.8558	-4.5362	-1.8618
O	0.1191	-2.6685	-3.0914	C	-1.8903	1.9631	3.8712
O	-0.1790	-2.1010	-0.1410	C	-3.6593	3.3649	1.2302
O	2.5404	-4.4111	1.0665	C	-4.6708	1.7368	-0.2374
N	-2.2821	-3.4750	1.4752	C	-4.6692	2.9871	0.3376
N	-3.0807	-1.5246	-0.1459	C	-6.1036	7.2889	-0.3850
N	1.0359	0.3916	-0.7719	C	-6.2173	4.2141	-1.0657
N	2.4217	-1.6492	-1.7690	C	-7.2533	6.3312	0.0181
C	-1.0804	3.2854	-1.3636	C	-7.4190	5.1394	-0.9494
C	-0.7254	-5.0445	4.3771	C	-0.7062	1.9293	-1.4933
C	-1.0030	-4.2850	-5.1703	C	0.9644	-3.7389	5.4772
C	0.7623	-2.6446	4.6387	C	0.2440	-4.9454	5.3551
C	1.4988	-1.3136	4.8830	C	2.5299	-1.4195	6.0287
C	-1.8695	-4.7060	-3.9570	C	0.4889	-4.2804	-4.8013
C	-1.4698	1.0262	-2.3033	C	0.4728	1.5522	-0.7601
C	-1.4407	-2.8706	-5.6254	C	0.9742	-3.3963	-3.7696
C	-0.9744	-3.9795	3.4780	C	1.3995	-5.1018	-5.4625
C	-1.3176	-5.2687	-6.3190	C	2.7802	-5.1050	-5.1747
C	0.4532	-0.2415	5.2776	C	2.3885	-3.3823	-3.4959
C	-0.2166	-2.7563	3.5774	C	2.2894	0.1064	-0.0523
C	2.2642	-0.8229	3.6278	C	3.2591	-4.2445	-4.2071
C	-2.1694	3.7525	-2.0663	C	3.0140	-2.4938	-2.5515
C	-1.9967	-4.2243	2.4889	C	3.2210	-0.6036	-1.0701
C	-2.5060	1.5817	-3.1395	C	3.0029	1.3115	0.5768
C	-2.3649	5.9855	-1.0768	C	4.5184	-1.0733	-0.3877
C	-2.8456	2.9190	-2.9706	C	4.3255	0.8692	1.2344
C	-3.0522	7.3129	-1.3710	C	5.2394	0.1413	0.2308
C	-1.8216	4.3640	3.1442	C	0.4198	-3.3706	0.2734
C	-0.1366	2.7724	2.2482	C	0.3500	-4.4815	-0.7766
C	-1.9809	0.4824	-5.3072	C	1.8424	-3.1721	0.8120
C	-3.7496	-0.5617	-3.8276	C	1.9846	-5.1448	2.1664
C	-3.5403	-5.2707	0.1742	H	-1.5836	-5.7047	-3.6001
C	-3.6347	7.9165	-0.0782	H	-1.3125	-5.9547	4.2741
C	-3.1194	0.7693	-4.2942	H	-0.0279	-0.5112	6.2263
C	-3.4338	-3.7991	0.6078	H	-1.7558	-3.9890	-3.1421
C	-4.8335	-5.4696	-0.6382	H	-0.8641	-2.5553	-6.5040
C	-3.3676	-2.8828	-0.6421	H	2.9935	-1.5739	3.2969
C	-1.6194	2.9056	2.6725	H	-1.2846	-2.1462	-4.8278
C	-2.5489	1.2181	0.9295	H	-0.7623	-5.0083	-7.2289
C	-2.6022	2.5158	1.5534	H	-1.0751	-6.3034	-6.0419
C	-4.8246	7.0964	0.4528	H	0.9453	0.7341	5.3963
C	-3.6292	0.8353	0.0662	H	2.8062	0.0987	3.8798
C	-4.2260	1.5530	-5.0362	H	-2.9208	-4.7324	-4.2738
C	-4.6517	-3.0585	-1.4687	H	-2.5495	-5.1559	2.6358
C	-3.7818	-0.4934	-0.4750	H	-1.1420	-0.0243	-4.8277

H	-2.6624	-5.5251	-0.4360
H	0.0882	3.4771	1.4384
H	-2.2964	7.9915	-1.7915
H	-1.7019	5.0678	2.3117
H	-2.8361	7.9415	0.6728
H	-3.0434	-1.1263	-3.2192
H	-2.5073	-2.8833	-5.8908
H	-0.3100	-0.1584	4.5058
H	-1.0695	4.5890	3.9108
H	-2.3901	-5.2144	-6.5430
H	-2.4916	-3.1749	-1.2370
H	0.5005	3.0208	3.1092
H	1.5712	-0.6151	2.8121
H	-1.6093	1.4280	-5.7218
H	-5.6959	-5.2489	0.0093
H	-4.6591	-0.3604	-3.2469
H	-3.9518	8.9524	-0.2660
H	-3.5457	-5.9364	1.0451
H	-2.8125	4.5052	3.5949
H	-4.9223	-6.5160	-0.9580
H	0.0776	1.7542	1.9230
H	-2.3605	-0.1394	-6.1301
H	-3.6566	3.3598	-3.5308
H	-3.8250	7.1662	-2.1311
H	-4.0320	-1.1583	-4.7056
H	-4.5532	6.0349	0.4750
H	-5.0413	7.3829	1.4919
H	-1.1747	2.1721	4.6778
H	-4.3355	-3.5120	1.1691
H	-3.8251	2.4585	-5.5084
H	-4.6081	-2.4439	-2.3707
H	-5.0377	1.8443	-4.3569
H	-4.0518	-4.8338	-2.5431
H	-4.6008	-0.6104	-1.1804
H	-3.7293	4.3470	1.6761
H	-4.6378	0.9114	-5.8253
H	-2.9087	2.1185	4.2482
H	-5.8026	-4.6439	-2.4072
H	-1.8015	0.9195	3.5675
H	-6.4290	8.3340	-0.2796
H	-5.8730	7.1435	-1.4504
H	-5.5054	-2.7127	-0.8665
H	-5.4601	1.4388	-0.9166
H	-7.0780	5.9479	1.0308
H	-7.6377	5.4981	-1.9604
H	-8.2079	6.8737	0.0365
H	-8.2691	4.5228	-0.6211
H	-0.5251	3.9311	-0.7020
H	1.7030	-3.6717	6.2664
H	0.4416	-5.7693	6.0329
H	3.0186	-0.4453	6.1502
H	1.0423	-5.7661	-6.2396
H	3.3000	-2.1696	5.8056
H	2.0476	-1.6801	6.9790
H	0.9168	2.3528	-0.1750
H	3.4494	-5.7657	-5.7165
H	2.0395	-0.6056	0.7403
H	3.4700	0.1395	-1.8409
H	2.3494	1.7771	1.3236
H	3.2033	2.0561	-0.2070
H	4.3215	-4.2117	-3.9740
H	4.1060	-2.5406	-2.5462
H	4.2878	-1.8090	0.3928
H	4.0950	0.1883	2.0631
H	5.1807	-1.5623	-1.1117
H	5.5250	0.8352	-0.5743
H	4.8390	1.7422	1.6586
H	6.1628	-0.1860	0.7261
H	-0.1628	-3.7235	1.1122
H	-0.6175	-4.4606	-1.2848
H	0.4703	-5.4483	-0.2711
H	1.1395	-4.4023	-1.5225
H	2.4422	-2.6748	0.0638
H	1.7979	-2.5676	1.7242
H	0.9802	-5.5280	1.9378
H	1.9176	-4.5266	3.0713
H	2.6563	-5.9919	2.3466

18:
-6626.0764

Cr	1.2196	-1.0040	-2.7171
Cr	-2.9269	-1.5469	2.1026
Cl	2.2060	-0.3742	-4.8652
Cl	-4.7494	-2.0451	3.3485
O	1.4199	-0.9746	1.9355
O	0.3625	-1.2746	-1.0280
O	0.6221	-2.7056	-3.4549
O	-6.4611	4.1181	0.2699
O	-5.2466	4.6061	-1.6179
O	-2.8752	0.3438	2.1737

O	-2.0872	5.1047	-1.9977	C	-3.7224	1.2384	1.6947
O	-1.4949	-1.7210	3.3196	C	-2.6472	2.9931	3.2507
O	-2.1628	5.0120	0.2931	C	-3.9221	-2.6572	-0.4583
O	-0.3608	0.0006	-3.2300	C	-4.6508	-5.4335	-1.1731
N	3.0579	-1.8141	-2.3253	C	-3.6654	-3.8464	0.5014
N	2.0654	0.6530	-1.8830	C	-3.0517	0.6095	-3.8641
N	-3.9635	-1.4233	0.3673	C	-3.2601	7.6386	0.4451
N	-2.6115	-3.4290	1.4542	C	-3.4150	-5.1281	-0.3021
C	1.0806	0.3228	1.4105	C	-3.1127	-0.7543	-3.1307
C	1.6230	-2.0088	0.9517	C	-2.5359	0.3761	-5.3078
C	0.4868	-3.6829	-0.5427	C	-1.2334	2.7944	2.6456
C	0.4361	-2.2411	-0.0073	C	-2.7877	4.4801	3.6408
C	6.3210	0.0173	-1.2404	C	-2.7316	7.0707	-0.8799
C	5.6538	1.1860	-0.4941	C	-2.5233	2.8634	-2.7789
C	5.3608	-1.1831	-1.3633	C	-2.3127	5.6121	-0.7547
C	4.3341	1.5996	-1.1750	C	-2.1150	1.5818	-3.1284
C	4.0668	-0.7508	-2.0747	C	-1.6570	-4.2223	1.8382
C	3.4338	-3.0099	-2.6590	C	-1.6473	3.7592	-2.1424
C	3.2279	-5.2993	-3.4643	C	0.4231	0.0209	4.7514
C	3.3890	0.3898	-1.2813	C	-0.6457	-2.6965	3.5732
C	2.6160	-4.0388	-3.2500	C	-1.1393	-1.2741	6.2650
C	2.5547	-6.3199	-4.1075	C	-1.3395	-5.8011	-5.8024
C	1.2472	-6.0804	-4.5901	C	-0.6613	-3.9214	2.8299
C	1.2643	-3.8120	-3.6934	C	-0.7645	-3.3728	-5.9550
C	1.4381	1.7686	-1.6901	C	-0.7602	1.1707	-2.8261
C	0.5922	-4.8650	-4.4197	C	-1.8219	-4.3091	-3.8643
C	1.3272	-1.3295	6.6434	C	0.2385	-1.2944	5.5481
C	1.2998	-4.7047	4.0311	C	0.3155	-2.5250	4.6271
C	1.2678	-3.5243	4.8081	C	-0.8055	-4.5958	-4.9991
C	0.0923	2.0836	-2.1056	C	0.3286	-4.9075	3.0720
C	-7.2395	5.8933	-1.0771	C	-0.3716	3.3842	-1.7919
C	-7.1215	7.0299	-0.0281	H	1.9492	0.8097	0.9446
C	-6.1943	4.8139	-0.8884	H	0.2799	0.2696	0.6687
C	-5.7632	7.7625	-0.0742	H	0.7747	0.9148	2.2722
C	-5.5186	3.1413	0.6850	H	1.7977	-2.9069	1.5560
C	-5.5304	1.8799	0.1401	H	2.5147	-1.8104	0.3371
C	-4.6136	3.4894	1.6992	H	1.4346	-3.8650	-1.0550
C	-2.7794	2.1431	4.5415	H	0.3977	-4.4109	0.2721
C	-4.9963	-4.2493	-2.0951	H	-0.3173	-3.8362	-1.2682
C	-4.6443	-0.3803	-0.0029	H	-0.4751	-2.1350	0.6132
C	-5.1692	-2.9321	-1.3137	H	7.2410	-0.2893	-0.7251
C	-4.4925	1.1613	-3.9405	H	6.3358	2.0447	-0.4403
C	-4.6380	0.9044	0.6440	H	6.6048	0.3489	-2.2503
C	-4.6622	7.0902	0.7699	H	5.8634	-1.9864	-1.9138
C	-3.6943	2.5784	2.2076	H	5.4391	0.8752	0.5392

H	5.1112	-1.5685	-0.3634
H	4.4819	-3.2944	-2.5343
H	4.2480	-5.4445	-3.1127
H	4.5289	1.9840	-2.1857
H	3.8694	2.4052	-0.5953
H	4.3044	-0.3541	-3.0720
H	3.2054	0.0061	-0.2705
H	3.0233	-7.2862	-4.2650
H	1.9366	2.5752	-1.1468
H	1.2362	-2.2254	7.2713
H	2.3333	-1.3028	6.2060
H	0.7497	-6.8811	-5.1258
H	1.2053	-0.4469	7.2821
H	2.0704	-5.4472	4.2080
H	2.0160	-3.4045	5.5821
H	0.2869	4.0822	-1.2839
H	-8.2342	5.4368	-1.0025
H	-7.9365	7.7395	-0.2237
H	-7.1107	6.3044	-2.0832
H	-7.2858	6.6108	0.9733
H	-6.2090	1.6311	-0.6690
H	-6.0469	-2.9796	-0.6533
H	-5.4358	7.8317	-1.1222
H	-5.8864	8.7951	0.2833
H	-2.6049	1.0855	4.3370
H	-5.9105	-4.4659	-2.6629
H	-3.7789	2.2641	4.9804
H	-5.1341	0.4171	-4.4296
H	-4.6364	4.5029	2.0698
H	-5.2649	-0.4382	-0.8958
H	-4.1865	-4.1153	-2.8183
H	-4.8875	1.3686	-2.9364
H	-5.3220	-2.1202	-2.0308
H	-4.5377	2.0884	-4.5254
H	-4.5718	-3.9699	1.1131
H	-2.0324	2.4877	5.2699
H	-4.8934	7.2362	1.8346
H	-4.6424	6.0115	0.5982
H	-3.8511	-1.4026	-3.6238
H	-3.4837	7.1368	-1.6748
H	-3.5268	3.2153	-2.9783
H	-3.1950	-0.3381	-5.8231
H	-1.0914	1.7507	2.3699
H	-4.4682	-6.3341	-1.7727
H	-3.7630	4.6811	4.1057
H	-3.2273	-5.9735	0.3712
H	-3.2943	8.7360	0.3905
H	-3.4106	-0.5950	-2.0928
H	-5.5058	-5.6432	-0.5131
H	-2.5373	1.3203	-5.8678
H	-0.3728	0.1457	4.0176
H	-0.4779	3.0675	3.3952
H	-3.0459	-2.5600	-1.1169
H	-2.3311	-5.5504	-6.1993
H	-2.0054	4.7244	4.3699
H	-1.9568	-1.2275	5.5424
H	-1.7707	-3.1990	-6.3619
H	-2.1363	-1.2384	-3.1388
H	-2.5621	7.3649	1.2447
H	-2.6637	5.1238	2.7627
H	-1.8569	7.6349	-1.2328
H	-1.1101	3.4210	1.7568
H	-2.5276	-4.9927	-0.9356
H	-1.5208	-0.0269	-5.2831
H	-1.5695	-5.2097	1.3834
H	-2.7986	-4.0918	-4.3174
H	0.4004	0.8692	5.4496
H	-1.1936	-0.3919	6.9172
H	-1.4354	-6.6957	-5.1725
H	-0.6797	-6.0388	-6.6469
H	-0.4318	-2.4775	-5.4275
H	1.3812	0.0070	4.2233
H	-0.0777	-3.5656	-6.7887
H	-1.5054	-3.4462	-3.2749
H	-1.2594	-2.1729	6.8845
H	0.3108	-5.8190	2.4795
H	-1.9255	-5.1848	-3.2080

19:
-6819.1694

Cr	1.1537	-0.9752	-2.8566
Cr	-2.8371	-1.4400	2.7439
Cl	1.7948	0.6085	-4.5723
Cl	-4.6963	-1.9595	4.0190
O	1.4275	-4.4099	0.5576
O	0.9100	-2.1486	-1.3454
O	0.7470	-2.2856	-4.2288
O	-6.8528	3.6050	0.0639
O	-5.4016	3.9706	-1.6759
O	-3.1014	0.4729	2.7090

O	-1.9193	5.1444	-1.7991	C	-4.1831	2.5757	2.4341
O	-1.5724	-1.4528	4.1928	C	-4.0189	1.1870	2.0874
O	-2.7238	4.8224	0.3236	C	-3.3004	3.2278	3.5121
O	-0.6208	-0.1787	-2.6797	C	-3.7126	-2.9332	0.3554
O	-1.2225	-1.1792	1.4761	C	-4.2135	-5.8313	-0.0312
N	3.0946	-1.6085	-2.8163	C	-3.3931	-3.9840	1.4580
N	1.8694	0.4049	-1.5250	C	-3.1609	0.7055	-3.6388
N	-3.9107	-1.6274	1.0283	C	-3.8751	7.4383	0.3918
N	-2.3939	-3.3802	2.3572	C	-3.0287	-5.3288	0.8190
C	2.7143	-3.8267	0.4448	C	-3.6315	-0.3944	-2.6526
C	0.7143	-4.4716	-0.6735	C	-2.5255	0.0627	-4.8988
C	-1.0215	-3.4759	-2.1450	C	-1.8133	3.1580	3.0767
C	-0.0186	-3.1699	-1.0280	C	-3.6458	4.7208	3.7096
C	6.1319	-0.1314	-0.8913	C	-3.0067	6.9755	-0.7870
C	5.3180	0.5142	0.2455	C	-2.4618	2.9461	-2.6365
C	5.3112	-1.2179	-1.6122	C	-2.5621	5.5270	-0.6528
C	3.9976	1.0993	-0.2882	C	-2.1582	1.6173	-2.9122
C	3.9908	-0.6453	-2.1496	C	-1.2468	-3.9169	2.6274
C	3.4695	-2.7831	-3.1996	C	-1.5677	3.7729	-1.9421
C	3.2591	-4.9724	-4.2492	C	0.0524	0.8211	5.0811
C	3.1801	0.0048	-0.9879	C	-0.4485	-2.1398	4.2548
C	2.6728	-3.7147	-3.9667	C	-0.7797	-0.6404	6.9649
C	2.6477	-5.8696	-5.1056	C	-0.7705	-4.8388	-7.4429
C	1.4568	-5.4847	-5.7606	C	-0.2382	-3.3369	3.4875
C	1.3988	-3.3709	-4.5469	C	-0.0472	-2.4721	-7.0856
C	1.2985	1.5309	-1.2548	C	-0.8912	1.0924	-2.4738
C	0.8327	-4.2595	-5.5379	C	-1.6386	-3.5826	-5.4700
C	1.6453	-0.0450	6.7926	C	0.3883	-0.4055	5.9707
C	2.0218	-3.5360	4.3642	C	0.6043	-1.6675	5.1152
C	1.8046	-2.3778	5.1393	C	-0.3892	-3.8033	-6.3607
C	0.0069	1.9567	-1.7528	C	1.0033	-4.0105	3.5557
C	-7.5077	5.1721	-1.5878	C	-0.3586	3.2985	-1.4894
C	-7.5407	6.4704	-0.7384	C	-0.1867	-0.1399	1.6697
C	-6.4573	4.1902	-1.1159	C	-1.0444	-0.1103	0.4648
C	-6.1957	7.2315	-0.7066	C	1.2130	-0.6794	1.6226
C	-5.9041	2.7657	0.7132	H	-0.4406	0.5272	2.4833
C	-5.7676	1.4470	0.3548	H	3.4126	-4.5156	-0.0659
C	-5.1313	3.3202	1.7419	H	2.6692	-2.8898	-0.1180
C	-3.4826	2.5102	4.8739	H	3.0656	-3.6427	1.4667
C	-4.5907	-4.8081	-1.1193	H	-0.0198	-5.2804	-0.5425
C	-4.7005	-0.7196	0.5538	H	1.3847	-4.7408	-1.5057
C	-4.8768	-3.4125	-0.5268	H	-0.5419	-4.0015	-2.9730
C	-4.4208	1.4790	-4.0883	H	-1.8303	-4.1111	-1.7617
C	-4.8344	0.6325	1.0410	H	-1.4428	-2.5475	-2.5350
C	-5.2550	6.7528	0.4148	H	-0.5789	-2.8686	-0.1234

H	7.0595	-0.5664	-0.4964
H	5.9051	1.2987	0.7402
H	6.4176	0.6462	-1.6153
H	5.9014	-1.6460	-2.4315
H	5.0872	-0.2491	1.0035
H	5.0781	-2.0317	-0.9088
H	4.4840	-3.1287	-2.9805
H	4.2124	-5.2144	-3.7828
H	4.2053	1.9081	-1.0036
H	3.4230	1.5281	0.5426
H	4.1885	0.1409	-2.8908
H	2.9832	-0.8008	-0.2729
H	3.0919	-6.8388	-5.3089
H	1.8044	2.2558	-0.6126
H	1.9308	-0.8595	7.4706
H	2.4976	0.1826	6.1388
H	1.0274	-6.1742	-6.4782
H	1.4272	0.8442	7.3964
H	2.9792	-4.0455	4.4051
H	2.6133	-2.0285	5.7704
H	0.3197	3.9485	-0.9451
H	-8.4914	4.6895	-1.5431
H	-8.3235	7.1135	-1.1620
H	-7.2777	5.4192	-2.6291
H	-7.8454	6.2198	0.2865
H	-6.3544	1.0322	-0.4582
H	-5.7894	-3.4391	0.0861
H	-5.6998	7.1243	-1.6820
H	-6.3857	8.3059	-0.5664
H	-3.2209	1.4541	4.7968
H	-5.4711	-5.1548	-1.6754
H	-4.5240	2.5922	5.2114
H	-5.0965	0.7814	-4.5998
H	-5.2808	4.3642	1.9708
H	-5.3165	-0.9497	-0.3153
H	-3.7661	-4.7269	-1.8381
H	-4.9504	1.9215	-3.2354
H	-5.0406	-2.7057	-1.3490
H	-4.1587	2.2809	-4.7902
H	-4.3022	-4.0976	2.0649
H	-2.8332	2.9857	5.6220
H	-5.7430	6.9393	1.3824
H	-5.0929	5.6764	0.3444
H	-4.3260	-1.0796	-3.1604
H	-3.5382	7.0750	-1.7411
H	-3.4042	3.3781	-2.9385
H	-3.2582	-0.6104	-5.3659
H	-1.5002	2.1202	2.9861
H	-3.9625	-6.7956	-0.4910
H	-4.6862	4.8513	4.0365
H	-2.7821	-6.0586	1.6005
H	-4.0046	8.5289	0.3395
H	-4.1526	0.0853	-1.8180
H	-5.0784	-5.9965	0.6291
H	-2.2541	0.8421	-5.6216
H	-0.9050	0.6834	4.5793
H	-1.1888	3.6470	3.8371
H	-2.8105	-2.8273	-0.2626
H	-1.6155	-4.4455	-8.0211
H	-2.9902	5.1310	4.4874
H	-1.6953	-0.8905	6.4238
H	-0.9189	-2.1413	-7.6677
H	-2.7824	-0.9631	-2.2696
H	-3.3461	7.2099	1.3252
H	-3.4861	5.2845	2.7827
H	-2.1015	7.5925	-0.8752
H	-1.6781	3.6627	2.1153
H	-2.1382	-5.2030	0.1881
H	-1.6292	-0.5031	-4.6458
H	-0.9813	-4.8740	2.1778
H	-2.4879	-3.2978	-6.1071
H	-0.0072	1.7217	5.7069
H	-0.9491	0.2714	7.5550
H	-1.0742	-5.7953	-6.9965
H	0.0644	-5.0216	-8.1315
H	0.2174	-1.6931	-6.3669
H	0.8381	0.9748	4.3291
H	0.7947	-2.6244	-7.7738
H	-1.4571	-2.7877	-4.7491
H	-0.5334	-1.4600	7.6530
H	1.1535	-4.8757	2.9195
H	-1.8975	-4.5041	-4.9320
H	-0.6451	-0.5047	-0.4632
H	-1.8685	0.5939	0.4122
H	1.2968	-1.3595	0.7695
H	1.4589	-1.2044	2.5510
H	1.9193	0.1506	1.4908

