Unravelling the chain growth mechanism in Cr/NNN-catalysed ethylene oligomerization

Jiale Peng, Mengyu Zhu, Long Chen and Zhen Liu*

School of Chemical Engineering, East China University of Science and Technology, Shanghai 200237, China

*Corresponding author:

Zhen Liu, Email: liuzhen@ecust.edu.cn

S1. Determination of the ground spin state

Table S1. Free energies (kcal mol^{-1}) of all intermediates and transition states via Cossee-Arlman mechanism under possible spin states.

	triplet	quintet
1A[a]	31.6	0.0
2A	10.4	0.9
TS[2A-3A]	12.4	6.1
3A	12.1	-14.2
4A	-6.9	-14.0
TS[4A-5A]	3.1	1.3
5A	0.0	-28.8
TS[5A-12A]	-3.9	-9.8
6A	-24.7	-29.0
TS[6A-7A]	-10.7	-11.9
7A	-30.8	-40.8
TS[7A-13A]	-16.9	-23.5
8A	-32.7	-40.6
TS[8A-9A]	-24.4	-24.9
9A	-43.6	-53.5
TS[9A-14A]	-30.0	-35.4
10A	-45.8	-52.7
TS[10A-11A]	-36.1	-36.1
11A	-37.9	-65.4

[a] Quintet 1A was chosen as the energy reference.

Table S2. Free energies (kcal mol^{-1}) of all intermediates and transition states via metallacycle mechanism under possible spin states.

	quartet	sextet[c]
1B[a]	0.0	4.1
2B	-8.9	-7.2
3B	-12.3	-3.7
TS[3B-4B]	0.1	—[b]
4B	-13.5	8.8
5B	-14.3	13.8
TS[5B-6B]	8.8	—[b]
6B	-24.7	0.1
TS[6B-11B]	-7.5	9.7
7B	-22.6	—[b]
TS[7B-8B]	0.4	—[b]
8B	-32.8	-0.3
TS[8B-12B]	-18.1	0.1
9B	-31.9	-13.7
TS[9B-10B]	-11.5	—[b]
10B	-48.6	-24.5
11B	-40.5	-37.4
12B	-51.9	-50.2

[a] Quartet 1B was chosen as the energy reference.

[b] Not successfully located.

[C] The intermediates and transition states under the sextet are energetically disfavoured and most of the chromacycle species can not maintain cyclic structure.

S2. *The formation of Cr-butyl species and comparation of two possible chain termination processes*

As illustrated in Figure S1, coordination and insertion of two molecule ethylene monomers to generate a Cr-butyl specie was exoergic by 28.8 kcal mol^{-1}. It is necessary to consider the two potential termination routes (β-H elimination versus β-H transfer) to decide which one can occur. Figure S2 shows these two possibilities and the activation barrier of β-H transfer route via **^{5}TS[6A-16A]** was calculated to be 0.7 kcal mol^{-1}. Due to the relatively high energy barrier (10.7 kcal mol^{-1}) compared to β-H elimination, the β-H transfer route can be immediately ruled out. It is notable that the original β-H elimination to give a Cr-hydride (**^{5}5A → ^{5}12A**) was endergonic by 10.5 kcal mol^{-1}, which means this reaction is not spontaneous and will return to Cr-butyl in the absence of ethylene. Similar results have been observed in all calculations towards Cossee-Arlman mechanism involving β-H elimination step.[1-4] Aiming at this phenomenon, a supplemental route was first proposed by McGuinness and co-workers.[1] Once the β-H elimination is achieved, the chromium centre tends to capture an incoming monomer to form a more stable Cr-ethyl species due to the relative low energy barrier of ethylene insertion. This process was also considered in this work and was found to do not impact the overall selectivity.