20:
-6819.1526

Cr	-2.6476	-1.1810	3.1666	C	-4.5368	-5.0808	2.7890
Cr	0.9216	-1.0711	-2.8988	C	-3.8897	7.7958	-1.0464
Cl	-4.3410	-0.5297	4.7497	C	-3.6860	-0.1020	-3.8977
Cl	1.4348	0.8138	-4.4320	C	-4.3359	-3.5614	2.9257
O	-1.3603	-1.9867	1.8430	C	-5.8440	-5.3985	2.0335
O	-1.0041	-0.6033	-2.8369	C	-4.3738	-2.8712	1.5321
O	-2.0044	5.5750	-0.6912	C	-1.9986	3.4940	2.9568
O	-1.2282	-1.2072	4.4944	C	-3.3343	1.4609	2.0437
O	-3.0396	4.5614	-2.4946	C	-3.1957	2.8862	2.1930
O	-2.3995	0.6424	2.5258	C	-5.0942	7.2328	-0.2646
O	-6.3803	3.4000	-1.6451	C	-4.4791	0.9442	1.3488
O	-6.2962	4.1108	0.5549	C	-5.0608	0.4720	-4.3173
O	0.9735	-2.2482	-4.4853	C	-5.6785	-3.1902	0.7834
O	0.6736	-2.5185	-1.5264	C	-4.7235	-0.4652	1.1705
O	2.5187	-5.2157	-1.2292	C	-5.8799	-4.7141	0.6562
N	-3.0837	-3.1268	3.5952	C	-2.0174	2.9992	4.4288
N	-4.0859	-1.4342	1.7560	C	-4.1924	3.7006	1.6619
N	1.1703	0.2693	-1.3909	C	-5.4474	1.8189	0.8032
N	2.9619	-1.1932	-2.7524	C	-5.2978	3.1741	0.9776
C	1.0298	-2.7043	1.9562	C	-6.4370	7.3322	-1.0218
C	-0.7228	-2.0638	0.1534	C	-6.7730	4.1451	-0.7448
C	0.0115	-1.7413	1.3925	C	-7.6031	6.5799	-0.3297
C	-1.3066	2.9249	-1.7710	C	-7.8834	5.1639	-0.8826
C	-0.5323	-4.5863	5.7984	C	-0.8111	1.6046	-1.8965
C	0.3924	-3.0565	-7.2453	C	1.0611	-3.0111	6.6750
C	0.4723	-1.9358	6.0106	C	0.5810	-4.3335	6.5755
C	0.9899	-0.4901	6.1865	C	2.2259	-0.4253	7.1163
C	-0.7298	-3.7666	-6.4457	C	1.7667	-3.1976	-6.5532
C	-1.5149	0.6172	-2.6619	C	0.4247	1.3210	-1.2145
C	0.0595	-1.5429	-7.3765	C	1.9933	-2.6578	-5.2313
C	-1.1775	-3.5442	5.0883	C	2.8481	-3.7733	-7.2180
C	0.3941	-3.6608	-8.6713	C	4.1572	-3.7999	-6.6930
C	-0.1292	0.3808	6.8242	C	3.3468	-2.5848	-4.7474
C	-0.6710	-2.2024	5.1700	C	2.4445	0.0336	-0.6797
C	1.4059	0.1172	4.8175	C	4.4009	-3.1789	-5.4859
C	-2.4902	3.2470	-2.3970	C	3.7335	-1.8375	-3.5777
C	-2.3580	-3.9053	4.3402	C	3.5212	-0.2254	-1.7648
C	-2.8115	0.9561	-3.1933	C	2.9000	1.1313	0.2939
C	-2.7470	5.6224	-1.6811	C	4.8590	-0.6212	-1.1084
C	-3.2484	2.2709	-3.0630	C	4.2417	0.7505	0.9515
C	-3.4310	6.8756	-2.1920	C	5.3207	0.4582	-0.1081
C	-2.0447	5.0412	2.9678	C	0.4222	-3.9400	-1.7285
C	-0.6657	3.0758	2.2770	C	-0.8426	-4.1790	-2.5676
C	-2.9678	-0.6233	-5.1709	C	1.6160	-4.7389	-2.2797
C	-3.9463	-1.2865	-2.9253	C	3.5230	-4.2602	-0.8178

H	1.9905	-2.5925	1.4424	H	-5.1945	7.7749	0.6874
H	1.1765	-2.5167	3.0239	H	-1.1654	3.4286	4.9740
H	0.6905	-3.7365	1.8298	H	-5.1530	-3.1327	3.5234
H	-1.1928	-1.2893	-0.4333	H	-4.9590	1.2685	-5.0643
H	-0.9730	-3.0921	-0.0273	H	-5.6598	-2.7385	-0.2159
H	-0.4936	-4.8274	-6.2960	H	-5.6165	0.8724	-3.4620
H	-0.9319	-5.5950	5.7206	H	-5.0886	-5.1343	0.0183
H	-0.3874	0.0017	7.8210	H	-5.5417	-0.7030	0.4885
H	-0.8603	-3.2916	-5.4759	H	-4.1378	4.7735	1.7754
H	0.7849	-1.0485	-8.0350	H	-5.6590	-0.3292	-4.7676
H	2.2100	-0.4752	4.3607	H	-2.9401	3.3175	4.9281
H	0.0850	-1.0406	-6.4072	H	-6.8329	-4.9200	0.1516
H	1.1337	-3.1773	-9.3205	H	-1.9574	1.9113	4.4790
H	0.5906	-4.7406	-8.6632	H	-6.6973	8.3973	-1.1174
H	0.2177	1.4163	6.9323	H	-6.3215	6.9566	-2.0484
H	1.7794	1.1392	4.9644	H	-6.5277	-2.7513	1.3279
H	-1.6764	-3.7011	-6.9981	H	-6.2972	1.4155	0.2656
H	-2.6507	-4.9525	4.4492	H	-7.4135	6.5127	0.7473
H	-2.0100	-1.0776	-4.9148	H	-8.1337	5.2099	-1.9470
H	-3.6828	-5.5125	2.2464	H	-8.5312	7.1535	-0.4516
H	-0.6312	3.4606	1.2510	H	-8.7565	4.7511	-0.3565
H	-2.7054	7.4016	-2.8292	H	-0.7508	3.6604	-1.2077
H	-2.0221	5.4532	1.9532	H	1.9240	-2.8348	7.3061
H	-3.0439	7.9347	-0.3622	H	1.0784	-5.1339	7.1138
H	-3.0003	-1.7405	-2.6260	H	2.5441	0.6191	7.2125
H	-0.9406	-1.4160	-7.8122	H	2.6920	-4.2066	-8.1982
H	-1.0263	0.3734	6.2036	H	3.0726	-0.9964	6.7150
H	-1.1651	5.4155	3.5052	H	2.0016	-0.7979	8.1235
H	-0.5932	-3.5063	-9.1225	H	0.7383	2.0857	-0.5017
H	-3.5247	-3.2642	0.9558	H	4.9605	-4.2657	-7.2550
H	0.1805	3.5005	2.8328	H	2.3063	-0.9036	-0.1267
H	0.5546	0.1495	4.1368	H	3.6490	0.7156	-2.3187
H	-2.7841	0.2006	-5.8700	H	2.1385	1.2886	1.0679
H	-6.7005	-5.0555	2.6322	H	3.0141	2.0809	-0.2483
H	-4.4758	-0.9357	-2.0296	H	5.4119	-3.1248	-5.0861
H	-4.1423	8.7845	-1.4560	H	4.8154	-1.7776	-3.4322
H	-4.5675	-5.5532	3.7780	H	4.7369	-1.5825	-0.5899
H	-2.9330	5.4178	3.4901	H	4.0963	-0.1396	1.5823
H	-5.9508	-6.4848	1.9218	H	5.6372	-0.7602	-1.8686
H	-0.5721	1.9885	2.2614	H	5.5510	1.3841	-0.6566
H	-3.5955	-1.3693	-5.6760	H	4.5699	1.5569	1.6190
H	-4.2016	2.5861	-3.4632	H	6.2534	0.1378	0.3752
H	-4.2613	6.5798	-2.8388	H	0.2602	-4.3745	-0.7273
H	-4.5669	-2.0472	-3.4182	H	-1.6822	-3.6068	-2.1637
H	-4.8917	6.1891	0.0042	H	-1.1138	-5.2429	-2.5698

H	-0.6829	-3.8488	-3.5938
H	2.1696	-4.1727	-3.0334
H	1.2445	-5.6600	-2.7401
H	4.0722	-4.7282	0.0032
H	3.0712	-3.3218	-0.4806
H	4.2197	-4.0387	-1.6405
H	0.2949	-0.6920	1.4965

21:
-6819.1526

Cr	0.7968	-0.8433	-2.6886
Cr	-2.4937	-1.2015	2.9968
Cl	1.3998	0.8607	-4.1524
Cl	-4.3779	-0.1957	4.1286
O	1.9638	-4.9529	-1.0260
O	0.2715	-2.3309	-1.1431
O	0.8364	-2.1313	-4.1519
O	-5.9441	3.8046	0.0754
O	-6.2371	3.0216	-2.0635
O	-1.9813	0.4360	2.0295
O	-3.1693	4.6964	-2.2137
O	-1.3466	-1.0363	4.5580
O	-1.8934	5.7134	-0.5874
O	-1.0797	-0.4202	-2.7173
O	-1.1859	-2.3112	2.1655
N	2.7942	-1.1371	-2.3488
N	1.0174	0.4035	-1.1217
N	-3.7540	-1.6112	1.4391
N	-3.1519	-3.0175	3.6576
C	3.0931	-4.1304	-0.8197
C	1.1038	-4.4783	-2.0551
C	-1.3174	-3.7054	-2.4102
C	-0.0950	-3.7235	-1.4912
C	5.0261	0.3172	0.4953
C	3.8838	0.6637	1.4700
C	4.5796	-0.7380	-0.5377
C	2.6338	1.1500	0.7113
C	3.3493	-0.2270	-1.3095
C	3.5816	-1.8013	-3.1325
C	4.2670	-3.1554	-5.0238
C	2.2074	0.0957	-0.3148
C	3.2084	-2.5256	-4.3223
C	4.0418	-3.7843	-6.2317
C	2.7464	-3.7446	-6.7888
C	1.8686	-2.5655	-4.8488
C	0.2690	1.4414	-0.9204
C	1.6620	-3.1383	-6.1557
C	2.7345	-0.3967	5.9796
C	0.7628	-4.1824	6.2705
C	1.3197	-2.8901	6.1757
C	-0.9304	1.7402	-1.6582
C	-7.7186	4.7315	-1.2035
C	-7.5713	6.0510	-0.4214
C	-6.5400	3.7674	-1.1495
C	-6.4515	6.9733	-0.9687
C	-4.9052	2.8978	0.4324
C	-4.9679	1.5432	0.1768
C	-3.8802	3.4386	1.2205
C	-1.9299	2.5935	4.1154
C	-5.5661	-4.9377	0.6185
C	-4.2607	-0.7288	0.6461
C	-5.2817	-3.4279	0.5209
C	-4.9348	0.7321	-4.4950
C	-4.0009	0.6936	0.7517
C	-5.1910	6.9899	-0.0840
C	-2.8753	2.6432	1.7690
C	-2.9172	1.2274	1.5294
C	-1.8136	3.2402	2.7103
C	-4.0938	-3.0408	1.4097
C	-5.8224	-5.3523	2.0801
C	-4.3256	-3.4805	2.8989
C	-3.6289	0.1299	-3.9319
C	-4.0225	7.7718	-0.7087
C	-4.6234	-4.9845	2.9740
C	-4.0213	-1.0524	-3.0055
C	-2.7966	-0.3971	-5.1280
C	-0.3870	2.9937	2.1605
C	-1.9842	4.7668	2.8753
C	-3.4177	7.0327	-1.9203
C	-3.2844	2.4609	-2.9504
C	-2.7274	5.7517	-1.4770
C	-2.8274	1.1579	-3.1181
C	-2.4587	-3.7634	4.4511
C	-2.5927	3.4013	-2.1680
C	1.3169	0.0286	3.9751
C	-0.6727	-2.0488	5.0482
C	0.4617	0.6019	6.2856
C	0.3143	-3.6226	-8.2749
C	-1.2148	-3.3834	5.0901
C	-0.0563	-1.5065	-6.9970

C	-1.5808	0.7918	-2.5120	H	-5.7715	1.1258	-0.4168
C	-0.8219	-3.7305	-6.0616	H	-6.1685	-2.8631	0.8445
C	1.2798	-0.4252	5.4597	H	-6.1872	6.6502	-1.9857
C	0.6472	-1.8232	5.5802	H	-6.8233	8.0045	-1.0610
C	0.2966	-3.0116	-6.8552	H	-1.7356	1.5220	4.0771
C	-0.4896	-4.4157	5.7268	H	-6.4265	-5.1994	-0.0111
C	-1.4485	3.0445	-1.4868	H	-2.9377	2.7377	4.5192
C	-0.1109	-1.8947	1.3619	H	-5.4804	-0.0537	-5.0324
C	-0.6579	-1.8383	-0.0863	H	-3.9019	4.5016	1.4164
C	1.0491	-2.8737	1.6122	H	-4.9904	-1.0205	-0.1107
H	0.2247	-0.8831	1.6375	H	-4.6981	-5.4940	0.2338
H	3.7813	-4.1748	-1.6812	H	-5.5764	1.1248	-3.6980
H	2.8048	-3.0871	-0.6668	H	-5.0742	-3.1478	-0.5203
H	3.6045	-4.5023	0.0751	H	-4.7186	1.5431	-5.2028
H	0.7207	-5.3654	-2.5760	H	-5.1823	-2.9016	3.2709
H	1.6455	-3.8690	-2.7785	H	-1.2001	3.0669	4.7878
H	-1.1702	-2.9759	-3.2036	H	-5.4516	7.4274	0.8901
H	-1.4849	-4.6956	-2.8506	H	-4.8761	5.9598	0.1129
H	-2.2159	-3.4192	-1.8540	H	-4.5368	-1.8246	-3.5934
H	-0.3401	-4.2124	-0.5413	H	-4.1782	6.8071	-2.6721
H	5.8994	-0.0532	1.0471	H	-4.2096	2.7827	-3.4037
H	4.2080	1.4301	2.1848	H	-3.4035	-1.1048	-5.7113
H	5.3372	1.2283	-0.0378	H	-0.2336	1.9270	1.9861
H	5.4098	-0.9583	-1.2196	H	-6.0193	-6.4307	2.1429
H	3.6177	-0.2275	2.0543	H	-2.9497	5.0056	3.3402
H	4.3126	-1.6708	-0.0234	H	-4.8228	-5.2742	4.0133
H	4.6545	-1.8047	-2.9236	H	-4.3647	8.7674	-1.0251
H	5.2650	-3.1242	-4.5914	H	-4.6992	-0.6926	-2.2222
H	2.8507	2.0955	0.1930	H	-6.7189	-4.8322	2.4498
H	1.8161	1.3327	1.4159	H	-2.5057	0.4346	-5.7821
H	3.6041	0.7092	-1.8276	H	0.3075	0.1103	3.5715
H	1.9777	-0.8305	0.2197	H	0.3498	3.3461	2.8953
H	4.8494	-4.2735	-6.7658	H	-3.1851	-3.5621	1.0762
H	0.5309	2.1531	-0.1422	H	-0.6699	-3.4702	-8.7335
H	2.7872	-0.6470	7.0475	H	-1.1893	5.1369	3.5348
H	3.3711	-1.0992	5.4250	H	-0.5677	0.6461	5.9255
H	2.6014	-4.1975	-7.7618	H	-1.0631	-1.4030	-7.4234
H	3.1345	0.6160	5.8437	H	-3.1341	-1.4880	-2.5410
H	1.3204	-4.9827	6.7470	H	-3.2275	7.9086	0.0337
H	2.3152	-2.7329	6.5752	H	-1.9112	5.2874	1.9126
H	-0.9381	3.7427	-0.8442	H	-2.6535	7.6642	-2.3941
H	-8.5890	4.1782	-0.8186	H	-0.2401	3.5550	1.2292
H	-8.5388	6.5681	-0.4700	H	-3.7321	-5.5387	2.6439
H	-7.9084	4.9334	-2.2637	H	-1.8923	-0.9003	-4.7878
H	-7.3803	5.8233	0.6343	H	-2.7761	-4.7927	4.6424

H	-1.7517	-3.7102	-6.6465
H	1.8127	1.0071	3.9046
H	0.9184	1.5979	6.1927
H	0.5171	-4.7023	-8.2496
H	1.0666	-3.1378	-8.9100
H	-0.0325	-0.9999	-6.0308
H	1.8812	-0.6938	3.3725
H	0.6615	-1.0141	-7.6653
H	-0.9967	-3.2305	-5.1135
H	0.4614	0.3148	7.3457
H	-0.9257	-5.4131	5.7589
H	-0.5509	-4.7777	-5.8703
H	-1.5456	-2.4695	-0.1087
H	-0.9543	-0.8320	-0.3601
H	0.8103	-3.8779	1.2478
H	1.1902	-2.9222	2.6976
H	1.9899	-2.5592	1.1488

F1:
-6708.3274

Cr	-1.7933	-1.4550	1.2799
Cr	0.2784	-0.8781	-2.0954
Cl	-3.3089	-1.6826	3.1089
Cl	1.5443	-0.1582	-3.9846
O	-1.2802	0.1279	-2.6538
O	-2.0546	5.9162	-0.3176
O	-0.2592	-1.7519	2.4759
O	-2.4398	5.5546	-2.5548
O	-1.8451	0.4868	1.3983
O	-5.4611	4.7085	-1.3560
O	-6.1685	3.9219	0.6838
O	-0.1896	-2.5545	-3.0100
O	-0.5762	-1.5369	-0.3598
N	-1.9419	-3.4777	1.0099
N	-3.3895	-1.4359	0.0370
N	0.9926	0.7124	-1.0725
N	1.9753	-1.7676	-1.3872
C	-0.9411	3.7136	-1.8597
C	1.0362	-5.1977	2.2877
C	-1.0491	-4.4543	-5.0119
C	1.4485	-2.8134	3.7561
C	1.5653	-1.6026	4.7089
C	-2.3921	-3.8506	-4.5263
C	-1.4492	1.4331	-2.6858
C	-0.3250	-3.4343	-5.9371
C	0.1585	-4.0993	2.0944
C	-1.3859	-5.7034	-5.8640
C	0.2068	-1.4060	5.4415
C	0.4114	-2.8428	2.7462
C	1.9299	-0.3108	3.9321
C	-2.0290	4.1955	-2.5509
C	-1.0380	-4.3511	1.3223
C	-2.5078	1.9906	-3.4959
C	-2.5104	6.2675	-1.3897
C	-2.7829	3.3488	-3.3797
C	-3.2059	7.5967	-1.6513
C	-1.9962	4.4453	3.3783
C	-0.4077	3.0566	2.0466
C	-2.3021	0.4113	-5.4622
C	-4.1041	0.0211	-3.7135
C	-3.3502	-5.2460	-0.2191
C	-3.6031	8.3162	-0.3513
C	-3.2932	1.0990	-4.4814
C	-3.2412	-3.8455	0.4040
C	-4.7859	-5.4813	-0.7314
C	-3.6137	-2.7429	-0.6277
C	-1.7594	3.0255	2.8086
C	-2.8875	1.2778	1.2436
C	-2.8968	2.5867	1.8601
C	-4.7475	7.6215	0.4175
C	-4.0249	0.8873	0.4550
C	-4.2965	1.9176	-5.3307
C	-5.0387	-2.9766	-1.1638
C	-4.1667	-0.4192	-0.1440
C	-5.2086	-4.3975	-1.7384
C	-1.6672	2.0364	4.0026
C	-3.9767	3.4297	1.6099
C	-5.0929	1.7879	0.2367
C	-5.0549	3.0388	0.8044
C	-6.1396	7.8221	-0.2163
C	-6.2590	4.7089	-0.4393
C	-7.2409	6.9291	0.4078
C	-7.4881	5.5957	-0.3495
C	-0.6347	2.3327	-1.9175
C	2.2760	-3.9224	3.8804
C	2.1284	-5.1244	3.1364
C	2.6530	-1.8176	5.7905
C	-0.1187	-4.7937	-3.8245
C	0.5059	1.9090	-1.1402
C	0.3572	-3.7414	-2.9542

C	0.3504	-6.0877	-3.6182	H	1.1861	-0.0990	3.1632
C	1.3330	-6.4414	-2.6564	H	-1.7669	1.1637	-6.0538
C	1.4509	-4.0574	-2.0733	H	-5.4756	-5.4725	0.1258
C	2.1347	0.3686	-0.1879	H	-4.8383	0.5041	-3.0571
C	1.8918	-5.3971	-1.9329	H	-3.8931	9.3508	-0.5866
C	2.2309	-3.0381	-1.4047	H	-3.1044	-6.0148	0.5237
C	2.9397	-0.7585	-0.8919	H	-2.9160	4.4958	3.9739
C	3.0676	1.5401	0.1754	H	-4.8617	-6.4759	-1.1891
C	4.0832	-1.2624	0.0014	H	-0.1880	2.0731	1.6289
C	4.2668	1.0674	1.0228	H	-2.8552	-0.2395	-6.1531
C	5.0266	-0.0939	0.3578	H	-3.5996	3.7988	-3.9278
C	3.1395	-6.2709	3.3383	H	-4.0712	7.4035	-2.2943
C	1.7273	-7.9136	-2.4100	H	-4.6432	-0.6184	-4.4254
C	2.8127	-7.4955	2.4552	H	-4.5148	6.5540	0.4970
C	3.1363	-6.7356	4.8207	H	-4.7765	8.0074	1.4472
C	4.5634	-5.7722	2.9676	H	-0.8473	2.3330	4.6712
C	1.5046	-8.7945	-3.6658	H	-3.9639	-3.7647	1.2292
C	0.8534	-8.4778	-1.2545	H	-3.7921	2.7013	-5.9087
C	3.2206	-8.0426	-2.0142	H	-5.2751	-2.2455	-1.9454
H	-2.9145	-4.5689	-3.8828	H	-5.0737	2.3843	-4.7130
H	0.8139	-6.1113	1.7443	H	-4.6022	-4.4946	-2.6476
H	-0.0246	-2.2849	6.0558	H	-5.0380	-0.5227	-0.7912
H	-2.2269	-2.9276	-3.9700	H	-4.0147	4.4194	2.0447
H	0.6040	-3.8660	-6.3302	H	-4.7919	1.2458	-6.0419
H	2.9148	-0.4204	3.4619	H	-2.5994	2.0414	4.5797
H	-0.0769	-2.5173	-5.3996	H	-6.2544	-4.5462	-2.0383
H	-0.4848	-6.1692	-6.2806	H	-1.4875	1.0188	3.6545
H	-1.9318	-6.4602	-5.2862	H	-6.4201	8.8799	-0.1079
H	0.2608	-0.5309	6.1023	H	-6.0925	7.6246	-1.2959
H	1.9756	0.5432	4.6207	H	-5.7541	-2.8209	-0.3427
H	-3.0390	-3.6337	-5.3866	H	-5.9420	1.4858	-0.3680
H	-1.1791	-5.3934	1.0294	H	-6.9924	6.7099	1.4554
H	-1.5649	-0.1883	-4.9268	H	-7.8030	5.8182	-1.3744
H	-2.6295	-5.3446	-1.0437	H	-8.1969	7.4695	0.4199
H	-0.4532	3.7920	1.2351	H	-8.2881	5.0406	0.1515
H	-2.5208	8.2213	-2.2431	H	-0.3367	4.3711	-1.2502
H	-2.0468	5.1979	2.5828	H	3.0755	-3.8838	4.6095
H	-2.7195	8.3685	0.2956	H	-0.0961	-2.3636	-0.2063
H	-3.4369	-0.5975	-3.1114	H	2.6772	-0.9430	6.4517
H	-0.9693	-3.1780	-6.7887	H	-0.0388	-6.8716	-4.2517
H	-0.6089	-1.2583	4.7316	H	3.6542	-1.9301	5.3547
H	-1.1595	4.7070	4.0371	H	2.4436	-2.6981	6.4104
H	-2.0239	-5.4010	-6.7030	H	0.9796	2.7066	-0.5685
H	-2.8875	-2.7961	-1.4516	H	1.6958	-0.0531	0.7282
H	0.4007	3.3449	2.7327	H	3.3683	-0.3203	-1.8060

H	2.5155	2.3041	0.7349
H	3.4235	2.0089	-0.7536
H	2.7000	-5.5818	-1.2308
H	3.1367	-3.4069	-0.9182
H	3.6757	-1.7148	0.9175
H	3.9038	0.7451	2.0068
H	4.6585	-2.0392	-0.5173
H	5.5120	0.2665	-0.5613
H	4.9460	1.9122	1.1980
H	5.8275	-0.4498	1.0193
H	1.8252	-7.9083	2.6907
H	3.5541	-8.2862	2.6226
H	2.8319	-7.2373	1.3905
H	2.1443	-7.1040	5.1059
H	3.4005	-5.9191	5.5011
H	3.8632	-7.5452	4.9694
H	4.5990	-5.4547	1.9190
H	5.3031	-6.5706	3.1129
H	4.8596	-4.9179	3.5861
H	-0.2099	-8.4247	-1.5151
H	1.0050	-7.8961	-0.3385
H	1.1067	-9.5259	-1.0450
H	0.4436	-8.8839	-3.9236
H	1.8811	-9.8076	-3.4767
H	2.0352	-8.3889	-4.5350
H	3.8697	-7.6175	-2.7883
H	3.4819	-9.1008	-1.8885
H	3.4419	-7.5383	-1.0681