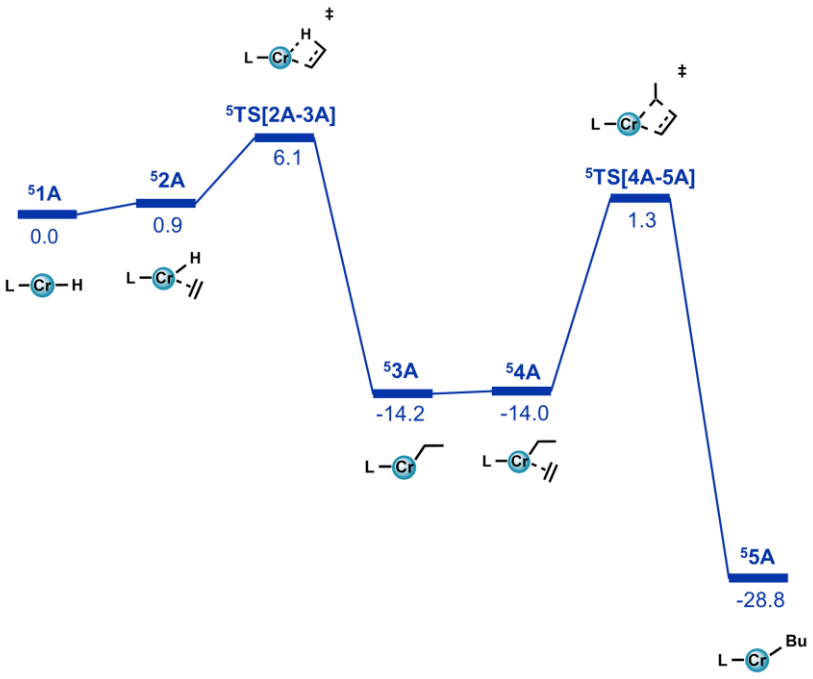


Figure S1. Calculated free energy diagrams for the formation of Cr-butyl species. The relative Gibbs free energies calculated at the M06L-D3/def2-TZVP//B3LYP-D3/def2-SVP level are given in kcal mol^{-1}. The superscript numbers in the diagrams refer to the spin multiplicity.

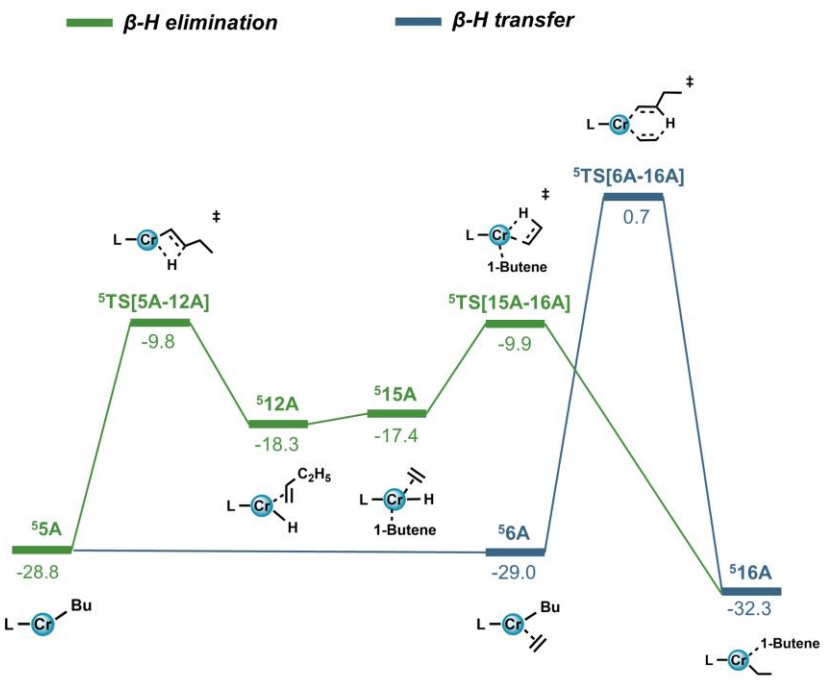


Figure S2. Calculated free energy diagrams for chain termination via stepwise β-H elimination (green line) and concerted β-H transfer (gray line). The relative Gibbs free energies calculated at the M06L-D3/def2-TZVP//B3LYP-D3/def2-SVP level are given in kcal mol^{-1}. The superscript numbers in the diagrams refer to the spin multiplicity.