F2:
-6708.294

Cr	0.5056	-0.2082	-4.3268
Cr	-0.8648	-1.2442	1.8544
Cl	2.0181	0.4524	-6.1204
Cl	1.0853	-0.8033	0.8071
O	-0.6247	-0.7198	-2.8615
O	0.0713	-1.9126	-5.2134
O	-5.0281	4.3105	0.6899
O	-5.2008	3.9058	-1.5678
O	-1.5261	0.4109	2.5364
O	-2.7387	6.0515	-3.9740
O	-0.1369	-1.7875	3.5514
O	-1.3304	6.8283	-2.3324
O	-0.9178	0.9252	-5.1000
N	2.0746	-1.1284	-3.4113
N	1.1706	1.3734	-3.2005
N	-2.0887	-1.0460	0.2554
N	-1.0577	-3.2064	1.3656
C	2.0067	-7.3776	-2.2255
C	-0.2595	-7.9669	-3.1158
C	1.7671	-8.0665	-4.6249
C	4.2458	-6.2466	5.0745
C	2.2499	-6.9480	6.4668
C	2.4811	-7.7380	4.0977
C	1.0889	-7.2823	-3.4671
C	2.7207	-6.5395	5.0438
C	5.1362	0.4683	-1.6177
C	4.3947	1.6806	-1.0234
C	4.1575	-0.6711	-1.9736
C	3.2699	2.1766	-1.9553
C	3.0719	-0.1544	-2.9293
C	2.1613	-2.3985	-3.1990
C	1.5166	-4.7413	-3.3401
C	2.2964	1.0292	-2.2899
C	1.2998	-3.4103	-3.7710
C	0.8514	-5.8217	-3.9021
C	-0.0208	-5.5346	-4.9867
C	0.3524	-3.1235	-4.8155
C	0.6049	2.5382	-3.1485
C	-0.2716	-4.2561	-5.4748
C	2.6012	-1.8355	7.0342
C	1.9538	-5.2815	4.5888
C	2.0726	-4.0756	5.3283
C	-0.5577	2.9764	-3.8820
C	-6.7647	5.4169	-0.4939
C	-6.5333	6.8076	0.1403
C	-5.5733	4.4769	-0.5637
C	-5.7146	7.7893	-0.7292
C	-4.0709	3.3103	0.9851
C	-3.8286	2.1723	0.2412
C	-3.4123	3.5088	2.2111
C	-2.2355	1.7657	5.1352
C	-2.9065	-3.6115	-2.5593
C	-2.7938	0.0001	-0.0495
C	-3.1012	-2.3210	-1.7393
C	-4.3929	2.6954	-7.1338
C	-2.9428	1.1925	0.7519
C	-4.1851	7.6714	-0.5799
C	-2.5255	2.5787	2.7497
C	-2.2981	1.3621	2.0165

C	-1.8169	2.8428	4.0959	H	2.8122	-7.5200	3.0758
C	-2.0143	-2.2217	-0.6606	H	3.0448	-8.6084	4.4534
C	-2.8567	-4.8698	-1.6759	H	1.4219	-8.0191	4.0645
C	-2.0173	-3.4680	0.2507	H	5.8938	0.1035	-0.9112
C	-3.2148	1.8945	-6.5265	H	5.1003	2.4990	-0.8281
C	-3.4053	8.6304	-1.5076	H	5.6726	0.7799	-2.5264
C	-1.7879	-4.7473	-0.5684	H	4.7113	-1.4955	-2.4402
C	-3.8087	0.6315	-5.8420	H	3.9587	1.3969	-0.0547
C	-2.2784	1.4704	-7.6932	H	3.6951	-1.0609	-1.0555
C	-0.2756	2.8150	3.8957	H	2.9674	-2.7853	-2.5696
C	-2.1866	4.2275	4.6800	H	2.2441	-4.8925	-2.5477
C	-3.2808	8.1213	-2.9572	H	3.6926	2.5675	-2.8917
C	-2.8140	4.0103	-5.1539	H	2.7419	3.0040	-1.4668
C	-2.3249	6.9344	-3.0325	H	3.5445	0.2261	-3.8468
C	-2.4251	2.7234	-5.4914	H	1.8471	0.6582	-1.3556
C	-0.4276	-4.1811	1.9497	H	1.0129	3.2936	-2.4723
C	-2.1220	4.7873	-4.2036	H	2.2460	-2.5998	7.7366
C	2.1924	-0.4731	4.9803	H	3.5970	-2.1241	6.6773
C	0.5559	-2.8743	3.8601	H	-0.5036	-6.3718	-5.4772
C	0.2540	-1.1699	6.4767	H	2.7083	-0.8976	7.5909
C	-1.6698	-5.3516	-7.3309	H	-0.5208	-0.0526	-2.1660
C	0.4357	-4.0769	3.0950	H	2.7188	-4.0863	6.1967
C	-0.2960	-3.3161	-7.8208	H	-0.4565	4.8809	-2.8579
C	-1.2656	2.1487	-4.8276	H	-7.5377	4.8926	0.0862
C	-2.3830	-3.1484	-6.3849	H	-7.5248	7.2429	0.3247
C	1.6122	-1.6123	5.8643	H	-7.1385	5.5245	-1.5166
C	1.4168	-2.8873	5.0143	H	-6.0580	6.6858	1.1221
C	-1.1471	-4.0246	-6.7269	H	-4.2946	2.0195	-0.7209
C	1.1270	-5.2526	3.4798	H	-4.1015	-2.3047	-1.2768
C	-0.9974	4.2909	-3.5820	H	-6.0041	7.6585	-1.7828
H	1.5865	-6.8310	-1.3730	H	-6.0008	8.8176	-0.4621
H	2.1240	-8.4279	-1.9302	H	-1.9758	0.7660	4.7844
H	3.0053	-6.9748	-2.4306	H	-3.7139	-3.7004	-3.2961
H	2.7303	-7.6101	-4.8807	H	-3.3171	1.8070	5.3160
H	1.9442	-9.1114	-4.3353	H	-4.9105	2.0671	-7.8684
H	1.1446	-8.0628	-5.5260	H	-3.6321	4.4280	2.7369
H	-0.0991	-9.0196	-2.8461	H	-3.3483	0.0026	-0.9866
H	-0.7396	-7.4647	-2.2676	H	-1.9735	-3.5235	-3.1273
H	-0.9560	-7.9381	-3.9599	H	-5.1250	2.9912	-6.3718
H	4.4877	-5.4305	5.7639	H	-2.9984	-1.4702	-2.4180
H	4.7972	-7.1383	5.3999	H	-4.0467	3.5986	-7.6520
H	4.6057	-5.9639	4.0787	H	-3.0139	-3.5282	0.7217
H	2.8010	-7.8320	6.8126	H	-1.7225	1.9469	6.0884
H	2.4148	-6.1428	7.1906	H	-3.9229	7.8886	0.4655
H	1.1799	-7.1857	6.4650	H	-3.8517	6.6422	-0.7676

H	-4.3455	0.0224	-6.5815
H	-4.2489	7.8358	-3.3801
H	-3.6861	4.4623	-5.6082
H	-2.8364	0.8608	-8.4167
H	0.0569	1.8423	3.5313
H	-2.6360	-5.7489	-2.2936
H	-3.2608	4.3143	4.8849
H	-1.8367	-5.6374	0.0711
H	-3.8906	9.6167	-1.5062
H	-4.5192	0.9212	-5.0564
H	-3.8414	-5.0418	-1.2124
H	-1.8934	2.3549	-8.2160
H	1.5436	-0.2554	4.1312
H	0.2260	3.0234	4.8497
H	-1.0538	-2.1304	-1.1904
H	-2.2694	-5.1249	-8.2209
H	-1.6567	4.3669	5.6294
H	-0.4749	-0.9630	5.6922
H	-0.9038	-3.1554	-8.7215
H	-3.0170	0.0280	-5.3963
H	-2.3903	8.7667	-1.1180
H	-1.8924	5.0447	4.0105
H	-2.8766	8.9190	-3.5974
H	0.0328	3.5815	3.1743
H	-0.7879	-4.7125	-1.0207
H	-1.4315	0.8924	-7.3203
H	-0.5532	-5.1936	1.5633
H	-2.9584	-2.9438	-7.2978
H	2.3056	0.4404	5.5784
H	0.3925	-0.2602	7.0757
H	-2.3113	-5.8990	-6.6282
H	-0.8502	-6.0127	-7.6391
H	0.0706	-2.3515	-7.4658
H	3.1801	-0.7537	4.5950
H	0.5664	-3.9364	-8.0963
H	-2.0726	-2.1997	-5.9467
H	-0.1459	-1.9536	7.1329
H	0.9882	-6.1366	2.8666
H	-3.0400	-3.6688	-5.6766

F3:
-6901.4151

Cr	4.7437	-0.3848	-1.0931
Cr	-2.1322	2.1048	-1.2718
Cl	6.7230	-1.5603	-1.3899
Cl	-3.7152	2.7347	-3.0222
N	4.1309	-0.7538	-2.9745
N	3.7408	-2.1198	-0.7195
N	-2.4344	3.8908	-0.3470
N	-0.7772	3.1992	-2.3589
O	4.9957	-0.1057	0.8132
O	5.4422	1.3407	-1.6538
O	2.9018	0.6793	-0.9588
O	-1.5485	0.4830	-2.2656
O	-3.6115	1.3204	-0.2335
O	-0.9164	1.7128	0.1577
C	1.5530	0.2751	-0.5286
C	2.3105	1.2390	0.2645
C	2.0395	2.7127	0.2253
O	0.4280	0.1401	-7.4424
O	2.6975	0.1377	-7.0950
O	4.1864	4.4543	-6.0883
O	1.8888	4.3925	-5.9926
C	2.2041	-4.6531	-3.2658
C	3.7386	-2.7319	0.4248
C	3.9276	0.1457	-3.8830
C	4.3507	-2.2758	1.6493
C	4.9732	-0.9909	1.7926
C	4.2896	-3.1698	2.7505
C	5.5556	-0.6557	3.0698
C	5.4586	-1.5838	4.1029
C	4.3116	1.5346	-3.7805
C	5.0875	2.0699	-2.6933
C	3.9699	2.3424	-4.8890
C	5.5331	3.4422	-2.7797
C	5.1519	4.2000	-3.8879
C	3.0524	-2.6732	-1.9176
C	3.8342	-2.1879	-3.1717
C	3.0931	-2.5832	-4.4557
C	2.8776	-4.2021	-1.9520
C	2.9342	-4.1160	-4.5112
C	-0.2137	2.8111	-3.4573
C	-3.4023	4.1781	0.4574
C	-0.3102	1.4994	-4.0583
C	-1.0249	0.3990	-3.4620
C	0.2361	1.3835	-5.3566
C	-1.1365	-0.8368	-4.2146
C	-0.5875	-0.8909	-5.4951
C	-4.4890	3.3046	0.8353

C	-4.5570	1.9202	0.4569	C	3.0110	5.3328	-7.9396
C	-5.4872	3.8733	1.6662	H	5.9486	6.1515	-2.0220
C	-5.7126	1.1631	0.8954	H	7.3748	5.6064	-2.9405
C	-6.6506	1.7886	1.7092	H	7.4885	5.8732	-1.1929
C	-0.8313	4.6516	-2.0292	H	4.8625	4.6303	-0.3191
C	-1.2697	4.7807	-0.5463	H	6.4424	4.3951	0.4604
C	-1.4546	6.2582	-0.1566	H	5.4836	2.9832	-0.0382
C	0.4562	5.4544	-2.3017	H	7.5736	2.1638	-1.4053
C	-0.1625	7.0544	-0.4265	H	8.4395	3.6237	-0.8641
C	0.2708	6.9317	-1.8979	H	8.3016	3.2618	-2.5991
C	6.4584	4.0329	-1.6944	H	5.4730	5.2282	-3.9883
C	7.7771	3.2108	-1.6366	H	2.0588	-2.2005	-1.9604
C	5.7626	4.0023	-0.3073	H	2.2642	-4.5390	-1.1073
C	6.8343	5.5050	-1.9917	H	3.8650	-4.6745	-1.8482
C	6.2690	0.6992	3.2719	H	1.1647	-4.2959	-3.2772
C	5.2603	1.8655	3.0803	H	2.1615	-5.7495	-3.2942
C	7.4368	0.8440	2.2571	H	3.9284	-4.5822	-4.5834
C	6.8690	0.8340	4.6931	H	2.3848	-4.3986	-5.4180
C	-5.9140	-0.2881	0.4083	H	3.6387	-2.2307	-5.3381
C	-4.7176	-1.1896	0.8212	H	2.1047	-2.1056	-4.4799
C	-6.0605	-0.2750	-1.1391	H	4.8150	-2.6849	-3.1521
C	-7.1941	-0.9329	0.9938	H	6.0974	0.8002	5.4722
C	-1.9425	-2.0190	-3.6391	H	7.3803	1.8005	4.7723
C	-3.4231	-1.5843	-3.4667	H	7.6062	0.0482	4.8972
C	-1.3730	-2.4561	-2.2607	H	7.0767	0.7814	1.2298
C	-1.9127	-3.2542	-4.5714	H	8.1783	0.0512	2.4136
C	4.3775	3.6588	-4.9238	H	7.9347	1.8121	2.4011
C	4.8319	-2.8525	3.9862	H	4.8537	1.8594	2.0684
C	0.0855	0.2060	-6.0565	H	5.7638	2.8266	3.2475
C	-6.5711	3.1433	2.1270	H	4.4328	1.7853	3.7971
C	-7.6596	3.7215	3.0519	H	3.8001	-4.1253	2.5918
C	-9.0537	3.5903	2.3797	H	5.8894	-1.3287	5.0626
C	-7.4234	5.2161	3.3664	H	-5.3735	4.9194	1.9345
C	-7.6699	2.9400	4.3946	H	-7.5025	1.2110	2.0473
C	4.7879	-3.7940	5.2055	H	-7.1519	-1.0045	2.0883
C	4.0823	-5.1311	4.8822	H	-7.2929	-1.9496	0.5944
C	4.0158	-3.1101	6.3665	H	-8.0971	-0.3760	0.7158
C	6.2336	-4.1155	5.6722	H	-4.5864	-1.1782	1.9114
C	1.7975	0.3298	-9.3493	H	-3.7958	-0.8456	0.3529
C	1.7304	0.1958	-7.8368	H	-4.9118	-2.2257	0.5117
C	2.9804	1.1805	-9.8551	H	-6.9854	0.2398	-1.4282
C	3.0949	2.6014	-9.2559	H	-6.1057	-1.3037	-1.5209
C	1.7597	3.3654	-9.1312	H	-5.2220	0.2414	-1.6085
C	1.8995	4.8917	-8.9147	H	-1.7187	6.3464	0.9043
C	2.9222	4.6772	-6.5710	H	-2.2854	6.6862	-0.7362

H	0.6398	6.6647	0.2179
H	-0.3066	8.1078	-0.1527
H	-0.4971	7.3890	-2.5397
H	1.2023	7.4860	-2.0714
H	-1.6495	5.0587	-2.6424
H	-0.4712	4.3423	0.0682
H	0.7333	5.3976	-3.3598
H	1.2870	5.0167	-1.7314
H	-0.6959	-1.7777	-6.1068
H	0.7251	2.2423	-5.8040
H	-0.3121	-2.7258	-2.3508
H	-1.9193	-3.3363	-1.8969
H	-1.4685	-1.6502	-1.5332
H	-3.8625	-1.3226	-4.4367
H	-3.4923	-0.7164	-2.8113
H	-4.0072	-2.4065	-3.0317
H	-2.3839	-3.0462	-5.5398
H	-2.4728	-4.0702	-4.0993
H	-0.8896	-3.6083	-4.7536
H	2.9733	3.2765	0.3264
H	1.3600	2.9691	1.0433
H	1.5462	2.9771	-0.7118
H	2.8138	0.8675	1.1528
H	3.4160	1.9029	-5.7083
H	2.9845	-2.8919	6.0665
H	4.4879	-2.1661	6.6594
H	3.9902	-3.7645	7.2477
H	6.7965	-4.6071	4.8703
H	6.2132	-4.7837	6.5430
H	6.7766	-3.2077	5.9568
H	3.0400	-4.9733	4.5802
H	4.0805	-5.7714	5.7724
H	4.5962	-5.6718	4.0786
H	-9.0790	4.1498	1.4374
H	-9.8374	3.9852	3.0405
H	-9.2939	2.5453	2.1564
H	-7.4336	5.8201	2.4517
H	-6.4644	5.3754	3.8734
H	-8.2189	5.5867	4.0247
H	-6.7044	3.0387	4.9050
H	-7.8543	1.8724	4.2319
H	-8.4551	3.3249	5.0596
H	3.4591	-0.1339	-4.8258
H	3.2385	-3.6994	0.5046
H	0.3571	3.5289	-4.0503
H	-3.4305	5.1635	0.9288
H	0.7546	0.6102	-1.1784
H	1.4948	-0.7524	-0.1781
H	-1.5141	1.4563	0.8774
H	1.8824	-0.6823	-9.7703
H	0.8426	0.7343	-9.6954

F4:
-6901.4262

Cr	4.5877	-0.3066	-1.0351
Cr	-2.1003	2.0731	-1.3462
Cl	6.5231	-1.6406	-1.1930
Cl	-3.8625	2.7581	-2.8447
N	4.0501	-0.7431	-2.9272
N	3.4563	-1.9572	-0.6250
N	-2.3659	3.7727	-0.2754
N	-0.8980	3.2789	-2.4930
O	4.7956	0.0419	0.8771
O	5.4574	1.3337	-1.6596
O	2.8936	0.8109	-1.0628
O	-1.5854	0.5584	-2.4942
O	-3.4131	1.1453	-0.2245
O	-0.6892	1.6048	-0.0693
C	1.1652	0.7483	-0.6386
C	2.2418	1.5082	-0.0088
C	2.2881	3.0142	-0.1232
O	0.4025	0.3921	-7.6722
O	2.6530	0.2125	-7.2454
O	4.4939	4.3192	-6.2485
O	2.1937	4.3974	-6.1859
C	1.9604	-4.5620	-3.1271
C	3.3492	-2.5005	0.5481
C	3.9429	0.1178	-3.8864
C	3.9385	-2.0263	1.7779
C	4.6691	-0.7951	1.8849
C	3.7552	-2.8525	2.9154
C	5.2414	-0.4591	3.1677
C	5.0224	-1.3209	4.2360
C	4.4103	1.4855	-3.8336
C	5.2074	2.0125	-2.7551
C	4.1352	2.2677	-4.9760
C	5.7838	3.3312	-2.9146
C	5.4643	4.0640	-4.0548
C	2.8088	-2.5408	-1.8324
C	3.6920	-2.1679	-3.0592

C	3.0266	-2.6084	-4.3693	C	4.1037	-3.3988	5.4142
C	2.5640	-4.0612	-1.7965	C	3.2839	-4.6776	5.1272
C	2.7972	-4.1331	-4.3471	C	3.3640	-2.5870	6.5141
C	-0.3788	2.9622	-3.6388	C	5.4961	-3.8314	5.9504
C	-3.2654	3.9605	0.6345	C	1.8405	0.4392	-9.5348
C	-0.4297	1.6683	-4.2810	C	1.7235	0.3347	-8.0226
C	-1.1154	0.5354	-3.7149	C	3.1046	1.1715	-10.0318
C	0.1380	1.5948	-5.5738	C	3.3294	2.5867	-9.4469
C	-1.2457	-0.6644	-4.5150	C	2.0583	3.4589	-9.3669
C	-0.6693	-0.6793	-5.7833	C	2.3083	4.9661	-9.1134
C	-4.2647	3.0081	1.0608	C	3.2529	4.6282	-6.7404
C	-4.3025	1.6457	0.6081	C	3.4159	5.3045	-8.0932
C	-5.2113	3.4792	2.0043	H	6.4972	6.0266	-2.3084
C	-5.3533	0.7966	1.1243	H	7.8408	5.2776	-3.2045
C	-6.2481	1.3311	2.0452	H	8.0073	5.6239	-1.4765
C	-1.0140	4.7105	-2.0894	H	5.2736	4.7084	-0.5068
C	-1.2895	4.7495	-0.5615	H	6.8349	4.3544	0.2648
C	-1.5316	6.1918	-0.0836	H	5.7284	3.0241	-0.1496
C	0.1775	5.6165	-2.4562	H	7.6917	1.9195	-1.4955
C	-0.3412	7.0976	-0.4565	H	8.7165	3.2994	-1.0313
C	-0.0613	7.0597	-1.9685	H	8.5197	2.8750	-2.7463
C	6.7788	3.8800	-1.8684	H	5.8744	5.0538	-4.2080
C	8.0043	2.9262	-1.7791	H	1.8447	-2.0242	-1.9594
C	6.1063	3.9942	-0.4735	H	1.8808	-4.3233	-0.9793
C	7.3047	5.2861	-2.2476	H	3.5186	-4.5688	-1.5987
C	6.0907	0.8220	3.3296	H	0.9409	-4.1655	-3.2321
C	5.2272	2.0786	3.0294	H	1.8703	-5.6557	-3.0956
C	7.3070	0.7712	2.3628	H	3.7711	-4.6445	-4.3197
C	6.6434	0.9780	4.7675	H	2.2995	-4.4487	-5.2730
C	-5.4960	-0.6568	0.6188	H	3.6578	-2.3387	-5.2243
C	-4.2028	-1.4696	0.9077	H	2.0681	-2.0867	-4.5039
C	-5.7811	-0.6349	-0.9087	H	4.6435	-2.7064	-2.9385
C	-6.6673	-1.4057	1.3013	H	5.8391	1.0777	5.5075
C	-2.1063	-1.8466	-4.0168	H	7.2544	1.8870	4.8161
C	-3.5826	-1.3704	-3.9254	H	7.2807	0.1334	5.0561
C	-1.6389	-2.3524	-2.6242	H	6.9838	0.6795	1.3251
C	-2.0517	-3.0541	-4.9847	H	7.9486	-0.0868	2.5986
C	4.6348	3.5460	-5.0602	H	7.9056	1.6858	2.4696
C	4.2790	-2.5270	4.1548	H	4.8550	2.0533	2.0049
C	0.0191	0.4308	-6.2989	H	5.8287	2.9872	3.1640
C	-6.2116	2.6692	2.5150	H	4.3731	2.1283	3.7167
C	-7.2600	3.1490	3.5379	H	3.1871	-3.7677	2.7804
C	-8.6880	2.9723	2.9512	H	5.4485	-1.0622	5.1970
C	-7.0757	4.6395	3.9043	H	-5.1305	4.5167	2.3132
C	-7.1428	2.3141	4.8434	H	-7.0310	0.6885	2.4297

H	-6.5225	-1.4967	2.3854
H	-6.7299	-2.4190	0.8868
H	-7.6306	-0.9140	1.1190
H	-3.9832	-1.4730	1.9834
H	-3.3518	-1.0435	0.3768
H	-4.3385	-2.5102	0.5846
H	-6.7620	-0.1851	-1.1073
H	-5.7872	-1.6588	-1.3053
H	-5.0256	-0.0549	-1.4390
H	-1.6766	6.2176	1.0032
H	-2.4529	6.5778	-0.5442
H	0.5547	6.7580	0.0844
H	-0.5381	8.1260	-0.1266
H	-0.9187	7.4899	-2.5078
H	0.8102	7.6812	-2.2109
H	-1.9219	5.0790	-2.5911
H	-0.3949	4.3522	-0.0621
H	0.3423	5.6240	-3.5386
H	1.0924	5.2175	-1.9974
H	-0.7697	-1.5452	-6.4250
H	0.6358	2.4642	-5.9907
H	-0.5835	-2.6507	-2.6589
H	-2.2324	-3.2295	-2.3341
H	-1.7581	-1.5776	-1.8685
H	-3.9542	-1.0771	-4.9146
H	-3.6719	-0.5121	-3.2580
H	-4.2168	-2.1815	-3.5443
H	-2.4498	-2.8060	-5.9760
H	-2.6662	-3.8652	-4.5768
H	-1.0296	-3.4362	-5.1058
H	3.3171	3.3622	0.0029
H	1.6591	3.4691	0.6504
H	1.9283	3.3294	-1.1059
H	2.5504	1.1551	0.9791
H	3.5469	1.8409	-5.7796
H	2.3686	-2.2862	6.1675
H	3.9162	-1.6791	6.7795
H	3.2458	-3.1896	7.4246
H	6.0350	-4.4144	5.1947
H	5.3865	-4.4490	6.8517
H	6.1153	-2.9658	6.2097
H	2.2734	-4.4380	4.7755
H	3.1873	-5.2694	6.0452
H	3.7715	-5.3052	4.3721
H	-8.8071	3.5664	2.0377
H	-9.4441	3.2977	3.6781
H	-8.8908	1.9262	2.6984
H	-7.1751	5.2829	3.0225
H	-6.0943	4.8255	4.3565
H	-7.8412	4.9407	4.6297
H	-6.1517	2.4408	5.2946
H	-7.2883	1.2455	4.6515
H	-7.8995	2.6328	5.5728
H	3.4937	-0.1804	-4.8348
H	2.7719	-3.4221	0.6536
H	0.1275	3.7296	-4.2277
H	-3.3010	4.9192	1.1570
H	0.7743	1.0722	-1.5847
H	0.9457	-0.2544	-0.2974
H	-1.1546	1.1882	0.6750
H	1.8338	-0.5842	-9.9379
H	0.9344	0.9240	-9.9083

F5:
-6901.464

Cr	4.5712	-0.2329	-0.9598
Cr	-2.1594	2.0559	-1.5757
Cl	6.6487	-1.4465	-1.0954
Cl	-3.9225	2.9428	-2.8138
N	4.1628	-0.7308	-2.8901
N	3.5974	-1.9911	-0.5886
N	-2.1315	3.6867	-0.3572
N	-0.8892	3.2000	-2.6785
O	4.7440	0.0893	0.9730
O	5.3698	1.4609	-1.5987
O	2.8503	0.6183	-1.0575
O	-1.8378	0.5537	-2.7543
O	-3.3503	1.1704	-0.3136
O	-0.6137	1.3146	-0.3263
C	0.5772	0.6307	-0.8156
C	1.9089	0.9487	-0.1011
C	2.0184	2.4219	0.3120
O	0.4101	0.2463	-7.8170
O	2.6516	0.1984	-7.3185
O	4.2435	4.3594	-6.2094
O	1.9426	4.3257	-6.1934
C	2.1350	-4.5730	-3.1241
C	3.4748	-2.5408	0.5767
C	4.0134	0.1182	-3.8505
C	4.0027	-2.0434	1.8265

C	4.6485	-0.7668	1.9631	C	-3.6741	-1.5046	-4.0782
C	3.8435	-2.8924	2.9507	C	-1.6738	-2.4026	-2.7951
C	5.1807	-0.4225	3.2651	C	-2.1060	-3.1483	-5.1385
C	4.9901	-1.3096	4.3188	C	4.4093	3.6051	-5.0057
C	4.3574	1.5234	-3.7894	C	4.3169	-2.5543	4.2069
C	5.0648	2.1219	-2.6829	C	-0.0115	0.3088	-6.4601
C	4.0433	2.2795	-4.9400	C	-5.9451	2.8115	2.5538
C	5.4862	3.5055	-2.8159	C	-6.9204	3.3439	3.6228
C	5.1351	4.2071	-3.9663	C	-8.3717	3.3154	3.0690
C	2.9723	-2.5656	-1.8061	C	-6.5960	4.7990	4.0340
C	3.8629	-2.1674	-3.0216	C	-6.8425	2.4565	4.8959
C	3.2265	-2.6237	-4.3432	C	4.1619	-3.4531	5.4495
C	2.7354	-4.0873	-1.7884	C	3.4247	-4.7732	5.1244
C	2.9948	-4.1473	-4.3281	C	3.3471	-2.7046	6.5409
C	-0.3497	2.8507	-3.8065	C	5.5615	-3.8145	6.0177
C	-2.9690	3.9201	0.6034	C	1.9067	0.3736	-9.6340
C	-0.4839	1.5715	-4.4642	C	1.7475	0.2641	-8.1270
C	-1.2467	0.4784	-3.9299	C	3.1351	1.1921	-10.0864
C	0.1270	1.4700	-5.7355	C	3.2584	2.6139	-9.4844
C	-1.3493	-0.7383	-4.7007	C	1.9357	3.4042	-9.4060
C	-0.7303	-0.7819	-5.9488	C	2.0933	4.9179	-9.1169
C	-4.0274	3.0442	1.0458	C	3.0052	4.6066	-6.7223
C	-4.1862	1.7062	0.5618	C	3.1571	5.3020	-8.0674
C	-4.9022	3.5591	2.0343	H	5.8288	6.2604	-2.1674
C	-5.2762	0.9213	1.0837	H	7.3076	5.6872	-2.9786
C	-6.1006	1.4954	2.0477	H	7.3234	6.0386	-1.2426
C	-0.8260	4.6124	-2.2090	H	4.6435	4.7601	-0.4603
C	-1.0001	4.5938	-0.6682	H	6.1868	4.6468	0.4152
C	-1.0848	6.0225	-0.1058	H	5.3201	3.1649	-0.0547
C	0.4386	5.4020	-2.5997	H	7.4637	2.3251	-1.2844
C	0.1689	6.8292	-0.5029	H	8.2777	3.8175	-0.7484
C	0.3790	6.8339	-2.0270	H	8.2484	3.3899	-2.4742
C	6.3431	4.1622	-1.7114	H	5.4387	5.2376	-4.0983
C	7.6685	3.3655	-1.5427	H	2.0084	-2.0498	-1.9350
C	5.5703	4.1795	-0.3646	H	2.0559	-4.3630	-0.9725
C	6.7165	5.6245	-2.0566	H	3.6920	-4.5944	-1.5985
C	5.9676	0.8938	3.4567	H	1.1232	-4.1562	-3.2378
C	5.0496	2.1119	3.1650	H	2.0244	-5.6653	-3.1020
C	7.1933	0.9126	2.5004	H	3.9662	-4.6616	-4.2811
C	6.5008	1.0542	4.9016	H	2.5150	-4.4611	-5.2645
C	-5.5433	-0.5009	0.5404	H	3.8740	-2.3539	-5.1862
C	-4.3115	-1.4193	0.7759	H	2.2691	-2.1044	-4.4989
C	-5.8586	-0.4134	-0.9791	H	4.8302	-2.6730	-2.8857
C	-6.7538	-1.1749	1.2309	H	5.6873	1.1060	5.6366
C	-2.1839	-1.9309	-4.1853	H	7.0696	1.9895	4.9675

H	7.1735	0.2349	5.1831
H	6.8827	0.8143	1.4595
H	7.8723	0.0832	2.7334
H	7.7475	1.8537	2.6200
H	4.6634	2.0590	2.1475
H	5.6140	3.0466	3.2827
H	4.2045	2.1310	3.8655
H	3.3359	-3.8388	2.7905
H	5.3844	-1.0407	5.2910
H	-4.7304	4.5751	2.3735
H	-6.9204	0.9036	2.4346
H	-6.5953	-1.3015	2.3093
H	-6.8998	-2.1707	0.7967
H	-7.6803	-0.6083	1.0790
H	-4.0749	-1.4803	1.8460
H	-3.4388	-1.0409	0.2431
H	-4.5287	-2.4338	0.4169
H	-6.7966	0.1309	-1.1439
H	-5.9712	-1.4222	-1.3969
H	-5.0644	0.1039	-1.5191
H	-1.1674	6.0016	0.9880
H	-1.9890	6.5148	-0.4929
H	1.0497	6.3877	-0.0151
H	0.0812	7.8565	-0.1269
H	-0.4470	7.3817	-2.5055
H	1.3022	7.3695	-2.2802
H	-1.7122	5.1057	-2.6362
H	-0.1082	4.1068	-0.2521
H	0.5481	5.4553	-3.6877
H	1.3264	4.8806	-2.2163
H	-0.8120	-1.6614	-6.5738
H	0.6755	2.3178	-6.1301
H	-0.6137	-2.6800	-2.8500
H	-2.2426	-3.2844	-2.4738
H	-1.7926	-1.6165	-2.0492
H	-4.0702	-1.2401	-5.0662
H	-3.7846	-0.6437	-3.4180
H	-4.2731	-2.3336	-3.6788
H	-2.5103	-2.9198	-6.1320
H	-2.7029	-3.9668	-4.7197
H	-1.0768	-3.5105	-5.2554
H	3.0156	2.5995	0.7210
H	1.2729	2.7005	1.0692
H	1.9002	3.0648	-0.5687
H	1.9964	0.3346	0.8159
H	3.5347	1.7967	-5.7668
H	2.3435	-2.4623	6.1725
H	3.8340	-1.7668	6.8284
H	3.2450	-3.3245	7.4421
H	6.1520	-4.3557	5.2695
H	5.4642	-4.4493	6.9088
H	6.1234	-2.9187	6.3031
H	2.4125	-4.5866	4.7459
H	3.3354	-5.3822	6.0324
H	3.9680	-5.3615	4.3759
H	-8.4552	3.9456	2.1763
H	-9.0762	3.6880	3.8239
H	-8.6770	2.3002	2.7943
H	-6.6776	5.4836	3.1818
H	-5.5865	4.8861	4.4530
H	-7.3055	5.1321	4.8008
H	-5.8325	2.4798	5.3216
H	-7.0899	1.4121	4.6764
H	-7.5464	2.8171	5.6574
H	3.6131	-0.2117	-4.8107
H	2.9348	-3.4873	0.6648
H	0.2572	3.5710	-4.3544
H	-2.8925	4.8569	1.1588
H	0.6919	0.9829	-1.8379
H	0.3896	-0.4475	-0.8418
H	-1.0366	0.8507	0.4145
H	1.9879	-0.6470	-10.0353
H	0.9829	0.7946	-10.0400

R1:
-6626.631

Cr	1.9850	0.7081	-2.6627
Cr	-1.6762	-1.5194	1.9195
Cl	3.3361	2.3054	-3.8502
Cl	-2.5266	-2.4081	3.8905
O	-1.1335	-0.5528	0.1205
O	3.7808	-7.6526	-1.2276
O	4.3039	-5.6642	-2.0651
O	2.5346	-0.7288	-3.8586
O	1.0365	-0.5487	-1.5558
O	0.3515	1.2424	-3.5701
O	-3.5612	-7.5929	-2.0304
O	-1.9920	-8.0901	-0.4214
O	-0.6422	-3.0598	1.4537
O	-0.2385	-0.6377	2.8318

N	3.5463	0.2881	-1.4235	C	-5.1345	1.0482	1.4467
N	1.6700	2.1924	-1.2871	C	-4.4807	-1.3871	1.1027
N	-3.2941	-2.2659	0.9604	C	-3.9743	0.0809	1.1702
N	-2.8390	0.1275	2.1158	C	-3.3849	-3.4780	0.5029
C	0.2976	-2.8432	-1.7156	C	-2.1969	2.2605	-6.9569
C	-0.7796	0.8583	0.1747	C	-2.5491	1.1670	2.8348
C	-1.3524	-0.9686	-1.2716	C	-1.6758	4.0071	-4.7417
C	-0.0288	-1.3646	-1.9817	C	-2.6972	-5.7453	-0.0084
C	4.7944	2.2079	1.7168	C	-2.3410	-4.4711	0.5045
C	4.6565	1.0081	0.7593	C	-1.9530	0.4471	-5.2592
C	3.9031	-4.3956	-2.5496	C	-1.4730	4.9731	-3.7319
C	3.3708	-6.6321	-1.7482	C	-2.7878	-8.3701	-1.5045
C	4.1133	-3.2930	-1.7505	C	-1.2789	1.7189	-5.8388
C	3.3711	-4.2502	-3.8431	C	-1.3637	1.3299	3.6424
C	3.8293	1.3820	-0.4776	C	-1.2794	2.5044	4.4328
C	4.0093	-0.9092	-1.3003	C	-1.0596	2.7577	-4.7235
C	3.7142	-2.0130	-2.1907	C	-2.5192	-9.7858	-1.9661
C	3.4167	2.7642	2.1269	C	-1.7703	-6.7642	0.0199
C	2.9564	-1.8727	-6.5735	C	-0.6143	4.6832	-2.6872
C	2.9134	-3.0229	-4.3104	C	-1.0266	-4.2402	1.0365
C	3.0377	-1.8648	-3.4542	C	-0.2769	0.3873	3.6524
C	2.9616	-0.1113	5.7728	C	-0.1836	2.7374	5.2415
C	1.9010	-6.4051	-2.0775	C	-0.1796	2.4402	-3.6266
C	2.5868	3.1523	0.8897	C	0.0544	3.4379	-2.6144
C	2.1641	-4.2399	-6.4240	C	-0.4910	-6.5607	0.5760
C	2.2110	-2.8916	-5.6727	C	-0.0906	-5.3362	1.0935
C	2.4396	1.9543	-0.0549	C	0.0746	1.3319	-6.4966
C	1.1847	-7.7505	-2.2992	H	1.1516	-3.1566	-2.3191
C	2.1444	-4.0816	1.0899	H	0.5476	-2.9601	-0.6620
C	2.0850	-6.4820	1.7861	H	-0.5605	-3.4907	-1.9518
C	1.8750	-0.5172	4.7527	H	-0.2428	1.0236	1.1060
C	2.6087	-0.8734	3.4340	H	-1.6971	1.4633	0.1440
C	1.1525	-1.7750	5.3075	H	-0.1424	1.0591	-0.6758
C	1.2763	-5.1648	1.7819	H	-1.8264	-0.1211	-1.7851
C	0.7448	-2.4185	-5.4699	H	-2.0503	-1.8079	-1.2267
C	-0.1313	-7.5996	-3.0791	H	5.6489	0.6562	0.4486
C	0.9182	3.2275	-1.4745	H	5.3690	3.0029	1.2178
C	0.8427	1.7680	5.3089	H	5.3602	1.9044	2.6074
C	0.8239	0.5941	4.5590	H	4.5604	-3.4142	-0.7690
C	-1.0645	-9.9638	-2.4693	H	4.6751	-1.1537	-0.4693
C	1.0490	-4.7480	3.2590	H	4.3403	2.1618	-1.0586
C	-0.6693	-8.9608	-3.5788	H	3.9647	-2.2396	-6.8076
C	-6.2177	0.8990	0.3606	H	4.1609	0.1781	1.2794
C	-6.7161	-0.5545	0.2685	H	3.2890	-5.1389	-4.4555
C	-5.5476	-1.5247	0.0027	H	3.6724	-0.9401	5.8755

H	3.1738	-4.6296	-6.6070
H	3.5400	3.6356	2.7837
H	3.0715	3.9772	0.3470
H	2.5300	0.0954	6.7602
H	3.5132	0.7762	5.4349
H	3.0335	-0.9046	-6.0741
H	2.8639	2.0065	2.6986
H	3.1277	-4.0576	1.5796
H	2.4027	-1.7485	-7.5148
H	1.0145	-8.2365	-1.3319
H	1.8525	-8.4185	-2.8607
H	3.0354	-6.3035	2.3029
H	2.3183	-6.8388	0.7768
H	1.4362	-5.8456	-1.2540
H	2.2974	-4.3055	0.0300
H	1.7899	-5.7734	-2.9589
H	3.3052	-1.7007	3.6271
H	1.5942	-4.9926	-5.8619
H	1.8648	-2.6073	5.3794
H	1.6706	-4.0903	-7.3920
H	1.9211	1.1368	0.4672
H	1.5974	3.5011	1.2131
H	3.1915	-0.0123	3.0891
H	0.7542	-1.5659	6.3089
H	1.6837	-3.0959	1.1737
H	1.5483	-7.2747	2.3239
H	1.6684	1.9483	5.9872
H	-0.3774	-9.8701	-1.6211
H	2.0242	-4.6265	3.7497
H	0.8885	4.0215	-0.7235
H	0.7717	0.9269	-5.7613
H	0.1181	-9.4156	-4.1972
H	0.7203	-1.4170	-5.0400
H	-0.9698	-10.9900	-2.8492
H	0.1789	-7.4094	0.5914
H	1.9102	-1.1719	2.6520
H	0.2101	-3.1083	-4.8035
H	0.2325	-2.4007	-6.4421
H	0.0548	-6.9665	-3.9596
H	0.3246	-2.0756	4.6633
H	-0.8723	-7.0641	-2.4748
H	0.5340	2.2132	-6.9619
H	-5.7904	1.1940	-0.6091
H	-7.0527	1.5784	0.5700
H	-7.4698	-0.6498	-0.5236
H	-5.9306	-2.5504	-0.0424
H	-5.5535	0.8286	2.4390
H	-7.2009	-0.8316	1.2166
H	-4.9231	-1.6242	2.0817
H	-4.7716	2.0826	1.4581
H	-5.0835	-1.3003	-0.9687
H	-4.3370	-3.8228	0.0939
H	-3.1982	2.5038	-6.5758
H	-3.5503	0.3105	0.1803
H	-2.9331	0.7009	-4.8312
H	-3.2331	2.0193	2.8475
H	-2.3338	4.2629	-5.5643
H	-3.6860	-5.9016	-0.4144
H	-2.3017	1.4888	-7.7295
H	-1.9761	5.9336	-3.7882
H	-1.7701	3.1594	-7.4211
H	-2.1010	-0.2867	-6.0640
H	-2.0999	3.2180	4.3914
H	-3.2270	-10.0049	-2.7715
H	-1.3238	0.0040	-4.4850
H	-0.4296	5.4163	-1.9042
H	-2.7030	-10.4777	-1.1339
H	-1.5363	-8.7943	-4.2346
H	0.4822	-5.5224	3.7913
H	0.5033	-3.8062	3.3177
H	-0.1168	3.6402	5.8400
H	-0.1080	0.5769	-7.2748
H	-0.2289	-1.2362	-3.0586

R2:
-6626.609

Cr	0.7141	-1.5893	-2.5372
Cr	-2.4954	-1.4903	2.6330
Cl	2.2300	-0.0159	-3.7176
Cl	-4.3600	-2.3707	3.7249
O	-0.3276	-2.8816	-1.5453
O	0.4986	-2.7305	-4.1327
O	-6.2149	4.0056	0.3354
O	-5.6749	3.7027	-1.8932
O	-2.8723	0.3651	2.8739
O	-1.6950	4.8418	-1.1393
O	-1.0056	-1.4956	3.8359
O	-0.6700	5.1778	0.9094
O	1.7050	2.3739	2.1648
O	-0.8112	-0.3801	-2.8273

N	2.4137	-2.6143	-2.0648	C	-2.4100	7.7429	0.7335
N	1.0852	-0.6223	-0.7945	C	-2.3390	-5.0191	0.1188
N	-3.2864	-1.3754	0.7738	C	-3.5418	-0.0185	-3.9741
N	-1.8720	-3.2924	1.9673	C	-1.6713	0.8948	-5.4273
C	4.7721	-2.0647	0.9904	C	-1.9799	2.9662	4.1641
C	3.7017	-1.5185	1.9507	C	-4.0844	4.1808	4.7721
C	4.1356	-2.8400	-0.1803	C	-1.5580	7.0657	-0.3625
C	2.6800	-0.6382	1.2052	C	-2.1203	2.9994	-2.5490
C	3.1217	-1.9609	-0.9336	C	-1.2569	5.6039	-0.0992
C	2.8743	-3.6569	-2.6856	C	-1.9422	1.7164	-3.0471
C	2.9696	-5.4619	-4.3194	C	-0.8618	-3.9886	2.3987
C	2.0408	-1.4006	0.0332	C	-1.4418	3.4557	-1.4064
C	2.3100	-4.2993	-3.8520	C	0.9840	0.4317	5.0332
C	2.5263	-6.1310	-5.4442	C	-0.0673	-2.3877	4.1752
C	1.4075	-5.6288	-6.1413	C	-0.6119	-0.6401	6.7002
C	1.1587	-3.7984	-4.5524	C	-0.8079	-4.8310	-7.7781
C	0.6032	0.5333	-0.4373	C	0.0351	-3.6282	3.4708
C	3.0188	4.1885	0.9452	C	-0.1671	-2.5173	-7.0636
C	0.7152	-4.4877	-5.7422	C	-1.0077	0.8449	-2.3710
C	1.8582	-0.6611	7.1074	C	-1.7616	-3.9104	-5.6593
C	1.9442	-4.2697	4.8256	C	0.7740	-0.7606	6.0071
C	1.8355	-3.0480	5.5194	C	1.4400	3.6279	2.9475
C	-0.3415	1.3278	-1.1935	C	0.8589	-2.0919	5.2310
C	2.7281	3.4668	2.2333	C	-0.4870	-3.9480	-6.5478
C	-6.7714	5.7664	-1.1561	C	1.0503	-4.5533	3.8094
C	-6.1472	6.7952	-0.1851	C	-0.5799	2.6381	-0.7059
C	-6.1607	4.3908	-0.9939	H	5.4761	-2.7143	1.5273
C	-4.6353	7.0474	-0.4214	H	4.1731	-0.9356	2.7528
C	-5.4075	2.9809	0.9121	H	5.3573	-1.2252	0.5855
C	-5.1048	1.7835	0.3030	H	4.9262	-3.1801	-0.8609
C	-4.9265	3.2911	2.1943	H	3.1832	-2.3570	2.4368
C	-3.8857	1.7532	5.3443	H	3.6258	-3.7379	0.2002
C	-3.6157	-4.1731	-1.9170	H	3.7955	-4.1215	-2.3251
C	-3.9601	-0.3618	0.3047	H	3.8407	-5.8200	-3.7741
C	-4.0260	-2.8992	-1.1490	H	3.1796	0.2634	0.8237
C	-3.6533	2.3223	-4.8566	H	1.9096	-0.2925	1.9017
C	-4.2710	0.8674	0.9905	H	3.6367	-1.0969	-1.3786
C	-3.8405	7.1870	0.8954	H	1.4736	-2.2597	0.4184
C	-4.0904	2.4327	2.9008	H	3.0328	-7.0233	-5.7983
C	-3.7329	1.1909	2.2738	H	3.6009	5.0981	1.1424
C	-3.5224	2.8247	4.2799	H	0.9298	0.9889	0.4990
C	-2.9746	-2.5684	-0.0755	H	2.0892	4.4742	0.4456
C	-3.3784	-5.3620	-0.9695	H	3.5969	3.5563	0.2619
C	-2.7829	-3.7635	0.8845	H	1.7619	-1.4606	7.8523
C	-2.6929	1.2394	-4.3085	H	2.8719	-0.6927	6.6895

H	1.0825	-6.1585	-7.0289
H	1.7448	0.2950	7.6313
H	2.7229	-4.9764	5.0927
H	-0.4583	-3.6514	-2.1357
H	2.5474	-2.8507	6.3112
H	-0.0760	2.9690	0.1907
H	0.6685	4.2537	2.5139
H	-7.8503	5.6918	-0.9650
H	-6.7050	7.7378	-0.2596
H	-6.6326	6.0588	-2.2012
H	-6.2995	6.4191	0.8327
H	-5.4659	1.5525	-0.6892
H	-5.0109	-3.0363	-0.6746
H	-4.2079	6.2181	-1.0002
H	-4.5012	7.9492	-1.0369
H	-3.4963	0.7735	5.0678
H	-4.3877	-4.4253	-2.6549
H	-4.9744	1.6762	5.4572
H	-4.1772	1.9202	-5.7324
H	-5.2229	4.2430	2.6129
H	-4.3336	-0.4178	-0.7170
H	-2.6957	-3.9570	-2.4732
H	-4.4058	2.6229	-4.1182
H	-4.1125	-2.0785	-1.8681
H	-3.1082	3.2173	-5.1817
H	-3.7404	-3.9596	1.3896
H	-3.4611	2.0402	6.3151
H	-4.3886	7.8478	1.5837
H	-3.8000	6.2030	1.3837
H	-4.0404	-0.3862	-4.8806
H	-2.0289	7.1567	-1.3424
H	-2.7951	3.6935	-3.0299
H	-2.2063	0.5392	-6.3186
H	-1.5277	2.0212	3.8607
H	-3.0415	-6.2384	-1.5378
H	-5.1771	4.1608	4.8671
H	-2.2343	-5.8701	0.8057
H	-2.4641	8.8144	0.4935
H	-4.3192	0.2298	-3.2382
H	-4.3278	-5.6417	-0.4874
H	-1.0945	1.7852	-5.7051
H	0.2098	0.4565	4.2662
H	-1.5580	3.2630	5.1336
H	-2.0006	-2.3936	-0.5745
H	-1.6655	-4.4005	-8.3085
H	-3.6675	4.3974	5.7621
H	-1.4205	-0.7057	5.9714
H	-1.0235	-2.1224	-7.6269
H	-2.9015	-0.8076	-3.5751
H	-1.8799	7.6576	1.6909
H	-3.8053	5.0072	4.1073
H	-0.5891	7.5817	-0.4148
H	-1.7223	3.7319	3.4226
H	-1.3629	-4.8201	-0.3407
H	-0.9734	0.1238	-5.0986
H	-0.6503	-4.9466	1.9237
H	-2.6156	-3.5474	-6.2464
H	1.3942	3.4726	4.0212
H	0.9502	1.3751	5.5943
H	-0.6843	0.3237	7.2204
H	-1.0730	-5.8562	-7.4897
H	0.0311	-4.8755	-8.4836
H	0.0506	-1.8449	-6.2328
H	1.9591	0.3653	4.5359
H	0.7030	-2.5375	-7.7319
H	-1.6134	-3.2452	-4.8076
H	-0.7402	-1.4387	7.4420
H	3.5964	3.1758	2.8231
H	1.1129	-5.4885	3.2586
H	-2.0045	-4.9163	-5.2913

R3:
-6819.721

Cr	-2.2932	-1.8357	2.0320
Cr	2.4473	-0.7841	-3.1186
Cl	-3.3590	-2.5341	3.9610
Cl	4.0970	0.8412	-3.8164
O	-1.5799	-1.1709	0.1897
O	-1.3677	-0.3672	2.8583
O	-0.8136	-3.0323	2.1544
O	0.1463	-8.1069	0.1512
O	-1.9680	-9.0054	0.2572
O	0.9788	0.3390	-3.7158
O	1.1282	-2.0174	-2.4690
O	2.6568	-1.7781	-4.7711
O	5.0588	-6.6693	-5.7216
O	4.6475	-8.8568	-5.5026
O	-1.2430	-3.7358	-2.1262
N	-3.8263	-0.5908	1.5417
N	-3.3313	-3.1539	0.9018

N	2.4374	0.1830	-1.3264	C	1.2576	0.8841	3.4404
N	3.9785	-1.8188	-2.2668	C	0.3423	0.9640	4.6912
C	-1.9432	0.7788	-1.3264	C	2.5916	-5.4004	3.5136
C	-0.2059	-0.7532	-0.0837	C	2.0594	-3.1112	2.6942
C	-1.2911	0.2394	-0.0841	C	2.1346	-8.5839	-4.1815
C	0.3427	1.4119	-6.3698	C	3.2317	-0.5280	-0.3071
C	0.4706	-5.0235	2.1427	C	1.9911	-3.0356	-7.2168
C	0.6606	-6.2934	1.6087	C	1.8443	-3.9298	-8.4662
C	1.0282	2.0478	-2.0212	C	3.7086	0.3190	0.8828
C	0.5964	1.5090	-3.2840	C	2.9179	-7.3682	-4.6765
C	-2.8399	3.1759	4.4504	C	1.0408	1.8912	5.7094
C	-1.8646	0.7333	3.3850	C	3.2981	-2.8858	-4.9993
C	-0.6749	-4.2680	1.7154	C	3.0236	-3.6014	-6.2282
C	0.5414	3.3057	-1.5908	C	2.4183	-1.6242	-7.7009
C	-0.2284	-6.8434	0.6717	C	4.5119	-0.5390	1.8764
C	-0.1161	-10.3433	-0.5829	C	4.2576	-3.4380	-4.0737
C	-0.3473	2.2617	-4.0772	C	4.5873	-2.8249	-2.8056
C	-3.6214	2.4562	3.5665	C	4.4560	-1.1736	-1.0194
C	-3.1655	1.2292	3.0250	C	3.6604	-4.8153	-6.4458
C	-0.8476	1.6684	-5.4060	C	4.8747	-4.6794	-4.3554
C	-0.7872	-9.1055	-0.0082	C	4.2501	-7.7247	-5.3208
C	-0.3507	4.0282	-2.3624	C	4.5568	-5.3609	-5.5084
C	-1.5930	0.3315	-5.1422	C	5.2148	-2.0742	-0.0301
C	-1.6044	-4.8698	0.8076	C	5.6889	-1.2497	1.1846
C	-1.3489	-6.1504	0.2675	C	1.2309	-3.4238	-2.3448
C	-0.7844	3.4924	-3.5972	C	-0.0517	-4.1100	-2.8515
C	-4.0268	0.5765	2.0655	C	-1.8564	-2.5602	-2.6831
C	-1.8350	2.6149	-6.1230	C	1.5252	-3.8120	-0.8898
C	-2.8616	-4.2671	0.4359	H	-1.7002	0.1689	-2.1976
C	-4.6495	-1.1447	0.4432	H	-3.0334	0.7974	-1.1887
C	-4.7105	-2.6850	0.6423	H	-1.6036	1.8014	-1.5108
C	-6.0534	-0.5463	0.2789	H	0.1990	-1.1665	-1.0123
C	-5.4470	-3.3563	-0.5242	H	0.4239	-0.8146	0.8019
C	-6.8585	-2.7588	-0.6796	H	2.0358	-3.8231	-2.9811
C	-6.7998	-1.2342	-0.8816	H	-0.0340	0.9748	-7.3056
C	0.0098	-9.3064	-2.9393	H	-3.1930	4.1131	4.8677
C	0.6502	-4.1751	4.5082	H	-0.1931	-3.5029	4.3382
C	0.7828	-10.0091	-1.7915	H	0.2715	-5.1218	4.9141
C	-1.0522	1.4884	4.3008	H	-0.9470	-8.9177	-2.5614
C	-1.5662	2.6817	4.8061	H	0.4862	-10.8117	0.2083
C	1.8790	1.3296	-1.1045	H	0.8776	3.6905	-0.6298
C	0.8071	-8.1403	-3.5459	H	-0.9253	-0.3916	-4.6705
C	0.6004	-2.9505	-6.5285	H	-0.9144	-11.0392	-0.8596
C	1.4283	-4.4373	3.1916	H	-4.6024	2.8231	3.2719
C	0.2308	-0.4435	5.3379	H	-1.9508	-0.0807	-6.0957

H	-1.3619	3.5769	-6.3588
H	-0.7177	4.9941	-2.0307
H	-2.1541	2.1487	-7.0634
H	-2.0455	-6.5830	-0.4377
H	-1.4881	4.0731	-4.1827
H	-4.9052	1.1538	1.7679
H	-2.4619	0.5013	-4.4910
H	-4.0760	-0.9724	-0.4795
H	-2.7279	2.8044	-5.5119
H	-3.4569	-4.8535	-0.2640
H	-4.8659	-3.2089	-1.4464
H	-5.9867	0.5305	0.0802
H	-5.2594	-2.8672	1.5785
H	-7.4409	-2.9788	0.2280
H	-6.6115	-0.6778	1.2173
H	-5.5224	-4.4362	-0.3503
H	-7.3740	-3.2358	-1.5224
H	-7.8133	-0.8217	-0.9660
H	-6.2803	-1.0130	-1.8259
H	0.8508	2.3558	-6.6051
H	1.0129	-7.4095	-2.7490
H	-0.2203	-1.1591	4.6493
H	0.1985	-7.6203	-4.3000
H	-0.1283	-2.5226	-7.2309
H	0.2587	-3.9546	-6.2405
H	0.8395	0.2015	2.6986
H	1.5120	-6.8942	1.8996
H	1.2543	-10.9310	-2.1536
H	0.6490	-2.3211	-5.6376
H	-0.2373	-10.0337	-3.7259
H	1.0649	0.7284	-5.9209
H	2.0191	1.8195	-0.1387
H	1.3244	-3.7211	5.2473
H	1.5892	-9.3531	-1.4435
H	-0.9716	3.2654	5.4987
H	2.2248	-6.3552	3.9111
H	1.2892	-2.3595	2.5127
H	-0.3835	-0.3933	6.2459
H	1.3763	1.8784	2.9883
H	2.8533	0.7611	1.4030
H	2.6041	-1.3510	0.0613
H	1.1182	-3.4690	-9.1465
H	1.2344	-0.7968	5.6141
H	1.4808	-4.9323	-8.2036
H	2.2493	0.5172	3.7374
H	2.3150	-6.7966	-5.3954
H	2.6245	-3.2789	1.7689
H	3.0982	-6.6712	-3.8478
H	3.2028	-5.6002	2.6234
H	3.2312	-4.9359	4.2734
H	1.9449	-9.2754	-5.0129
H	2.7386	-9.1368	-3.4510
H	1.6493	-1.2271	-8.3779
H	2.7475	-2.7376	3.4649
H	3.8426	-1.2869	2.3161
H	2.5383	-0.9409	-6.8588
H	1.2027	2.8945	5.2940
H	0.4554	1.9818	6.6330
H	4.3291	1.1413	0.4981
H	4.8775	0.0922	2.6970
H	2.8000	-4.0299	-8.9971
H	2.0183	1.4636	5.9633
H	3.4580	-5.3984	-7.3360
H	4.5474	-2.8828	0.3028
H	3.3676	-1.6851	-8.2495
H	5.1037	-0.3481	-1.3462
H	5.4238	-3.2941	-2.2814
H	5.5643	-5.1185	-3.6401
H	6.2077	-1.9044	1.8967
H	6.4153	-0.4976	0.8416
H	6.0842	-2.5375	-0.5109
H	0.0492	-5.1966	-2.7208
H	-0.1796	-3.8875	-3.9213
H	-1.1180	-1.7633	-2.8005
H	-2.6359	-2.2538	-1.9779
H	-2.3019	-2.7837	-3.6685
H	0.7372	-3.4214	-0.2423
H	2.4855	-3.3874	-0.5793
H	1.5660	-4.9010	-0.7592
H	-1.3890	0.8485	0.8101

R4:
-6819.701

Cr	-2.3524	-1.5199	1.7427
Cr	2.4801	-0.7255	-2.7352
Cl	-3.5460	-1.0855	3.7974
Cl	3.8893	0.9895	-3.4269
O	-1.7836	-2.0028	-0.0072
O	-1.1509	-0.0095	1.9978
O	-1.1955	-2.8677	2.5635

O	-0.3304	-8.0191	0.6968	C	0.1067	-9.0193	-3.0200
O	-2.1731	-8.5412	-0.5803	C	0.7516	-3.8293	4.6226
O	0.9229	0.3256	-2.9786	C	0.8158	-9.4434	-1.7129
O	1.3193	-2.3654	-1.8795	C	-0.8362	2.0643	3.1340
O	2.4024	-1.5718	-4.4732	C	-1.1729	3.4172	3.2026
O	4.7525	-6.2036	-6.3344	C	1.9265	0.7932	-0.2753
O	4.5572	-8.4049	-5.9788	C	0.8406	-7.8789	-3.7385
O	-0.2736	-5.2174	-1.9672	C	0.1279	-2.6859	-6.0198
N	-3.6934	-0.3202	0.7996	C	1.2809	-4.1295	3.1957
N	-3.7342	-2.9638	1.3378	C	-0.3814	0.2750	4.8673
N	2.6216	-0.1594	-0.8212	C	1.4309	0.9149	3.2462
N	4.1631	-1.7936	-2.2952	C	0.2312	1.4494	4.0600
C	-1.5188	-1.6473	-2.3394	C	2.5274	-5.0316	3.3250
C	0.3780	-2.3043	-0.7529	C	1.7439	-2.8056	2.5390
C	-0.9060	-1.4771	-0.9469	C	2.2164	-8.2551	-4.3137
C	0.6293	2.3625	-5.2277	C	3.5737	-1.0052	-0.0685
C	0.1712	-4.7967	2.3647	C	1.3829	-2.5724	-6.9276
C	0.3203	-6.0769	1.8463	C	1.0737	-3.3171	-8.2444
C	0.9507	1.6132	-0.9456	C	4.0582	-0.4459	1.2737
C	0.5311	1.3904	-2.3000	C	2.8808	-7.0090	-4.9102
C	-2.2233	3.9801	2.4496	C	0.7843	2.4784	5.0699
C	-1.5646	1.2227	2.2199	C	3.0796	-2.5672	-4.9852
C	-1.0702	-4.0944	2.1293	C	2.6054	-3.1676	-6.2089
C	0.3785	2.6697	-0.1953	C	1.6293	-1.0810	-7.2778
C	-0.7136	-6.7270	1.1493	C	5.0633	-1.4135	1.9260
C	-0.1856	-9.9436	-0.6369	C	4.2310	-3.1340	-4.3307
C	-0.3739	2.3156	-2.9174	C	4.7438	-2.6564	-3.0628
C	-2.9987	3.1499	1.6570	C	4.7599	-1.3225	-1.0206
C	-2.7169	1.7707	1.5546	C	3.2198	-4.3342	-6.6538
C	-0.6889	2.2079	-4.4224	C	4.8207	-4.3151	-4.8389
C	-1.0460	-8.7798	-0.1725	C	4.1143	-7.3003	-5.7534
C	-0.5472	3.5191	-0.7720	C	4.2885	-4.9235	-5.9533
C	-1.3376	0.8491	-4.7928	C	5.7575	-2.2828	-0.3544
C	-2.1281	-4.7926	1.4468	C	6.2459	-1.7042	0.9881
C	-1.9426	-6.1158	0.9828	C	1.6420	-3.7394	-2.2920
C	-0.8958	3.3415	-2.1264	C	0.4341	-4.4254	-2.9318
C	-3.6579	0.9698	0.7988	C	-1.5323	-5.6651	-2.4932
C	-1.6552	3.3206	-4.8856	C	2.2891	-4.5425	-1.1598
C	-3.4269	-4.2046	1.1705	H	-1.8972	-2.6733	-2.4283
C	-4.6789	-1.1229	0.0495	H	-2.3635	-0.9575	-2.4526
C	-5.0194	-2.3678	0.9373	H	-0.7953	-1.4454	-3.1314
C	-5.9562	-0.3831	-0.3739	H	0.0383	-3.3212	-0.5630
C	-5.9958	-3.3010	0.2112	H	0.9212	-1.9404	0.1197
C	-7.2773	-2.5432	-0.1819	H	2.3699	-3.6014	-3.0775
C	-6.9407	-1.3368	-1.0778	H	0.4145	2.2571	-6.3008

H	-2.4420	5.0403	2.5281	H	2.2907	-5.9759	3.8318
H	-0.1065	-3.1551	4.5776	H	0.9023	-2.1251	2.4002
H	0.4494	-4.7609	5.1191	H	-1.2450	0.6171	5.4476
H	-0.9092	-8.6771	-2.7843	H	1.9628	1.7421	2.7542
H	0.3608	-10.3617	0.2156	H	3.2078	-0.3015	1.9441
H	0.6545	2.7886	0.8476	H	3.0605	-1.9572	0.1159
H	-0.6320	0.0346	-4.6363	H	0.2192	-2.8306	-8.7291
H	-0.8428	-10.7100	-1.0597	H	0.3784	-0.1231	5.5558
H	-3.8512	3.5476	1.1097	H	0.8089	-4.3678	-8.0664
H	-1.6287	0.8698	-5.8530	H	2.1352	0.4096	3.9221
H	-1.2312	4.3174	-4.7096	H	2.1627	-6.4689	-5.5433
H	-1.0075	4.3042	-0.1846	H	2.2001	-3.0253	1.5677
H	-1.8309	3.2067	-5.9623	H	3.1349	-6.2997	-4.1123
H	-2.7519	-6.6248	0.4808	H	2.9532	-5.2630	2.3394
H	-1.5993	4.0392	-2.5648	H	3.2877	-4.5048	3.9153
H	-4.4091	1.5374	0.2433	H	2.1093	-9.0275	-5.0860
H	-2.2325	0.6603	-4.1869	H	2.8593	-8.6806	-3.5317
H	-4.1481	-1.5066	-0.8325	H	0.7445	-0.6830	-7.7930
H	-2.6221	3.2540	-4.3688	H	2.4962	-2.3237	3.1781
H	-4.1655	-4.8978	0.7584	H	4.5452	-2.3528	2.1631
H	-5.5101	-3.6938	-0.6948	H	1.8090	-0.4936	-6.3762
H	-5.7005	0.4472	-1.0444	H	1.2799	3.3170	4.5619
H	-5.4750	-1.9865	1.8617	H	-0.0149	2.8770	5.7073
H	-7.7813	-2.1881	0.7293	H	4.5276	0.5346	1.1071
H	-6.4288	0.0466	0.5215	H	5.4211	-0.9926	2.8739
H	-6.2410	-4.1583	0.8514	H	1.9280	-3.2804	-8.9322
H	-7.9712	-3.2197	-0.6978	H	1.5227	1.9800	5.7104
H	-7.8551	-0.7933	-1.3496	H	2.8552	-4.8473	-7.5343
H	-6.4866	-1.7014	-2.0116	H	5.2641	-3.2518	-0.1848
H	1.0649	3.3543	-5.0526	H	2.4937	-0.9884	-7.9481
H	0.9482	-7.0569	-3.0192	H	5.2561	-0.3714	-1.2565
H	-0.7249	-0.5230	4.2084	H	5.6767	-3.1244	-2.7415
H	0.2153	-7.4975	-4.5599	H	5.6440	-4.7833	-4.3071
H	-0.7457	-2.2975	-6.5593	H	6.9463	-2.4054	1.4592
H	-0.0609	-3.7360	-5.7606	H	6.7959	-0.7709	0.7957
H	1.0818	0.2008	2.4986	H	6.6180	-2.4575	-1.0123
H	1.2477	-6.6219	1.9692	H	0.7838	-5.0757	-3.7512
H	1.5554	-10.2289	-1.9126	H	-0.2169	-3.6615	-3.3676
H	0.2549	-2.1097	-5.1018	H	-2.1882	-4.8087	-2.7076
H	0.0037	-9.8878	-3.6876	H	-1.9827	-6.3038	-1.7321
H	1.3577	1.6042	-4.9327	H	-1.3863	-6.2450	-3.4185
H	2.0731	1.0211	0.7757	H	1.6024	-4.6985	-0.3240
H	1.5487	-3.3598	5.2163	H	3.1839	-4.0192	-0.8060
H	1.3591	-8.5851	-1.2939	H	2.5802	-5.5310	-1.5379
H	-0.6242	4.0676	3.8740	H	-0.6979	-0.4134	-0.7680

R5:
-6819.747

Cr	-2.3524	-1.5199	1.7427
Cr	2.4801	-0.7255	-2.7352
Cl	-3.5460	-1.0855	3.7974
Cl	3.8893	0.9895	-3.4269
O	-1.7836	-2.0028	-0.0072
O	-1.1509	-0.0095	1.9978
O	-1.1955	-2.8677	2.5635
O	-0.3304	-8.0191	0.6968
O	-2.1731	-8.5412	-0.5803
O	0.9229	0.3256	-2.9786
O	1.3193	-2.3654	-1.8795
O	2.4024	-1.5718	-4.4732
O	4.7525	-6.2036	-6.3344
O	4.5572	-8.4049	-5.9788
O	-0.2736	-5.2174	-1.9672
N	-3.6934	-0.3202	0.7996
N	-3.7342	-2.9638	1.3378
N	2.6216	-0.1594	-0.8212
N	4.1631	-1.7936	-2.2952
C	-1.5188	-1.6473	-2.3394
C	0.3780	-2.3043	-0.7529
C	-0.9060	-1.4771	-0.9469
C	0.6293	2.3625	-5.2277
C	0.1712	-4.7967	2.3647
C	0.3203	-6.0769	1.8463
C	0.9507	1.6132	-0.9456
C	0.5311	1.3904	-2.3000
C	-2.2233	3.9801	2.4496
C	-1.5646	1.2227	2.2199
C	-1.0702	-4.0944	2.1293
C	0.3785	2.6697	-0.1953
C	-0.7136	-6.7270	1.1493
C	-0.1856	-9.9436	-0.6369
C	-0.3739	2.3156	-2.9174
C	-2.9987	3.1499	1.6570
C	-2.7169	1.7707	1.5546
C	-0.6889	2.2079	-4.4224
C	-1.0460	-8.7798	-0.1725
C	-0.5472	3.5191	-0.7720
C	-1.3376	0.8491	-4.7928
C	-2.1281	-4.7926	1.4468
C	-1.9426	-6.1158	0.9828
C	-0.8958	3.3415	-2.1264
C	-3.6579	0.9698	0.7988
C	-1.6552	3.3206	-4.8856
C	-3.4269	-4.2046	1.1705
C	-4.6789	-1.1229	0.0495
C	-5.0194	-2.3678	0.9373
C	-5.9562	-0.3831	-0.3739
C	-5.9958	-3.3010	0.2112
C	-7.2773	-2.5432	-0.1819
C	-6.9407	-1.3368	-1.0778
C	0.1067	-9.0193	-3.0200
C	0.7516	-3.8293	4.6226
C	0.8158	-9.4434	-1.7129
C	-0.8362	2.0643	3.1340
C	-1.1729	3.4172	3.2026
C	1.9265	0.7932	-0.2753
C	0.8406	-7.8789	-3.7385
C	0.1279	-2.6859	-6.0198
C	1.2809	-4.1295	3.1957
C	-0.3814	0.2750	4.8673
C	1.4309	0.9149	3.2462
C	0.2312	1.4494	4.0600
C	2.5274	-5.0316	3.3250
C	1.7439	-2.8056	2.5390
C	2.2164	-8.2551	-4.3137
C	3.5737	-1.0052	-0.0685
C	1.3829	-2.5724	-6.9276
C	1.0737	-3.3171	-8.2444
C	4.0582	-0.4459	1.2737
C	2.8808	-7.0090	-4.9102
C	0.7843	2.4784	5.0699
C	3.0796	-2.5672	-4.9852
C	2.6054	-3.1676	-6.2089
C	1.6293	-1.0810	-7.2778
C	5.0633	-1.4135	1.9260
C	4.2310	-3.1340	-4.3307
C	4.7438	-2.6564	-3.0628
C	4.7599	-1.3225	-1.0206
C	3.2198	-4.3342	-6.6538
C	4.8207	-4.3151	-4.8389
C	4.1143	-7.3003	-5.7534
C	4.2885	-4.9235	-5.9533
C	5.7575	-2.2828	-0.3544
C	6.2459	-1.7042	0.9881
C	1.6420	-3.7394	-2.2920

C	0.4341	-4.4254	-2.9318	H	1.0818	0.2008	2.4986
C	-1.5323	-5.6651	-2.4932	H	1.2477	-6.6219	1.9692
C	2.2891	-4.5425	-1.1598	H	1.5554	-10.2289	-1.9126
H	-1.8972	-2.6733	-2.4283	H	0.2549	-2.1097	-5.1018
H	-2.3635	-0.9575	-2.4526	H	0.0037	-9.8878	-3.6876
H	-0.7953	-1.4454	-3.1314	H	1.3577	1.6042	-4.9327
H	0.0383	-3.3212	-0.5630	H	2.0731	1.0211	0.7757
H	0.9212	-1.9404	0.1197	H	1.5487	-3.3598	5.2163
H	2.3699	-3.6014	-3.0775	H	1.3591	-8.5851	-1.2939
H	0.4145	2.2571	-6.3008	H	-0.6242	4.0676	3.8740
H	-2.4420	5.0403	2.5281	H	2.2907	-5.9759	3.8318
H	-0.1065	-3.1551	4.5776	H	0.9023	-2.1251	2.4002
H	0.4494	-4.7609	5.1191	H	-1.2450	0.6171	5.4476
H	-0.9092	-8.6771	-2.7843	H	1.9628	1.7421	2.7542
H	0.3608	-10.3617	0.2156	H	3.2078	-0.3015	1.9441
H	0.6545	2.7886	0.8476	H	3.0605	-1.9572	0.1159
H	-0.6320	0.0346	-4.6363	H	0.2192	-2.8306	-8.7291
H	-0.8428	-10.7100	-1.0597	H	0.3784	-0.1231	5.5558
H	-3.8512	3.5476	1.1097	H	0.8089	-4.3678	-8.0664
H	-1.6287	0.8698	-5.8530	H	2.1352	0.4096	3.9221
H	-1.2312	4.3174	-4.7096	H	2.1627	-6.4689	-5.5433
H	-1.0075	4.3042	-0.1846	H	2.2001	-3.0253	1.5677
H	-1.8309	3.2067	-5.9623	H	3.1349	-6.2997	-4.1123
H	-2.7519	-6.6248	0.4808	H	2.9532	-5.2630	2.3394
H	-1.5993	4.0392	-2.5648	H	3.2877	-4.5048	3.9153
H	-4.4091	1.5374	0.2433	H	2.1093	-9.0275	-5.0860
H	-2.2325	0.6603	-4.1869	H	2.8593	-8.6806	-3.5317
H	-4.1481	-1.5066	-0.8325	H	0.7445	-0.6830	-7.7930
H	-2.6221	3.2540	-4.3688	H	2.4962	-2.3237	3.1781
H	-4.1655	-4.8978	0.7584	H	4.5452	-2.3528	2.1631
H	-5.5101	-3.6938	-0.6948	H	1.8090	-0.4936	-6.3762
H	-5.7005	0.4472	-1.0444	H	1.2799	3.3170	4.5619
H	-5.4750	-1.9865	1.8617	H	-0.0149	2.8770	5.7073
H	-7.7813	-2.1881	0.7293	H	4.5276	0.5346	1.1071
H	-6.4288	0.0466	0.5215	H	5.4211	-0.9926	2.8739
H	-6.2410	-4.1583	0.8514	H	1.9280	-3.2804	-8.9322
H	-7.9712	-3.2197	-0.6978	H	1.5227	1.9800	5.7104
H	-7.8551	-0.7933	-1.3496	H	2.8552	-4.8473	-7.5343
H	-6.4866	-1.7014	-2.0116	H	5.2641	-3.2518	-0.1848
H	1.0649	3.3543	-5.0526	H	2.4937	-0.9884	-7.9481
H	0.9482	-7.0569	-3.0192	H	5.2561	-0.3714	-1.2565
H	-0.7249	-0.5230	4.2084	H	5.6767	-3.1244	-2.7415
H	0.2153	-7.4975	-4.5599	H	5.6440	-4.7833	-4.3071
H	-0.7457	-2.2975	-6.5593	H	6.9463	-2.4054	1.4592
H	-0.0609	-3.7360	-5.7606	H	6.7959	-0.7709	0.7957

H	6.6180	-2.4575	-1.0123
H	0.7838	-5.0757	-3.7512
H	-0.2169	-3.6615	-3.3676
H	-2.1882	-4.8087	-2.7076
H	-1.9827	-6.3038	-1.7321
H	-1.3863	-6.2450	-3.4185
H	1.6024	-4.6985	-0.3240
H	3.1839	-4.0192	-0.8060
H	2.5802	-5.5310	-1.5379
H	-0.6979	-0.4134	-0.7680

A1:
-6394.244

Cr	-1.8110	-1.4892	1.1730
Cr	0.3640	-0.9169	-1.9613
Cl	-3.4994	-1.5725	2.8336
Cl	1.5905	-0.0610	-3.7990
N	-2.0714	-3.4752	0.7874
N	-3.2645	-1.2770	-0.2169
N	0.8995	0.6916	-0.8677
N	2.0798	-1.6946	-1.1703
O	-1.2722	-0.0697	-2.5193
O	-2.2935	5.8489	-0.3159
O	-0.4245	-1.9546	2.4583
O	-2.8112	5.2543	-2.4747
O	-1.6105	0.4247	1.3015
O	-5.5050	4.5039	-1.6592
O	-5.5746	4.2457	0.6214
O	0.0375	-2.6075	-2.8677
O	-0.4578	-1.6483	-0.2898
C	-1.2976	3.4967	-1.6069
C	0.9552	-5.2939	1.7625
C	-0.9054	-4.6742	-4.5721
C	1.4701	-3.0267	3.3898
C	1.6664	-1.8576	4.3715
C	-2.2148	-3.9626	-4.1552
C	-1.5429	1.2187	-2.5384
C	-0.1540	-3.7938	-5.6071
C	0.0506	-4.2050	1.7299
C	-1.3037	-5.9912	-5.2746
C	0.4416	-1.7670	5.3203
C	0.3269	-3.0227	2.5068
C	1.8210	-0.5150	3.6152
C	-2.3399	3.9218	-2.4020
C	-1.1733	-4.3863	0.9742
C	-2.5687	1.7112	-3.4210
C	-2.8144	6.0787	-1.3940
C	-2.9527	3.0443	-3.3111
C	-3.5494	7.3654	-1.7433
C	-1.6149	4.1464	3.6282
C	-0.0250	2.7050	2.3717
C	-2.0238	0.2353	-5.3991
C	-3.9235	-0.3978	-3.8692
C	-3.5186	-5.0679	-0.5968
C	-3.7675	8.2421	-0.5002
C	-3.1625	0.7915	-4.5021
C	-3.3483	-3.7099	0.0951
C	-4.9481	-5.1809	-1.1655
C	-3.5841	-2.5446	-0.9146
C	-1.4605	2.7693	2.9474
C	-2.5624	1.3168	1.1210
C	-2.5171	2.5567	1.8470
C	-4.8009	7.6168	0.4570
C	-3.6351	1.0969	0.1935
C	-4.1593	1.5410	-5.4129
C	-5.0222	-2.6426	-1.4569
C	-3.8606	-0.1624	-0.4814
C	-5.2871	-4.0124	-2.1112
C	-1.6192	1.6731	4.0353
C	-3.4983	3.5137	1.5922
C	-4.5916	2.1063	-0.0441
C	-4.5207	3.2876	0.6625
C	-6.2524	7.7851	-0.0424
C	-6.0337	4.7071	-0.5827
C	-7.2183	6.7214	0.5261
C	-7.3293	5.4743	-0.3816
C	-0.8717	2.1525	-1.6853
C	2.3290	-4.1219	3.3595
C	2.1000	-5.2483	2.5369
C	2.9287	-2.0437	5.2414
C	0.0077	-4.9234	-3.3586
C	0.2656	1.8158	-0.8658
C	0.5179	-3.7943	-2.6127
C	0.4213	-6.2010	-2.9927
C	1.3641	-6.4337	-1.9651
C	1.5577	-4.0260	-1.6410
C	2.0281	0.4260	0.0509
C	1.9484	-5.3514	-1.3330
C	2.3207	-2.9577	-1.0280
C	2.9435	-0.6275	-0.6345

C	2.8576	1.6686	0.4215
C	4.0788	-1.0511	0.3029
C	4.0801	1.3072	1.2887
C	4.9306	0.1851	0.6603
H	-2.7562	-4.5860	-3.4365
H	0.7392	-6.1615	1.1448
H	0.3542	-2.6857	5.9153
H	-2.0033	-2.9908	-3.7075
H	0.7634	-4.2998	-5.9361
H	2.6629	-0.5860	2.9205
H	0.1102	-2.8247	-5.1767
H	-0.4217	-6.5312	-5.6425
H	-1.8636	-6.6532	-4.5998
H	0.5769	-0.9181	6.0046
H	2.0247	0.2916	4.3335
H	-2.8535	-3.8169	-5.0377
H	-1.3100	-5.3840	0.5525
H	-1.3130	-0.3508	-4.8146
H	-2.7680	-5.1717	-1.3919
H	0.1222	3.5167	1.6471
H	-2.9628	7.8959	-2.5065
H	-1.5045	4.9626	2.9019
H	-2.8080	8.3553	0.0175
H	-3.2818	-0.9238	-3.1612
H	-0.7980	-3.6339	-6.4835
H	-0.4785	-1.6211	4.7493
H	-0.8364	4.2519	4.3940
H	-1.9449	-5.7524	-6.1319
H	-2.8555	-2.6490	-1.7291
H	0.7011	2.8335	3.1869
H	0.9152	-0.2748	3.0574
H	-1.4817	1.0587	-5.8808
H	-5.6561	-5.1742	-0.3229
H	-4.8228	-0.0332	-3.3550
H	-4.1042	9.2424	-0.8087
H	-3.3497	-5.8789	0.1235
H	-2.5924	4.2397	4.1179
H	-5.0696	-6.1383	-1.6892
H	0.1487	1.7434	1.8872
H	-2.4632	-0.4015	-6.1801
H	-3.7395	3.4519	-3.9306
H	-4.4993	7.0878	-2.2164
H	-4.2375	-1.0971	-4.6562
H	-4.5597	6.5565	0.5867
H	-4.7148	8.0722	1.4535
H	-0.8795	1.8416	4.8311
H	-4.1133	-3.6032	0.8777
H	-3.6760	2.3806	-5.9282
H	-5.2050	-1.8598	-2.1962
H	-5.0126	1.9254	-4.8390
H	-4.6846	-4.0922	-3.0228
H	-4.6436	-0.1353	-1.2365
H	-3.5031	4.4568	2.1204
H	-4.5395	0.8434	-6.1698
H	-2.6236	1.7176	4.4732
H	-6.3410	-4.0733	-2.4138
H	-1.4741	0.6765	3.6150
H	-6.6020	8.7934	0.2225
H	-6.2766	7.7293	-1.1414
H	-5.7125	-2.4815	-0.6159
H	-5.3844	1.9372	-0.7635
H	-6.8892	6.4123	1.5267
H	-7.6795	5.7723	-1.3751
H	-8.2276	7.1412	0.6301
H	-8.0596	4.7779	0.0522
H	-0.8066	4.1728	-0.9233
H	3.2023	-4.1257	4.0015
H	0.0303	-2.4604	-0.0921
H	2.8003	-6.0775	2.5431
H	3.0147	-1.1931	5.9286
H	0.0289	-7.0588	-3.5271
H	3.8363	-2.0824	4.6240
H	2.8708	-2.9629	5.8382
H	0.6007	2.6189	-0.2150
H	1.6552	-7.4488	-1.7143
H	1.6013	-0.0342	0.9510
H	3.3708	-0.1429	-1.5248
H	2.2397	2.3887	0.9674
H	3.1852	2.1454	-0.5135
H	2.7130	-5.4989	-0.5750
H	3.1702	-3.2826	-0.4228
H	3.6603	-1.5115	1.2092
H	3.7347	0.9917	2.2794
H	4.7094	-1.8031	-0.1885
H	5.3977	0.5623	-0.2623
H	4.6976	2.2036	1.4359
H	5.7403	-0.1030	1.3436

A2:
-6587.287

Cr	0.0799	-1.5667	-3.1510	C	-3.2799	1.9985	5.1239
Cr	-2.4763	-1.3445	2.3173	C	-4.2532	-3.9507	-2.0751
Cl	1.4956	-0.0081	-4.4623	C	-4.1134	-0.1270	0.1566
Cl	-4.2507	-2.0768	3.6314	C	-4.5059	-2.6588	-1.2696
O	-0.8672	-2.8345	-2.0405	C	-4.4348	2.2988	-5.2465
O	-0.2478	-2.7372	-4.6965	C	-4.2714	1.1140	0.8739
O	-6.2141	4.2973	0.5055	C	-4.2640	7.1136	0.6504
O	-5.8291	4.0276	-1.7597	C	-3.7497	2.6711	2.7251
O	-2.6522	0.5401	2.5486	C	-3.5449	1.4131	2.0666
O	-2.1601	4.9268	-1.7823	C	-2.9766	3.0356	4.0075
O	-0.8858	-1.4682	3.3871	C	-3.3271	-2.3947	-0.3154
O	-1.2510	5.1264	0.3377	C	-3.9795	-5.1577	-1.1599
O	4.6921	-6.4211	3.4098	C	-3.1123	-3.6018	0.6233
O	-1.4735	-0.3689	-3.3407	C	-3.4384	1.2270	-4.7423
N	1.8174	-2.5698	-2.7791	C	-2.8384	7.6581	0.4326
N	0.5819	-0.5529	-1.4672	C	-2.8201	-4.8764	-0.1798
N	-3.4653	-1.1860	0.5563	C	-4.2633	-0.0157	-4.3088
N	-2.0712	-3.1953	1.6116	C	-2.5042	0.8434	-5.9231
C	5.7779	-4.1162	3.5841	C	-1.4529	3.0651	3.6987
C	4.3825	-1.9394	0.0901	C	-3.3722	4.4331	4.5413
C	3.3706	-1.3999	1.1146	C	-2.1346	7.0890	-0.8165
C	3.6816	-2.7396	-1.0258	C	-2.7131	3.0433	-3.1007
C	2.2874	-0.5403	0.4347	C	-1.7969	5.6187	-0.6596
C	2.6009	-1.8888	-1.7161	C	-2.5901	1.7391	-3.5602
C	2.2344	-3.6259	-3.4076	C	-1.0915	-3.9732	1.9688
C	2.2225	-5.4594	-5.0105	C	-1.9377	3.5372	-2.0380
C	1.5829	-1.3189	-0.6876	C	1.3139	0.2549	4.4952
C	1.5904	-4.2917	-4.5181	C	-0.0242	-2.4523	3.6732
C	1.7042	-6.1504	-6.0888	C	-0.2477	-0.7128	6.2526
C	0.5361	-5.6658	-6.7132	C	-1.7832	-4.9097	-8.2118
C	0.3882	-3.8096	-5.1432	C	-0.0882	-3.6948	2.9674
C	0.1372	0.6199	-1.1236	C	-1.1170	-2.5792	-7.5800
C	-0.1341	-4.5214	-6.2863	C	-1.6148	0.8805	-2.9281
C	2.2352	-0.9466	6.4873	C	-2.6057	-3.9551	-6.0513
C	1.8442	-4.5249	4.1887	C	1.0737	-0.9354	5.4651
C	1.8907	-3.3031	4.8916	C	4.5375	-5.8234	2.0447
C	-0.8457	1.4033	-1.8331	C	0.9910	-2.2568	4.6699
C	5.6995	-5.4442	2.8805	C	-1.3908	-4.0027	-7.0198
C	-7.1741	5.9038	-0.9734	C	0.8576	-4.7124	3.2367
C	-6.7462	7.1119	-0.1075	C	-1.0235	2.7377	-1.3874
C	-6.3270	4.6616	-0.8275	H	6.2798	-4.2181	4.5531
C	-5.3074	7.6330	-0.3627	H	6.3481	-3.3978	2.9815
C	-5.3365	3.2654	0.9591	H	4.7781	-3.7065	3.7550
C	-5.1592	2.0622	0.3118	H	5.1287	-2.5736	0.5873
C	-4.6565	3.5582	2.1514	H	3.8838	-0.8071	1.8827

H	4.9311	-1.0983	-0.3593
H	4.4281	-3.0725	-1.7577
H	2.8932	-2.2416	1.6361
H	3.2185	-3.6437	-0.6015
H	3.1795	-4.0819	-3.1027
H	3.1322	-5.8027	-4.5218
H	2.7488	0.3669	0.0165
H	1.5552	-0.2155	1.1839
H	3.0715	-1.0287	-2.2148
H	1.0369	-2.1715	-0.2595
H	2.1894	-7.0464	-6.4626
H	0.5333	1.0967	-0.2251
H	2.1173	-1.7426	7.2323
H	3.2098	-1.0675	5.9987
H	0.1541	-6.2123	-7.5671
H	2.2475	0.0106	7.0206
H	2.5784	-5.2987	4.3863
H	-1.1127	-3.5930	-2.6085
H	2.6613	-3.1828	5.6431
H	-0.4463	3.1131	-0.5540
H	4.6593	-6.5275	1.2267
H	-8.2070	5.6314	-0.7145
H	-7.4669	7.9152	-0.3113
H	-7.1571	6.1658	-2.0358
H	-6.8617	6.8492	0.9509
H	-5.6634	1.8433	-0.6190
H	-5.4410	-2.7390	-0.6933
H	-5.0020	7.3758	-1.3871
H	-5.3105	8.7318	-0.3128
H	-3.0470	0.9853	4.7944
H	-5.1144	-4.1557	-2.7235
H	-4.3394	2.0359	5.4070
H	-5.0281	1.8747	-6.0654
H	-4.8547	4.5171	2.6088
H	-4.5949	-0.1521	-0.8202
H	-3.3904	-3.7829	-2.7315
H	-5.1243	2.6235	-4.4576
H	-4.6198	-1.8316	-1.9774
H	-3.9155	3.1824	-5.6369
H	-4.0251	-3.7438	1.2220
H	-2.6796	2.2281	6.0138
H	-4.5982	7.3956	1.6600
H	-4.2331	6.0178	0.6385
H	-4.8466	-0.3935	-5.1591
H	-2.7348	7.2191	-1.7198
H	-3.4226	3.7269	-3.5444
H	-3.1040	0.4691	-6.7637
H	-1.1059	2.0785	3.3892
H	-3.7440	-6.0437	-1.7638
H	-4.4403	4.4929	4.7850
H	-2.6976	-5.7358	0.4930
H	-2.8691	8.7544	0.3550
H	-4.9686	0.2506	-3.5091
H	-4.8883	-5.3973	-0.5870
H	-1.9416	1.7200	-6.2658
H	0.5054	0.3279	3.7666
H	-0.9006	3.3656	4.5990
H	-2.4049	-2.2831	-0.9188
H	-2.6758	-4.4944	-8.6942
H	-2.8103	4.6326	5.4610
H	-1.1032	-0.6692	5.5775
H	-2.0068	-2.2069	-8.1051
H	-3.5966	-0.8045	-3.9560
H	-2.2215	7.4148	1.3063
H	-3.1294	5.2267	3.8247
H	-1.1872	7.6237	-0.9739
H	-1.2355	3.7833	2.8992
H	-1.8841	-4.7335	-0.7347
H	-1.7903	0.0745	-5.6240
H	-0.9965	-4.9479	1.4895
H	-3.5005	-3.6180	-6.5915
H	3.7021	-5.1350	1.9563
H	1.3579	1.1937	5.0619
H	-0.1933	0.2312	6.8101
H	-2.0215	-5.9318	-7.8910
H	-0.9898	-4.9602	-8.9678
H	-0.8677	-1.8878	-6.7743
H	2.2664	0.1340	3.9626
H	-0.2823	-2.6003	-8.2917
H	-2.4095	-3.2642	-5.2306
H	-0.4071	-1.5258	6.9719
H	0.7927	-5.6481	2.6867
H	-2.8115	-4.9529	-5.6413
H	6.6531	-5.9184	2.6531

A3: -6587.320

Cr	1.4645	-1.0526	-3.2520
Cr	-2.8345	-1.3959	2.0870
Cl	2.3607	0.1840	-5.1324

Cl	-4.6813	-1.9595	3.3807	C	-5.1821	-2.8851	-1.2620
O	0.8990	-1.9779	-1.6690	C	-4.3073	1.3742	-4.0891
O	0.9781	-2.6135	-4.3111	C	-4.7177	0.9757	0.6467
O	-6.5300	4.1724	0.0371	C	-4.4854	6.7758	0.8345
O	-5.0852	4.4605	-1.7293	C	-4.2019	2.5936	2.4510
O	-3.0833	0.4991	2.3549	C	-3.9740	1.3114	1.8324
O	-1.7553	4.9899	-1.7658	C	-3.5207	2.9563	3.7809
O	-1.5234	-1.6811	3.4689	C	-3.9422	-2.5958	-0.4001
O	-1.9695	4.5448	0.4743	C	-4.7807	-5.3890	-0.9488
O	-1.2384	-1.0724	0.8047	C	-3.6873	-3.7530	0.6047
O	-0.2379	-0.0901	-3.3887	C	-2.9171	0.7064	-3.9968
N	3.3352	-1.8383	-3.0035	C	-3.0112	7.2120	0.9027
N	2.1975	0.3893	-2.0162	C	-3.5133	-5.0881	-0.1249
N	-3.9914	-1.3430	0.3963	C	-3.1174	-0.6686	-3.3097
N	-2.5856	-3.3150	1.4767	C	-2.3891	0.4773	-5.4369
C	-0.1599	1.2155	1.2591	C	-1.9798	2.9752	3.6196
C	6.4380	-0.2153	-1.3180	C	-3.9428	4.3578	4.2755
C	5.6536	0.5552	-0.2422	C	-2.2369	6.8208	-0.3637
C	5.5882	-1.3631	-1.8975	C	-2.2802	2.8421	-2.7566
C	4.3355	1.1120	-0.8120	C	-1.9978	5.3202	-0.4606
C	4.2693	-0.8274	-2.4717	C	-1.9195	1.5775	-3.2129
C	3.6629	-3.0693	-3.2134	C	-1.5044	-3.9980	1.6665
C	3.2362	-5.4361	-3.6425	C	-1.3687	3.6573	-2.0684
C	3.4765	-0.0203	-1.3998	C	0.3165	0.1875	4.8233
C	2.7634	-4.1035	-3.6803	C	-0.4959	-2.5063	3.4477
C	2.4113	-6.4971	-3.9756	C	-0.7862	-1.4957	6.3526
C	1.0671	-6.2380	-4.3205	C	-1.7558	-5.9772	-4.8153
C	1.4240	-3.8322	-4.1319	C	-0.4207	-3.6203	2.5417
C	1.6259	1.5183	-1.7571	C	-1.1460	-3.8242	-5.9330
C	0.5460	-4.9480	-4.3895	C	-0.5762	1.0969	-2.9632
C	1.6921	-1.1750	6.3943	C	-1.5337	-3.9140	-3.4290
C	1.7879	-4.2030	3.3812	C	0.4578	-1.2149	5.4664
C	1.6882	-3.1474	4.3116	C	-1.2878	-0.3447	-0.4797
C	0.3168	1.9333	-2.2004	C	0.5769	-2.3087	4.3897
C	-0.1961	-0.0595	0.4669	C	-0.9449	-4.6736	-4.6507
C	-6.9269	6.0096	-1.3928	C	0.7290	-4.4450	2.5257
C	-6.7766	7.1127	-0.3124	C	-0.0992	3.2176	-1.7795
C	-6.0633	4.8023	-1.0966	H	0.1583	1.0340	2.2893
C	-5.3255	7.6196	-0.1445	H	0.5555	1.8984	0.7852
C	-5.7002	3.1730	0.6111	H	-1.1353	1.7030	1.2714
C	-5.5574	1.9366	0.0333	H	7.3700	-0.6157	-0.8976
C	-5.0565	3.4875	1.8177	H	6.2610	1.3741	0.1652
C	-3.9157	1.9245	4.8705	H	6.7130	0.4738	-2.1303
C	-5.0645	-4.2579	-1.9550	H	6.1516	-1.8856	-2.6809
C	-4.6631	-0.3102	-0.0015	H	5.4216	-0.1274	0.5894

H	5.3646	-2.0952	-1.1074
H	4.6793	-3.4083	-2.9953
H	4.2634	-5.6126	-3.3283
H	4.5465	1.8470	-1.6022
H	3.7874	1.6297	-0.0148
H	4.4725	-0.1403	-3.3040
H	3.2113	-0.7291	-0.6009
H	2.7783	-7.5179	-3.9452
H	2.1345	2.2435	-1.1177
H	1.8294	-2.1276	6.9228
H	2.6085	-0.9495	5.8326
H	0.4183	-7.0827	-4.5241
H	1.5430	-0.3857	7.1414
H	2.6778	-4.8233	3.3549
H	0.8776	-2.9332	-1.8300
H	2.5155	-2.9929	4.9942
H	0.5853	3.8492	-1.2215
H	-1.0698	-0.9736	-1.3320
H	-7.9766	5.6936	-1.4405
H	-7.4321	7.9450	-0.6012
H	-6.6269	6.3988	-2.3708
H	-7.1446	6.7218	0.6452
H	-6.0726	1.6948	-0.8903
H	-6.0704	-2.8590	-0.6146
H	-4.8413	7.6399	-1.1315
H	-5.3396	8.6571	0.2203
H	-3.6583	0.9090	4.5617
H	-5.9882	-4.4657	-2.5104
H	-4.9955	1.9689	5.0633
H	-4.9862	0.7038	-4.6309
H	-5.2413	4.4643	2.2388
H	-5.2573	-0.3808	-0.9132
H	-4.2470	-4.2207	-2.6853
H	-4.7234	1.5672	-3.0911
H	-5.2942	-2.1104	-2.0281
H	-4.2578	2.3263	-4.6312
H	-4.5684	-3.8110	1.2589
H	-3.3834	2.1627	5.8020
H	-4.9412	6.8423	1.8329
H	-4.5050	5.7200	0.5552
H	-3.8565	-1.2517	-3.8780
H	-2.7506	7.1508	-1.2724
H	-3.2742	3.2369	-2.9127
H	-3.0859	-0.1738	-5.9840
H	-1.6090	1.9750	3.4057
H	-4.6692	-6.3450	-1.4761
H	-5.0285	4.4245	4.4248
H	-3.3358	-5.8893	0.6035
H	-2.9491	8.2996	1.0497
H	-3.4921	-0.5282	-2.2909
H	-5.6348	-5.4899	-0.2619
H	-2.3150	1.4355	-5.9669
H	-0.5668	0.2270	4.1860
H	-1.5244	3.3250	4.5569
H	-3.0574	-2.5224	-1.0503
H	-2.8133	-5.7234	-4.9624
H	-3.4517	4.5497	5.2367
H	-1.6965	-1.5026	5.7485
H	-2.2205	-3.6478	-6.0857
H	-2.1812	-1.2232	-3.2765
H	-2.5314	6.7278	1.7619
H	-3.6329	5.1384	3.5676
H	-1.2472	7.3010	-0.3728
H	-1.6904	3.6484	2.8048
H	-2.6398	-5.0393	-0.7888
H	-1.4040	0.0065	-5.4097
H	-1.3722	-4.9521	1.1503
H	-2.5499	-3.5765	-3.6668
H	-2.0982	0.3735	-0.5488
H	0.2169	0.9443	5.6135
H	-0.8702	-0.7129	7.1194
H	-1.6734	-6.6084	-3.9208
H	-1.4152	-6.5542	-5.6850
H	-0.6317	-2.8666	-5.8407
H	1.2070	0.4252	4.2258
H	-0.7529	-4.3612	-6.8067
H	-0.9307	-3.0411	-3.1711
H	-0.6801	-2.4665	6.8546
H	0.7656	-5.2716	1.8193
H	-1.5792	-4.5848	-2.5602
H	0.7385	-0.5721	0.2601

A4:
-6587.258

Cr	1.6043	-0.7493	-3.2531
Cr	-3.0749	-1.6935	2.3402
Cl	2.4548	0.0836	-5.4001
Cl	-5.0005	-2.1082	3.7732
O	1.0241	-1.3663	-1.4592
O	1.0164	-2.4613	-4.0110

O	-6.4825	4.0822	0.1191	C	-4.3961	6.9448	0.5761
O	-5.1904	4.1819	-1.7993	C	-4.2201	2.4442	2.5749
O	-3.2597	0.2499	2.5593	C	-4.0964	1.1187	2.0129
O	-1.5715	5.4356	-2.1384	C	-3.4798	2.8207	3.8751
O	-1.7695	-2.0699	3.7495	C	-4.3838	-2.9045	-0.0188
O	-1.5993	5.0355	0.1414	C	-5.4157	-5.6706	-0.4138
O	-1.5701	-1.5341	1.0802	C	-4.1499	-4.0463	1.0065
O	-0.0471	0.2672	-3.5292	C	-2.7017	1.1125	-4.3072
N	3.4568	-1.5837	-2.9588	C	-2.9774	7.5580	0.5493
N	2.4569	0.8585	-2.3565	C	-4.0834	-5.4124	0.3120
N	-4.3659	-1.6202	0.7433	C	-2.9952	-0.2044	-3.5375
N	-3.0143	-3.6788	1.8726	C	-2.1068	0.7741	-5.7029
C	0.2061	0.9596	0.8865	C	-1.9445	2.7444	3.6461
C	6.7113	0.2065	-1.7670	C	-3.8109	4.2618	4.3319
C	6.0166	1.1657	-0.7857	C	-2.1937	7.2427	-0.7336
C	5.8021	-0.9889	-2.1109	C	-2.0448	3.2812	-3.1324
C	4.6770	1.6676	-1.3592	C	-1.7711	5.7942	-0.8156
C	4.4531	-0.5122	-2.6805	C	-1.7035	1.9914	-3.5242
C	3.8055	-2.7991	-3.2685	C	-1.9281	-4.3860	1.9852
C	3.4685	-5.1886	-3.6290	C	-1.1334	4.1156	-2.4676
C	3.7544	0.4901	-1.7244	C	0.3290	-0.3187	4.9584
C	2.9189	-3.8839	-3.6125	C	-0.8008	-2.9755	3.7550
C	2.6843	-6.2814	-3.9417	C	-0.9552	-1.7620	6.6036
C	1.3207	-6.0836	-4.2449	C	-1.4842	-5.9966	-4.8518
C	1.5380	-3.6804	-3.9488	C	-0.8229	-4.1065	2.8661
C	1.8722	2.0041	-2.1437	C	-0.9543	-3.7525	-5.8366
C	0.7182	-4.8266	-4.2576	C	-0.3801	1.5052	-3.2045
C	1.5525	-1.7315	6.6231	C	-1.4997	-3.9828	-3.3643
C	1.3192	-4.8729	3.7277	C	0.3096	-1.6829	5.7022
C	1.3207	-3.7866	4.6287	C	-1.4644	-0.7739	-0.1276
C	0.5420	2.3874	-2.5384	C	0.2953	-2.8437	4.6845
C	-0.0577	-0.3500	0.1378	C	-0.7820	-4.6455	-4.5753
C	-6.9622	5.8224	-1.4285	C	0.2481	-5.0312	2.8697
C	-6.7929	7.0212	-0.4581	C	0.1410	3.6987	-2.1784
C	-6.1043	4.6244	-1.1006	H	0.5826	0.6749	1.8730
C	-5.3732	7.6338	-0.3977	H	0.8901	1.6827	0.4334
C	-5.7063	3.0407	0.7289	H	-0.7352	1.4982	1.0385
C	-5.6581	1.7729	0.2041	H	7.6595	-0.1542	-1.3494
C	-5.0221	3.3663	1.9114	H	6.6658	2.0198	-0.5565
C	-3.8955	1.8531	5.0182	H	6.9591	0.7504	-2.6911
C	-5.7084	-4.5603	-1.4394	H	6.3135	-1.6312	-2.8375
C	-4.8956	-0.5308	0.2570	H	5.8327	0.6407	0.1633
C	-5.6891	-3.1582	-0.7989	H	5.6230	-1.5941	-1.2097
C	-4.0537	1.8340	-4.5246	H	4.8491	-3.0959	-3.1426
C	-4.8764	0.7826	0.8505	H	4.5201	-5.3163	-3.3815

H	4.8567	2.2752	-2.2579
H	4.1926	2.3161	-0.6201
H	4.6110	-0.0010	-3.6401
H	3.4984	-0.0670	-0.8101
H	3.1021	-7.2828	-3.9490
H	2.4131	2.7718	-1.5865
H	1.5910	-2.6582	7.2098
H	2.4875	-1.6410	6.0563
H	0.7249	-6.9586	-4.4752
H	1.5086	-0.8932	7.3288
H	2.1463	-5.5756	3.7222
H	0.8577	-2.3252	-1.3954
H	2.1667	-3.6925	5.2996
H	0.8371	4.3551	-1.6665
H	-1.5744	-1.3556	-1.0484
H	-8.0114	5.5032	-1.4074
H	-7.4940	7.7951	-0.7989
H	-6.7073	6.1274	-2.4478
H	-7.1140	6.7172	0.5462
H	-6.2087	1.5231	-0.6966
H	-6.5329	-3.0508	-0.1027
H	-4.9520	7.6554	-1.4128
H	-5.4654	8.6844	-0.0822
H	-3.7018	0.8148	4.7457
H	-6.6809	-4.7319	-1.9183
H	-4.9646	1.9572	5.2405
H	-4.7302	1.1636	-5.0682
H	-5.1346	4.3720	2.2911
H	-5.4931	-0.5991	-0.6546
H	-4.9531	-4.6020	-2.2390
H	-4.5339	2.1095	-3.5784
H	-5.8231	-2.4048	-1.5839
H	-3.9371	2.7449	-5.1243
H	-5.0180	-4.0356	1.6814
H	-3.3303	2.0934	5.9286
H	-4.7971	7.0481	1.5954
H	-4.3296	5.8688	0.3853
H	-3.7255	-0.8038	-4.0977
H	-2.7551	7.4973	-1.6369
H	-3.0342	3.6784	-3.3122
H	-2.8004	0.1254	-6.2545
H	-1.6447	1.7194	3.4269
H	-5.3988	-6.6438	-0.9208
H	-4.8836	4.3950	4.5180
H	-3.9014	-6.1984	1.0566
H	-3.0554	8.6494	0.6568
H	-3.4200	0.0167	-2.5496
H	-6.2192	-5.7098	0.3360
H	-1.9538	1.6886	-6.2890
H	-0.5488	-0.2243	4.3179
H	-1.4179	3.0800	4.5494
H	-3.5326	-2.8845	-0.7154
H	-2.5469	-5.8142	-5.0515
H	-3.2811	4.4664	5.2693
H	-1.8624	-1.7029	6.0001
H	-2.0220	-3.6292	-6.0617
H	-2.0831	-0.7879	-3.4099
H	-2.4068	7.1780	1.4046
H	-3.4870	5.0100	3.5971
H	-1.2744	7.8474	-0.7771
H	-1.6490	3.3919	2.8104
H	-3.2540	-5.4497	-0.4095
H	-1.1484	0.2613	-5.6047
H	-1.8766	-5.3566	1.4841
H	-2.5351	-3.7357	-3.6341
H	-2.1436	0.0856	-0.1580
H	0.3254	0.5053	5.6843
H	-0.9533	-0.9355	7.3272
H	-1.4166	-6.6762	-3.9933
H	-1.0634	-6.5023	-5.7295
H	-0.5090	-2.7698	-5.6758
H	1.2350	-0.2291	4.3442
H	-0.4735	-4.2196	-6.7054
H	-0.9932	-3.0609	-3.0738
H	-0.9669	-2.7055	7.1652
H	0.2096	-5.8773	2.1862
H	-1.5215	-4.6686	-2.5067
H	0.5976	-1.1023	0.5615

A5:
-6587.339

Cr	1.3801	-0.2790	-3.0121
Cr	-2.6192	-1.7325	2.1562
Cl	2.4177	1.2350	-4.4174
Cl	-4.1347	-0.7806	3.7954
O	0.5619	-1.7000	-1.7442
O	1.2516	-1.7208	-4.2857
O	-5.9943	3.8273	0.0726
O	-4.9979	4.5595	-1.8617
O	-2.1690	0.0221	1.4183

O	-2.2256	5.5568	-2.4757	C	-1.7005	2.7013	2.3776
O	-1.1647	-1.8177	3.4361	C	-4.7177	-3.2061	0.7840
O	-2.0623	5.6584	-0.1929	C	-6.5182	-5.4194	1.5936
O	-1.7458	-2.8410	0.8488	C	-4.6673	-3.8165	2.2253
O	-0.4115	0.3806	-3.2373	C	-3.0239	1.0123	-4.2364
N	3.1790	-1.0027	-2.3510	C	-3.6080	8.0280	-0.0754
N	1.5941	0.9305	-1.4251	C	-5.1116	-5.2861	2.2095
N	-4.2218	-1.8242	0.8939	C	-3.3370	-0.2032	-3.3215
N	-3.3222	-3.5467	2.7603	C	-2.3288	0.5205	-5.5324
C	0.7002	-2.8857	0.9745	C	-0.3873	2.5107	1.5824
C	5.3737	0.3101	0.5908	C	-1.7735	4.1824	2.8150
C	4.2174	0.8909	1.4257	C	-3.0996	7.4825	-1.4196
C	4.8658	-0.7291	-0.4307	C	-2.5242	3.3251	-3.2755
C	3.1380	1.5119	0.5190	C	-2.4188	6.1347	-1.2533
C	3.7968	-0.1066	-1.3434	C	-2.1258	2.0107	-3.4885
C	3.6973	-2.1369	-2.6947	C	-2.5830	-4.4226	3.3497
C	3.8478	-4.2914	-3.8306	C	-1.7415	4.2271	-2.5377
C	2.6331	0.4717	-0.4870	C	1.5096	-0.5774	3.6324
C	3.1452	-3.0751	-3.6484	C	-0.6329	-2.8921	3.9595
C	3.3745	-5.2671	-4.6893	C	0.1978	-0.5580	5.7942
C	2.1608	-5.0513	-5.3770	C	-0.3318	-4.9004	-6.7943
C	1.9314	-2.8434	-4.3818	C	-1.2545	-4.1907	3.8823
C	1.0005	2.0796	-1.3285	C	0.1579	-2.4531	-6.9262
C	1.4202	-3.8781	-5.2429	C	-0.8530	1.5936	-2.9666
C	2.5354	-1.4447	5.7260	C	-1.0553	-3.4168	-4.9214
C	0.6751	-5.2066	4.9750	C	1.2091	-1.3657	4.9356
C	1.2476	-3.9244	5.1172	C	-0.5011	-1.4841	-0.7427
C	-0.1224	2.4973	-2.1221	C	0.6255	-2.7658	4.6573
C	-0.5664	-2.7574	0.1141	C	0.0749	-3.6651	-5.9614
C	-7.1743	5.4177	-1.2016	C	-0.5748	-5.3219	4.3920
C	-7.2506	6.5589	-0.1572	C	-0.5755	3.8242	-1.9314
C	-5.9240	4.5680	-1.0728	H	0.7401	-2.0533	1.6785
C	-6.1190	7.5961	-0.3249	H	0.6644	-3.8145	1.5529
C	-4.9703	2.8696	0.3455	H	1.6028	-2.8793	0.3472
C	-5.2177	1.5505	0.0371	H	6.1216	-0.1547	1.2459
C	-3.8345	3.2445	1.0753	H	4.5950	1.6464	2.1263
C	-1.6566	1.8449	3.6701	H	5.8749	1.1275	0.0501
C	-6.5505	-4.8382	0.1681	H	5.7095	-1.0987	-1.0267
C	-4.7394	-0.8160	0.2803	H	3.7587	0.0938	2.0257
C	-6.1132	-3.3616	0.1665	H	4.4259	-1.5874	0.0981
C	-4.3770	1.6484	-4.6246	H	4.6309	-2.4594	-2.2283
C	-4.3075	0.5563	0.4541	H	4.7696	-4.4470	-3.2737
C	-4.8282	7.2400	0.4405	H	3.5534	2.3708	-0.0279
C	-2.8945	2.3012	1.4921	H	2.2999	1.8710	1.1271
C	-3.0924	0.9213	1.1308	H	4.2305	0.7317	-1.9075

H	2.1949	-0.3706	0.0701	H	-0.3064	1.4786	1.2284
H	3.9164	-6.1973	-4.8249	H	-6.8256	-6.4737	1.5859
H	1.3178	2.7855	-0.5626	H	-2.6927	4.3763	3.3835
H	2.3958	-1.9385	6.6961	H	-5.1082	-5.6866	3.2315
H	3.3028	-1.9917	5.1617	H	-3.8763	9.0880	-0.1888
H	1.7953	-5.8388	-6.0261	H	-3.7985	0.1321	-2.3842
H	2.9005	-0.4257	5.9066	H	-7.2382	-4.8733	2.2217
H	1.2002	-6.0808	5.3471	H	-2.1356	1.3681	-6.2029
H	0.2912	-2.4488	-2.3030	H	0.5952	-0.3886	3.0673
H	2.2059	-3.8511	5.6187	H	0.4716	2.7389	2.2313
H	-0.0209	4.4975	-1.2905	H	-3.9711	-3.7461	0.1867
H	-1.4457	-1.2836	-1.2512	H	-1.2979	-4.7003	-7.2729
H	-8.0475	4.7647	-1.0831	H	-0.9175	4.3920	3.4694
H	-8.2273	7.0481	-0.2723	H	-0.7491	-0.4339	5.2653
H	-7.1797	5.8428	-2.2103	H	-0.8185	-2.3050	-7.4072
H	-7.2185	6.1249	0.8506	H	-2.4222	-0.7510	-3.0885
H	-6.1386	1.2687	-0.4651	H	-2.7932	7.9642	0.6549
H	-6.8278	-2.7605	0.7478	H	-1.7327	4.8622	1.9593
H	-5.8981	7.6998	-1.3977	H	-2.3737	8.1710	-1.8756
H	-6.4623	8.5832	0.0173	H	-0.3855	3.1942	0.7276
H	-1.5027	0.7891	3.4544	H	-4.3911	-5.8729	1.6202
H	-7.5562	-4.9328	-0.2616	H	-1.3804	0.0310	-5.3020
H	-2.5974	1.9351	4.2240	H	-2.9554	-5.4419	3.4877
H	-4.9967	0.8855	-5.1121	H	-2.0172	-3.3275	-5.4438
H	-3.7131	4.2880	1.3290	H	-0.2082	-0.6043	-0.1689
H	-5.6071	-0.9532	-0.3691	H	1.9711	0.3858	3.8926
H	-5.8652	-5.4158	-0.4702	H	0.6133	0.4351	6.0159
H	-4.9062	2.0190	-3.7375	H	-0.4366	-5.7932	-6.1642
H	-6.1148	-2.9766	-0.8613	H	0.4047	-5.1105	-7.5807
H	-4.2439	2.4826	-5.3256	H	0.4292	-1.5449	-6.3854
H	-5.3563	-3.2245	2.8440	H	2.2124	-1.1418	3.0059
H	-0.8331	2.2065	4.3029	H	0.9075	-2.6430	-7.7055
H	-4.9836	7.4458	1.5086	H	-0.8800	-2.4911	-4.3688
H	-4.6095	6.1701	0.3644	H	0.0126	-1.0807	6.7420
H	-4.0337	-0.8763	-3.8410	H	-1.0567	-6.2950	4.3112
H	-3.9136	7.3606	-2.1433	H	-1.1213	-4.2606	-4.2201
H	-3.4705	3.6898	-3.6444	H	-0.5626	-3.6032	-0.6126
H	-2.9861	-0.1914	-6.0516				

VII. X-ray Crystallography Conditions and Coordinates

X-ray diffraction quality crystals of the μ-hydroxide non-tethered chromium salen complex were obtained by refluxing (*R,R*-salcy)CrCl in acetonitrile at 75 °C for 16 hours and allowing the solvent volume to be reduced by three fourths. Crystals were collected and rinsed with cold acetonitrile.

X-ray diffraction data was collected on a Bruker APEX 2 CCD Kappa diffractometer (Mo Kα, λ = 0.71073 Å) at 173 K. The structures were solved through intrinsic phasing using SHELXT[18] and refined against F^2 on all data by full-matrix least squares with SHELXL[19] following established refinement strategies.[20] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. Hydrogen atoms bound to oxygen were located in the difference Fourier synthesis and subsequently refined semi-freely with the help of distance restraints. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). A partially occupied solvent molecule of acetonitrile was included in the unit cell but could not be satisfactorily modeled. Therefore, that solvent was treated as a diffuse contribution to the overall scattering without using specific atom positions by the solvent masking function in Olex2.[21] Details of the data quality and a summary of the residual values of all the refinements are listed in Table S4-S8.

Table S4. Crystal data and structure refinement for μ-hydroxide non-tethered chromium salen complex complex.

Identification code	μ-hydroxide non-tethered chromium salen complex
Empirical formula	C75 H109.5 Cl Cr2 N5.5 O5
Formula weight	1307.62
Temperature	173.15 K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	P 21 21 21
Unit cell dimensions	a = 17.0512(8) Å α= 90°.
	b = 20.0506(9) Å β= 90°.
	c = 22.7296(10) Å γ = 90°.
Volume	7771.0(6) $Å^3$
Z	4
Density (calculated)	1.118 Mg/m^3
Absorption coefficient	0.361 mm^{-1}
F(000)	2768
Crystal size	0.15 x 0.1 x 0.05 mm^3
Theta range for data collection	1.354 to 26.372°.
Index ranges	-20<=h<=21
Reflections collected	63537
Independent reflections	15881 [R(int) = 0.0647]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15881 / 1 / 812
Goodness-of-fit on F2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0511
R indices (all data)	R1 = 0.0673
Absolute structure parameter	0.024(8)
Extinction coefficient	n/a
Largest diff. peak and hole	0.280 and -0.307 e.$Å^{-3}$

Table S5. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2x10^3$) for the μ-hydroxide non-tethered chromium salen complex. U(eq) is defined as one third of the trace of orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cr(1)	9716(1)	529(1)	7328(1)	19(1)
Cr(2)	8702(1)	2247(1)	7257(1)	21(1)
Cl(1)	10426(1)	-450(1)	7519(1)	33(1)
O(1)	10550(2)	862(1)	6832(1)	22(1)
O(2)	9128(2)	80(1)	6726(1)	22(1)
O(3)	8013(2)	1999(2)	7896(1)	28(1)
O(4)	7980(2)	2134(1)	6616(1)	24(1)
O(5)	9068(2)	1337(1)	7146(1)	22(1)
N(1)	10243(2)	951(2)	8031(1)	20(1)
N(2)	8921(2)	262(2)	7938(1)	20(1)
N(3)	9528(2)	2498(2)	7850(2)	23(1)
N(4)	9522(2)	2587(2)	6691(2)	23(1)
N(5)	8256(2)	3209(2)	7363(2)	31(1)
C(1)	10979(2)	1071(2)	8057(2)	23(1)
C(2)	11529(2)	1038(2)	7575(2)	23(1)
C(3)	12321(2)	1118(2)	7708(2)	25(1)
C(4)	12902(2)	1095(2)	7292(2)	26(1)
C(5)	12655(2)	984(2)	6711(2)	25(1)
C(6)	11885(2)	902(2)	6536(2)	22(1)
C(7)	11283(2)	928(2)	6978(2)	21(1)
C(8)	13766(2)	1194(2)	7467(2)	32(1)
C(9)	13861(3)	1874(2)	7766(2)	41(1)
C(10)	14320(3)	1176(3)	6940(2)	48(1)
C(11)	14019(3)	646(3)	7895(2)	50(1)
C(12)	11657(3)	762(2)	5895(2)	30(1)
C(13)	11111(3)	1306(2)	5661(2)	39(1)
C(14)	12377(3)	749(3)	5484(2)	47(1)
C(15)	11255(3)	78(2)	5847(2)	39(1)
C(16)	8225(2)	55(2)	7822(2)	21(1)

C(17)	7928(2)	-120(2)	7249(2)	22(1)
C(18)	8398(2)	-131(2)	6734(2)	20(1)
C(19)	8064(2)	-390(2)	6202(2)	21(1)
C(20)	7303(2)	-614(2)	6216(2)	24(1)
C(21)	6825(2)	-603(2)	6719(2)	23(1)
C(22)	7147(2)	-354(2)	7224(2)	23(1)
C(23)	8575(2)	-422(2)	5642(2)	22(1)
C(24)	8914(3)	276(2)	5487(2)	32(1)
C(25)	8109(3)	-658(3)	5105(2)	38(1)
C(26)	9248(3)	-921(2)	5735(2)	29(1)
C(27)	5976(3)	-866(2)	6688(2)	33(1)
C(28)	5957(3)	-1549(2)	6381(3)	52(2)
C(29)	5608(3)	-933(4)	7297(3)	79(2)
C(30)	5479(3)	-388(3)	6320(3)	48(1)
C(31)	9713(2)	986(2)	8543(2)	26(1)
C(32)	9218(2)	344(2)	8546(2)	25(1)
C(33)	8622(3)	355(3)	9040(2)	37(1)
C(34)	9038(3)	451(3)	9628(2)	43(1)
C(35)	9495(3)	1098(3)	9632(2)	41(1)
C(36)	10110(2)	1111(3)	9128(2)	32(1)
C(37)	9377(3)	2670(2)	8385(2)	29(1)
C(38)	8629(2)	2606(2)	8677(2)	26(1)
C(39)	7976(2)	2281(2)	8419(2)	25(1)
C(40)	7259(2)	2253(2)	8744(2)	27(1)
C(41)	7249(3)	2539(2)	9301(2)	30(1)
C(42)	7895(3)	2857(2)	9564(2)	33(1)
C(43)	8577(3)	2883(2)	9246(2)	30(1)
C(44)	6519(2)	1944(2)	8468(2)	31(1)
C(45)	5815(3)	1971(3)	8893(2)	42(1)
C(46)	6654(3)	1209(2)	8302(2)	39(1)
C(47)	6303(3)	2354(3)	7918(2)	43(1)
C(48)	7800(3)	3177(2)	10178(2)	38(1)
C(49)	7439(3)	2666(3)	10610(2)	48(1)

C(50)	7245(4)	3766(3)	10125(3)	63(2)
C(51)	8575(4)	3420(4)	10421(2)	69(2)
C(52)	9513(2)	2475(2)	6138(2)	26(1)
C(53)	8879(2)	2184(2)	5804(2)	24(1)
C(54)	9008(3)	2089(2)	5200(2)	31(1)
C(55)	8429(3)	1880(2)	4825(2)	31(1)
C(56)	7681(3)	1789(2)	5078(2)	28(1)
C(57)	7500(2)	1876(2)	5665(2)	25(1)
C(58)	8123(2)	2065(2)	6053(2)	24(1)
C(59)	8545(3)	1769(3)	4168(2)	36(1)
C(60)	8081(4)	2317(3)	3840(2)	54(2)
C(61)	9408(3)	1830(4)	3993(3)	71(2)
C(62)	8245(3)	1081(2)	3982(2)	43(1)
C(63)	6672(3)	1786(2)	5905(2)	34(1)
C(64)	6088(3)	1586(3)	5422(3)	62(2)
C(65)	6671(3)	1232(2)	6383(2)	41(1)
C(66)	6379(3)	2440(3)	6172(2)	47(1)
C(67)	10166(2)	2943(2)	6986(2)	27(1)
C(68)	10304(2)	2580(2)	7575(2)	24(1)
C(69)	10931(3)	2928(2)	7951(2)	29(1)
C(70)	11686(2)	3018(2)	7605(2)	37(1)
C(71)	11511(3)	3394(2)	7034(2)	37(1)
C(72)	10927(3)	3013(2)	6650(2)	34(1)
C(73)	7972(3)	3689(3)	7486(2)	44(1)
C(74)	7596(3)	4318(3)	7674(4)	84(2)

Table S6. Bond lengths (Å) and angles (^{o}) for the μ-hydroxide non-tethered chromium salen complex.

Cr(1)-Cl(1)	2.3477(12)
Cr(1)-O(1)	1.934(3)
Cr(1)-O(2)	1.920(3)
Cr(1)-O(5)	2.003(3)
Cr(1)-N(1)	2.019(3)
Cr(1)-N(2)	2.012(3)
Cr(2)-O(3)	1.934(3)
Cr(2)-O(4)	1.922(3)
Cr(2)-O(5)	1.945(3)
Cr(2)-N(3)	2.013(3)
Cr(2)-N(4)	2.018(3)
Cr(2)-N(5)	2.088(4)
O(1)-C(7)	1.300(5)
O(2)-C(18)	1.313(5)
O(3)-C(39)	1.317(5)
O(4)-C(58)	1.309(5)
N(1)-C(1)	1.280(5)
N(1)-C(31)	1.475(5)
N(2)-C(16)	1.285(5)
N(2)-C(32)	1.481(5)
N(3)-C(37)	1.289(5)
N(3)-C(68)	1.472(5)
N(4)-C(52)	1.278(5)
N(4)-C(67)	1.472(5)
N(5)-C(73)	1.112(6)
C(1)-C(2)	1.444(6)
C(2)-C(3)	1.394(5)
C(2)-C(7)	1.437(6)
C(3)-C(4)	1.370(6)
C(4)-C(5)	1.404(6)
C(4)-C(8)	1.539(6)
C(5)-C(6)	1.382(6)
C(6)-C(7)	1.437(6)

C(6)-C(12)	1.535(6)
C(8)-C(9)	1.533(6)
C(8)-C(10)	1.527(6)
C(8)-C(11)	1.529(7)
C(12)-C(13)	1.529(7)
C(12)-C(14)	1.542(6)
C(12)-C(15)	1.537(6)
C(16)-C(17)	1.441(6)
C(17)-C(18)	1.419(6)
C(17)-C(22)	1.415(5)
C(18)-C(19)	1.433(5)
C(19)-C(20)	1.373(5)
C(19)-C(23)	1.545(6)
C(20)-C(21)	1.406(6)
C(21)-C(22)	1.366(6)
C(21)-C(27)	1.543(6)
C(23)-C(24)	1.554(6)
C(23)-C(25)	1.532(6)
C(23)-C(26)	1.537(6)
C(27)-C(28)	1.536(7)
C(27)-C(29)	1.526(7)
C(27)-C(30)	1.528(7)
C(31)-C(32)	1.538(6)
C(31)-C(36)	1.515(6)
C(32)-C(33)	1.515(6)
C(33)-C(34)	1.526(6)
C(34)-C(35)	1.513(7)
C(35)-C(36)	1.553(6)
C(37)-C(38)	1.446(6)
C(38)-C(39)	1.417(6)
C(38)-C(43)	1.409(6)
C(39)-C(40)	1.430(6)
C(40)-C(41)	1.388(6)
C(40)-C(44)	1.539(6)
C(41)-C(42)	1.406(6)

C(42)-C(43)	1.371(6)
C(42)-C(48)	1.546(6)
C(44)-C(45)	1.541(6)
C(44)-C(46)	1.538(7)
C(44)-C(47)	1.542(6)
C(48)-C(49)	1.548(7)
C(48)-C(50)	1.517(8)
C(48)-C(51)	1.512(8)
C(52)-C(53)	1.443(6)
C(53)-C(54)	1.404(6)
C(53)-C(58)	1.428(6)
C(54)-C(55)	1.369(6)
C(55)-C(56)	1.412(6)
C(55)-C(59)	1.523(6)
C(56)-C(57)	1.379(6)
C(57)-C(58)	1.431(6)
C(57)-C(63)	1.525(6)
C(59)-C(60)	1.546(7)
C(59)-C(61)	1.528(7)
C(59)-C(62)	1.532(7)
C(63)-C(64)	1.535(7)
C(63)-C(65)	1.554(7)
C(63)-C(66)	1.529(7)
C(67)-C(68)	1.541(6)
C(67)-C(72)	1.511(6)
C(68)-C(69)	1.536(5)
C(69)-C(70)	1.520(6)
C(70)-C(71)	1.531(7)
C(71)-C(72)	1.529(6)
C(73)-C(74)	1.479(7)

O(1)-Cr(1)-Cl(1)	91.01(9)
O(1)-Cr(1)-O(5)	90.37(12)
O(1)-Cr(1)-N(1)	89.40(12)
O(1)-Cr(1)-N(2)	171.62(13)

O(2)-Cr(1)-Cl(1)	90.52(9)
O(2)-Cr(1)-O(1)	97.54(11)
O(2)-Cr(1)-O(5)	86.81(11)
O(2)-Cr(1)-N(1)	173.00(13)
O(2)-Cr(1)-N(2)	90.79(12)
O(5)-Cr(1)-Cl(1)	177.14(9)
O(5)-Cr(1)-N(1)	94.03(12)
O(5)-Cr(1)-N(2)	89.21(12)
N(1)-Cr(1)-Cl(1)	88.49(10)
N(2)-Cr(1)-Cl(1)	89.79(10)
N(2)-Cr(1)-N(1)	82.28(13)
O(3)-Cr(2)-O(5)	92.92(12)
O(3)-Cr(2)-N(3)	89.23(13)
O(3)-Cr(2)-N(4)	170.60(13)
O(3)-Cr(2)-N(5)	85.96(14)
O(4)-Cr(2)-O(3)	98.65(11)
O(4)-Cr(2)-O(5)	89.81(12)
O(4)-Cr(2)-N(3)	170.23(13)
O(4)-Cr(2)-N(4)	90.02(13)
O(4)-Cr(2)-N(5)	87.87(13)
O(5)-Cr(2)-N(3)	95.59(12)
O(5)-Cr(2)-N(4)	90.72(12)
O(5)-Cr(2)-N(5)	177.24(13)
N(3)-Cr(2)-N(4)	81.79(13)
N(3)-Cr(2)-N(5)	86.92(14)
N(4)-Cr(2)-N(5)	90.77(14)
C(7)-O(1)-Cr(1)	126.4(3)
C(18)-O(2)-Cr(1)	129.5(3)
C(39)-O(3)-Cr(2)	126.6(3)
C(58)-O(4)-Cr(2)	129.4(3)
Cr(2)-O(5)-Cr(1)	155.29(15)
C(1)-N(1)-Cr(1)	123.5(3)
C(1)-N(1)-C(31)	123.7(3)
C(31)-N(1)-Cr(1)	111.8(2)
C(16)-N(2)-Cr(1)	124.6(3)

C(16)-N(2)-C(32)	122.9(3)
C(32)-N(2)-Cr(1)	112.6(2)
C(37)-N(3)-Cr(2)	124.0(3)
C(37)-N(3)-C(68)	123.3(3)
C(68)-N(3)-Cr(2)	111.9(2)
C(52)-N(4)-Cr(2)	124.0(3)
C(52)-N(4)-C(67)	122.9(3)
C(67)-N(4)-Cr(2)	113.0(3)
C(73)-N(5)-Cr(2)	170.6(4)
N(1)-C(1)-C(2)	126.4(4)
C(3)-C(2)-C(1)	117.3(4)
C(3)-C(2)-C(7)	120.4(4)
C(7)-C(2)-C(1)	122.3(3)
C(4)-C(3)-C(2)	123.2(4)
C(3)-C(4)-C(5)	115.9(4)
C(3)-C(4)-C(8)	120.6(4)
C(5)-C(4)-C(8)	123.4(4)
C(6)-C(5)-C(4)	125.1(4)
C(5)-C(6)-C(7)	118.2(4)
C(5)-C(6)-C(12)	122.4(4)
C(7)-C(6)-C(12)	119.3(4)
O(1)-C(7)-C(2)	122.5(4)
O(1)-C(7)-C(6)	120.3(4)
C(6)-C(7)-C(2)	117.2(3)
C(9)-C(8)-C(4)	109.3(3)
C(10)-C(8)-C(4)	112.7(4)
C(10)-C(8)-C(9)	107.7(4)
C(10)-C(8)-C(11)	107.9(4)
C(11)-C(8)-C(4)	110.1(4)
C(11)-C(8)-C(9)	109.1(4)
C(6)-C(12)-C(14)	112.1(4)
C(6)-C(12)-C(15)	110.1(4)
C(13)-C(12)-C(6)	110.7(4)
C(13)-C(12)-C(14)	106.7(4)
C(13)-C(12)-C(15)	109.9(4)

C(15)-C(12)-C(14)	107.3(4)
N(2)-C(16)-C(17)	126.0(4)
C(18)-C(17)-C(16)	123.5(3)
C(22)-C(17)-C(16)	116.6(4)
C(22)-C(17)-C(18)	119.6(4)
O(2)-C(18)-C(17)	122.7(4)
O(2)-C(18)-C(19)	118.8(3)
C(17)-C(18)-C(19)	118.4(4)
C(18)-C(19)-C(23)	119.1(3)
C(20)-C(19)-C(18)	118.4(4)
C(20)-C(19)-C(23)	122.5(3)
C(19)-C(20)-C(21)	124.1(4)
C(20)-C(21)-C(27)	120.0(4)
C(22)-C(21)-C(20)	117.2(4)
C(22)-C(21)-C(27)	122.7(4)
C(21)-C(22)-C(17)	122.2(4)
C(19)-C(23)-C(24)	111.0(3)
C(25)-C(23)-C(19)	112.2(3)
C(25)-C(23)-C(24)	106.9(3)
C(25)-C(23)-C(26)	107.2(4)
C(26)-C(23)-C(19)	109.5(3)
C(26)-C(23)-C(24)	109.8(3)
C(28)-C(27)-C(21)	110.2(4)
C(29)-C(27)-C(21)	111.9(4)
C(29)-C(27)-C(28)	109.0(4)
C(29)-C(27)-C(30)	108.8(5)
C(30)-C(27)-C(21)	109.4(4)
C(30)-C(27)-C(28)	107.4(4)
N(1)-C(31)-C(32)	107.5(3)
N(1)-C(31)-C(36)	115.3(3)
C(36)-C(31)-C(32)	112.3(3)
N(2)-C(32)-C(31)	106.0(3)
N(2)-C(32)-C(33)	117.7(3)
C(33)-C(32)-C(31)	111.1(4)
C(32)-C(33)-C(34)	109.8(4)

C(35)-C(34)-C(33)	110.6(4)
C(34)-C(35)-C(36)	111.0(4)
C(31)-C(36)-C(35)	110.0(3)
N(3)-C(37)-C(38)	125.9(4)
C(39)-C(38)-C(37)	123.0(4)
C(43)-C(38)-C(37)	116.2(4)
C(43)-C(38)-C(39)	120.9(4)
O(3)-C(39)-C(38)	122.2(4)
O(3)-C(39)-C(40)	119.4(4)
C(38)-C(39)-C(40)	118.3(4)
C(39)-C(40)-C(44)	120.3(4)
C(41)-C(40)-C(39)	117.7(4)
C(41)-C(40)-C(44)	121.9(4)
C(40)-C(41)-C(42)	124.4(4)
C(41)-C(42)-C(48)	119.4(4)
C(43)-C(42)-C(41)	117.2(4)
C(43)-C(42)-C(48)	123.3(4)
C(42)-C(43)-C(38)	121.4(4)
C(40)-C(44)-C(45)	111.6(4)
C(40)-C(44)-C(47)	108.1(4)
C(45)-C(44)-C(47)	107.6(4)
C(46)-C(44)-C(40)	111.4(4)
C(46)-C(44)-C(45)	107.7(4)
C(46)-C(44)-C(47)	110.3(4)
C(42)-C(48)-C(49)	109.9(4)
C(50)-C(48)-C(42)	108.4(4)
C(50)-C(48)-C(49)	108.5(4)
C(51)-C(48)-C(42)	111.8(4)
C(51)-C(48)-C(49)	109.2(5)
C(51)-C(48)-C(50)	108.9(5)
N(4)-C(52)-C(53)	126.7(4)
C(54)-C(53)-C(52)	116.9(4)
C(54)-C(53)-C(58)	120.3(4)
C(58)-C(53)-C(52)	122.4(4)
C(55)-C(54)-C(53)	122.6(4)

C(54)-C(55)-C(56)	115.9(4)
C(54)-C(55)-C(59)	124.2(4)
C(56)-C(55)-C(59)	119.9(4)
C(57)-C(56)-C(55)	125.4(4)
C(56)-C(57)-C(58)	117.6(4)
C(56)-C(57)-C(63)	122.5(4)
C(58)-C(57)-C(63)	119.9(4)
O(4)-C(58)-C(53)	122.4(4)
O(4)-C(58)-C(57)	119.5(4)
C(53)-C(58)-C(57)	118.1(4)
C(55)-C(59)-C(60)	107.6(4)
C(55)-C(59)-C(61)	111.6(4)
C(55)-C(59)-C(62)	111.0(4)
C(61)-C(59)-C(60)	108.1(5)
C(61)-C(59)-C(62)	108.8(5)
C(62)-C(59)-C(60)	109.6(4)
C(57)-C(63)-C(64)	112.1(4)
C(57)-C(63)-C(65)	109.6(4)
C(57)-C(63)-C(66)	110.1(4)
C(64)-C(63)-C(65)	108.3(4)
C(66)-C(63)-C(64)	107.2(4)
C(66)-C(63)-C(65)	109.6(4)
N(4)-C(67)-C(68)	106.3(3)
N(4)-C(67)-C(72)	117.1(3)
C(72)-C(67)-C(68)	110.6(4)
N(3)-C(68)-C(67)	106.6(3)
N(3)-C(68)-C(69)	116.1(3)
C(69)-C(68)-C(67)	112.0(3)
C(70)-C(69)-C(68)	110.8(3)
C(69)-C(70)-C(71)	109.4(4)
C(72)-C(71)-C(70)	111.3(4)
C(67)-C(72)-C(71)	108.6(4)
N(5)-C(73)-C(74)	177.7(7)

Table S7. Anisotropic displacement parameters ($Å^2x10^3$) for the μ-hydroxide non-tethered chromium salen complex. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{11}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cr(1)	13(1)	25(1)	18(1)	-3(1)	1(1)	-2(1)
Cr(2)	15(1)	26(1)	22(1)	-6(1)	0(1)	-1(1)
Cl(1)	26(1)	27(1)	46(1)	4(1)	2(1)	2(1)
O(1)	14(2)	32(2)	20(2)	-3(1)	2(1)	-2(1)
O(2)	16(2)	30(2)	19(2)	-8(1)	4(1)	-3(1)
O(3)	19(2)	42(2)	25(2)	-12(1)	6(1)	-5(1)
O(4)	20(2)	33(2)	19(2)	-3(1)	-4(1)	-1(1)
O(5)	17(2)	24(2)	23(2)	-7(1)	-4(1)	1(1)
N(1)	18(2)	23(2)	18(2)	-5(1)	3(2)	-2(2)
N(2)	18(2)	25(2)	18(2)	2(1)	2(1)	-1(1)
N(3)	15(2)	31(2)	24(2)	-9(2)	-1(1)	-1(1)
N(4)	18(2)	25(2)	25(2)	-3(1)	-2(2)	-3(1)
N(5)	24(2)	26(2)	43(2)	-5(2)	-3(2)	3(2)
C(1)	20(2)	26(2)	21(2)	-1(2)	-2(2)	-2(2)
C(2)	17(2)	26(2)	27(2)	-2(2)	1(2)	-3(2)
C(3)	21(2)	28(2)	25(2)	-1(2)	0(2)	-6(2)
C(4)	18(2)	25(2)	33(2)	-3(2)	2(2)	-2(2)
C(5)	22(2)	23(2)	31(2)	-2(2)	13(2)	-1(2)
C(6)	20(2)	22(2)	24(2)	0(2)	4(2)	0(2)
C(7)	17(2)	18(2)	27(2)	-3(2)	2(2)	-5(2)
C(8)	16(2)	40(2)	39(3)	-4(2)	0(2)	0(2)
C(9)	23(2)	51(3)	47(3)	-3(3)	-4(2)	-12(2)
C(10)	19(2)	75(4)	51(3)	-11(3)	4(2)	-1(2)
C(11)	21(2)	62(3)	66(4)	9(3)	-12(2)	4(2)
C(12)	22(2)	42(3)	26(3)	-8(2)	6(2)	-5(2)
C(13)	42(3)	52(3)	23(3)	-5(2)	6(2)	-3(2)
C(14)	32(3)	75(4)	33(3)	-19(3)	9(2)	-9(3)
C(15)	37(3)	46(3)	32(3)	-18(2)	2(2)	-1(2)
C(16)	16(2)	22(2)	25(2)	-1(2)	6(2)	-1(2)

C(17)	18(2)	25(2)	23(2)	-2(2)	0(2)	-2(2)
C(18)	18(2)	16(2)	25(2)	-1(2)	0(2)	2(2)
C(19)	12(2)	23(2)	28(2)	-3(2)	-4(2)	4(2)
C(20)	28(2)	24(2)	20(2)	-2(2)	-4(2)	-5(2)
C(21)	17(2)	29(2)	24(2)	2(2)	-3(2)	-2(2)
C(22)	17(2)	27(2)	24(2)	2(2)	4(2)	3(2)
C(23)	19(2)	32(2)	16(2)	-1(2)	-2(2)	-2(2)
C(24)	36(3)	33(2)	27(2)	8(2)	0(2)	0(2)
C(25)	34(3)	57(3)	22(2)	-8(2)	-2(2)	-6(2)
C(26)	34(3)	32(2)	20(2)	0(2)	6(2)	1(2)
C(27)	20(2)	48(3)	31(3)	1(2)	-4(2)	-14(2)
C(28)	33(3)	44(3)	79(4)	7(3)	-11(3)	-21(2)
C(29)	34(3)	163(7)	40(3)	-2(4)	7(3)	-56(4)
C(30)	20(3)	49(3)	75(4)	3(3)	-10(3)	-1(2)
C(31)	19(2)	41(2)	17(2)	-4(2)	2(2)	-8(2)
C(32)	15(2)	44(3)	18(2)	2(2)	-1(2)	-2(2)
C(33)	23(2)	68(3)	20(2)	1(2)	5(2)	-10(2)
C(34)	27(3)	89(4)	15(2)	-3(2)	3(2)	-5(3)
C(35)	30(3)	74(4)	18(2)	-7(2)	2(2)	-8(2)
C(36)	24(2)	53(3)	18(2)	-4(2)	4(2)	-11(2)
C(37)	26(2)	33(2)	28(3)	-9(2)	-2(2)	-2(2)
C(38)	23(2)	28(2)	28(2)	-6(2)	4(2)	-2(2)
C(39)	20(2)	30(2)	24(2)	-3(2)	-2(2)	2(2)
C(40)	20(2)	34(2)	28(2)	4(2)	3(2)	4(2)
C(41)	24(2)	39(2)	26(2)	-5(2)	5(2)	8(2)
C(42)	37(3)	38(3)	23(2)	-5(2)	8(2)	2(2)
C(43)	26(2)	35(3)	30(2)	-7(2)	-4(2)	3(2)
C(44)	14(2)	52(3)	28(2)	5(2)	6(2)	-3(2)
C(45)	24(3)	70(4)	34(3)	-2(3)	4(2)	0(2)
C(46)	23(2)	53(3)	40(3)	-3(2)	1(2)	-9(2)
C(47)	21(2)	71(4)	36(3)	0(2)	-2(2)	2(2)
C(48)	47(3)	40(3)	28(3)	-15(2)	15(2)	-7(2)
C(49)	66(4)	57(3)	22(3)	-4(2)	14(2)	-6(3)
C(50)	89(5)	51(4)	49(4)	-9(3)	28(3)	6(3)
C(51)	72(4)	104(5)	31(3)	-29(3)	20(3)	-31(4)

C(52)	19(2)	26(2)	32(3)	5(2)	4(2)	-4(2)
C(53)	21(2)	26(2)	26(2)	0(2)	1(2)	-5(2)
C(54)	27(2)	40(3)	27(2)	7(2)	0(2)	-11(2)
C(55)	36(3)	30(2)	25(2)	4(2)	-4(2)	-8(2)
C(56)	24(2)	38(3)	24(2)	-3(2)	-4(2)	-5(2)
C(57)	23(2)	22(2)	31(3)	8(2)	-3(2)	0(2)
C(58)	26(2)	17(2)	28(2)	2(2)	-1(2)	3(2)
C(59)	29(3)	55(3)	26(3)	1(2)	2(2)	-13(2)
C(60)	74(4)	53(3)	35(3)	9(3)	-5(3)	-20(3)
C(61)	39(3)	138(6)	36(3)	-25(4)	8(3)	-30(4)
C(62)	62(4)	44(3)	24(3)	-2(2)	-4(2)	-5(3)
C(63)	22(2)	49(3)	31(3)	-6(2)	-3(2)	-2(2)
C(64)	24(3)	103(5)	59(4)	-19(3)	-2(3)	-19(3)
C(65)	26(3)	44(3)	53(3)	-3(2)	8(2)	-13(2)
C(66)	33(3)	57(3)	52(3)	3(3)	-2(2)	17(3)
C(67)	24(2)	25(2)	31(2)	-8(2)	0(2)	-1(2)
C(68)	18(2)	27(2)	27(2)	-8(2)	-4(2)	-2(2)
C(69)	26(2)	32(2)	29(2)	-11(2)	0(2)	-6(2)
C(70)	18(2)	47(3)	46(3)	-19(2)	-1(2)	-9(2)
C(71)	29(3)	42(3)	40(3)	-14(2)	8(2)	-19(2)
C(72)	30(3)	41(3)	30(3)	-10(2)	5(2)	-15(2)
C(73)	31(3)	42(3)	61(4)	-4(3)	-5(3)	-5(2)
C(74)	45(3)	42(3)	166(8)	-32(4)	20(5)	10(3)

Table S8. Hydrogen coordinates ($x10^4$) and isotropic parameters ($Å^2x10^3$) for the μ-hydroxide non-tethered chromium salen complex.

	x	y	z	U(eq)
H(5)	8860(20)	1150(20)	6876(15)	26
H(1)	11184	1195	8430	27
H(3)	12465	1192	8106	30
H(5A)	13048	964	6415	30
H(9A)	13535	1890	8121	61
H(9B)	13696	2227	7494	61
H(9C)	14411	1941	7874	61
H(10A)	14260	750	6733	73
H(10B)	14862	1222	7076	73
H(10C)	14193	1543	6672	73
H(11A)	13707	677	8256	74
H(11B)	14576	701	7990	74
H(11C)	13937	208	7713	74
H(13A)	10987	1217	5248	59
H(13B)	11369	1741	5695	59
H(13C)	10625	1309	5892	59
H(14A)	12741	401	5614	70
H(14B)	12640	1184	5496	70
H(14C)	12206	656	5081	70
H(15A)	11619	-271	5976	58
H(15B)	11102	-3	5437	58
H(15C)	10787	72	6097	58
H(16)	7873	13	8144	25
H(20)	7087	-788	5862	29
H(22)	6835	-339	7570	27
H(24A)	8487	601	5466	48
H(24B)	9182	254	5106	48
H(24C)	9288	412	5792	48
H(25A)	7686	-341	5022	56
H(25B)	7885	-1099	5185	56
H(25C)	8459	-686	4763	56
H(26A)	9581	-931	5384	43

H(26B)	9032	-1366	5807	43
H(26C)	9562	-782	6075	43
H(28A)	6128	-1499	5972	79
H(28B)	5421	-1726	6390	79
H(28C)	6310	-1857	6586	79
H(29A)	5918	-1244	7534	118
H(29B)	5071	-1101	7258	118
H(29C)	5599	-495	7489	118
H(30A)	5708	-345	5927	72
H(30B)	5466	50	6511	72
H(30C)	4944	-563	6288	72
H(31)	9345	1366	8472	31
H(32)	9583	-35	8625	30
H(33A)	8326	-70	9044	44
H(33B)	8245	723	8976	44
H(34A)	8647	456	9950	52
H(34B)	9400	73	9698	52
H(35A)	9764	1149	10015	49
H(35B)	9128	1477	9584	49
H(36A)	10375	1551	9121	38
H(36B)	10513	765	9199	38
H(37)	9796	2855	8606	35
H(41)	6774	2518	9518	36
H(43)	9025	3093	9412	36
H(45A)	5347	1799	8694	64
H(45B)	5724	2434	9013	64
H(45C)	5927	1699	9241	64
H(46A)	6179	1029	8118	58
H(46B)	6775	951	8657	58
H(46C)	7093	1177	8025	58
H(47A)	5816	2180	7748	64
H(47B)	6726	2319	7627	64
H(47C)	6230	2822	8028	64
H(49A)	6904	2558	10485	72
H(49B)	7426	2857	11007	72
H(49C)	7757	2260	10613	72

H(50A)	6738	3612	9974	95
H(50B)	7468	4095	9854	95
H(50C)	7172	3970	10513	95
H(51A)	8953	3052	10421	103
H(51B)	8500	3581	10824	103
H(51C)	8773	3784	10175	103
H(52)	9970	2596	5924	31
H(54)	9516	2173	5045	38
H(56)	7267	1658	4824	34
H(60A)	7518	2256	3911	81
H(60B)	8186	2285	3417	81
H(60C)	8243	2756	3983	81
H(61A)	9457	1783	3565	106
H(61B)	9712	1479	4188	106
H(61C)	9607	2268	4113	106
H(62A)	7691	1037	4091	65
H(62B)	8551	734	4181	65
H(62C)	8300	1031	3555	65
H(64A)	5567	1526	5595	93
H(64B)	6259	1168	5239	93
H(64C)	6066	1938	5123	93
H(65A)	6963	1387	6728	62
H(65B)	6920	829	6225	62
H(65C)	6130	1130	6496	62
H(66A)	6715	2565	6504	71
H(66B)	5838	2382	6310	71
H(66C)	6395	2792	5873	71
H(67)	9976	3403	7079	32
H(68)	10504	2124	7480	29
H(69A)	10734	3369	8079	35
H(69B)	11036	2658	8307	35
H(70A)	11916	2576	7513	45
H(70B)	12070	3271	7843	45
H(71A)	11294	3839	7129	45
H(71B)	12005	3460	6812	45
H(72A)	10835	3258	6279	40

H(72B)	11139	2567	6553	40
H(74A)	7494	4598	7329	127
H(74B)	7945	4556	7945	127
H(74C)	7099	4218	7873	127

VIII. References

[1] Morris, L. S.; Childers, M. I.; Coates, G. W., Bimetallic Chromium Catalysts with Chain Transfer Agents: A Route to Isotactic Poly(propylene oxide)s with Narrow Dispersities. *Angew. Chem. Int. Ed.* **2018**, *57*, 5731–5734.

[2] Konsler, R. G.; Karl, J.; Jacobsen, E. N., Cooperative Asymmetric Catalysis with Dimeric Salen Complexes. *J. Am. Chem. Soc.* **1998**, *120*, 10780–10781.

[3] DiCiccio, A. M.; Longo, J. M.; Coates, G. W., Development of Highly Active and Regioselective Catalysts for the Copolymerization of Epoxides with Cyclic Anhydrides: An Unanticipated Effect of Electronic Variation. *J. Am. Chem. Soc.* **2016**, *138*, 7107–7113.

[4] Martinez, L. E.; Leighton, J. L.; Carsten, D. H.; Jacobsen, E. N., Highly Enantioselective Ring Opening of Epoxides Catalyzed by (salen)Cr(III) Complexes. *J. Am. Chem. Soc.* **1995**, *117*, 5897–5898.

[5] Connelly, N. G.; Damhus, T.; Hartshorn, R. M.; Hutton, A.T. *Nomenclature of Inorganic Chemistry IUPAC Recommendations 2005*; the Royal Society of Chemistry: Cambridge, U.K., 2005; pp 80 – 81.

[6] Ford, D. D.; Nielsen, L. P. C.; Zuend, S. J.; Musgrave, C. B.; Jacobsen, E. N., Mechanistic Basis for High Stereoselectivity and Broad Substrate Scope in the (salen)Co(III)-Catalyzed Hydrolytic Kinetic Resolution. *J. Am. Chem. Soc.* **2013**, *135*, 15595–15608.

[7] Becke, A. D., Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648–5652

[8] Rassolov, V. A.; Pople, J. A.; Ratner, M. A.; Windus, T.L.; 6-31G* basis set for atoms K through Zn. *J. Chem. Phys.,* **1998,** *109*, 1223–1229.

[9] Childers, M. I.; Vitek, A. K.; Morris, L. S.; Widger, P. C. B.; Ahmed, S. M.; Zimmerman, P. M.; Coates, G. W., Isospecific, Chain Shuttling Polymerization of Propylene Oxide Using a Bimetallic Chromium Catalyst: A New Route to Semicrystalline Polyols. *J. Am. Chem. Soc.* **2017**, *139*, 11048–11054.

[10] Weingend, F.; Ahlrichs, R., Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.,* **2005**, *7*, 3297–3305.

[11] Neese, F., Software update: the ORCA program system, version 4.0. *Comp. Mol. Sci.,* **2017**, *8*, 1327.

[12] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H., A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys*., **2010**, *132*, 154104.

[13] Marenich, A. V.; Cramer, C .J.; Truhlar, D. G., Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B*, **2009**, *113*, 6378–6396.

[14] Zimmerman, P. M., Growing string method with interpolation and optimization in internal coordinates: Method and examples. *J. Chem. Phys.,* **2013**, *138*, 184102.

[15] Zimmerman, P. M., Single-ended transition state finding with the growing string method. *J. Comp. Chem.,* **2015,** *36*, 601–611.

[16] Zimmerman, P. M., Reliable Transition State Searches Integrated with the Growing String Method. *J. Chem. Theory and Comp.*, **2013,** *9*, 3043–3050.

[17] Schuchardt, K. L., Didier, B. T., Elsethagen, T., Sun, L., Gurumoorthi, V., Chase, J., Li, J., Windus, T.L., Basis set exchange: a community database for computational sciences. *J. Chem. Inf. Model.* **2007**, *47*, 1045–1052.
[18] Sheldrick, G. M., *SHELXL-97, A program for crystal structure refinement*. Göttingen, 1997
[19] Sheldrick, G. M., A short history of SHELX. *Acta Crystallographica Section A* **2008,** *64*, 112-122.
[20] Muller, P., Practical suggestions for better crystal structures AU. *Crystallography Reviews* **2009,** *15*, 57-83.
[21] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H., OLEX2: a complete structure solution, refinement and analysis program. *Journal of Applied Crystallography* **2009,** *42*, 339-341