S3. *The formation of metallacyclopentane*

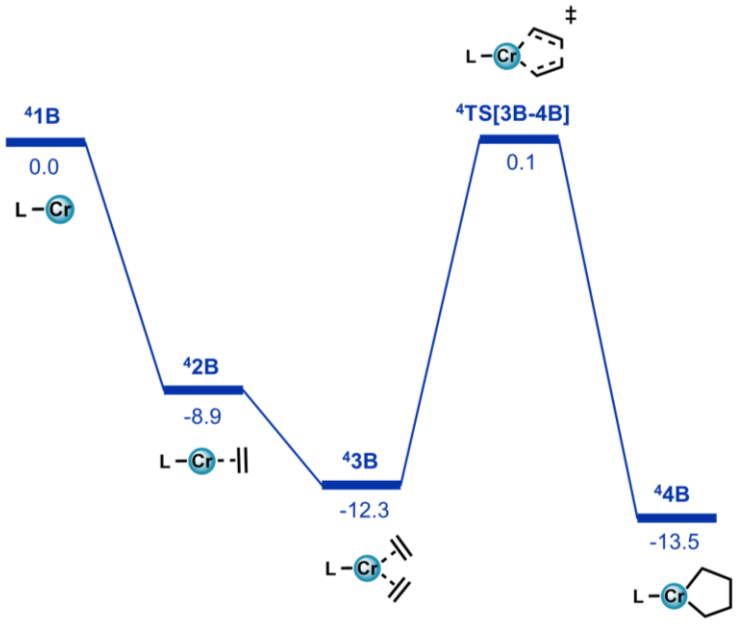


Figure S3. Calculated free energy diagrams for the formation of metallacyclopentane. The relative Gibbs free energies calculated at the M06L-D3/def2-TZVP//B3LYP-D3/def2-SVP level are given in kcal mol^{-1}. The superscript numbers in the diagrams refer to the spin multiplicity.

S4. Conformational searching

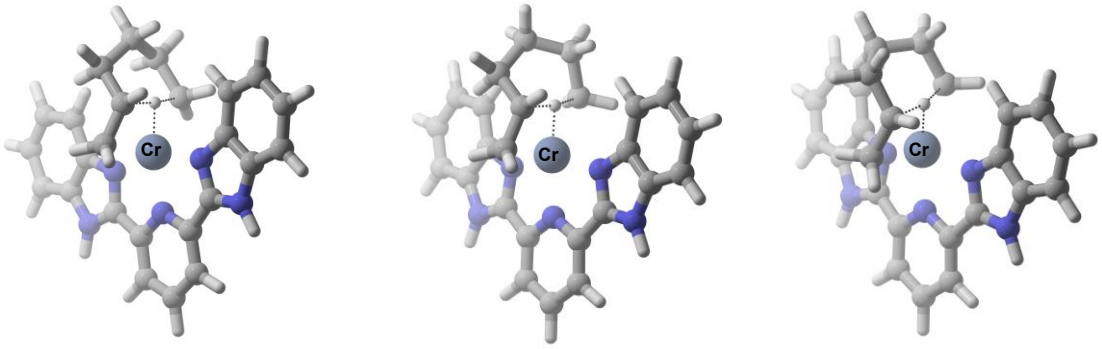
Various conformers exist for the key intermediate due to the flexibility of alkyl groups. The capture of lowest conformer is critical for the establishment of decisive free energy surface.[5] As for 3,7-H shift structure **^{4}TS[6B-11B]**, conformational searching furnished three unique conformers which were called chair conformation, half-chair conformation, and boat conformation (Figure S4). Among them, chair form was found to be most stable. The results of conformational searching along the Cossee-Arlman route and metallacycle route are listed in Table S3 and Table S4, respectively.

Table S3. Various conformers of key intermediates and transition states for Cr/NNN-catalysed ethylene oligomerization via a Cossee-Arlman mechanism.

Structure	Number of conformers
^{5}5A	43
^{5}6A	46
^{5}7A	616
^{5}8A	173
^{5}9A	622
^{5}10A	1230
^{5}TS[6A-7A]	62
^{5}TS[5A-12A]	6
^{5}TS[8A-9A]	277
^{5}TS[7A-13A]	30
^{5}TS[10A-11A]	799
^{5}TS[9A-14A]	215
^{5}TS[6A-16A]	198
^{5}TS[15A-16A]	7

Table S4. Various conformers of key intermediates and transition states for Cr/NNN-catalysed ethylene oligomerization via a metallacycle mechanism.

Structure	Number of conformers
^{4}6B	11
^{4}7B	14
^{4}8B	67
^{4}9B	72
^{4}10B	187
^{4}TS[7B-8B]	18
^{4}TS[6B-11B]	3
^{4}TS[9B-10B]	58
^{4}TS[8B-12B]	10



Chair form

-11.5 kcal mol^{-1}

Half-chair form

-8.8 kcal mol^{-1}

Boat form

-7.4 kcal mol^{-1}

Figure S4. Three unique conformers for the 3,7-H shift structure.

S5. *Lowest energy conformers of key intermediates and transition states along the catalytic cycle*

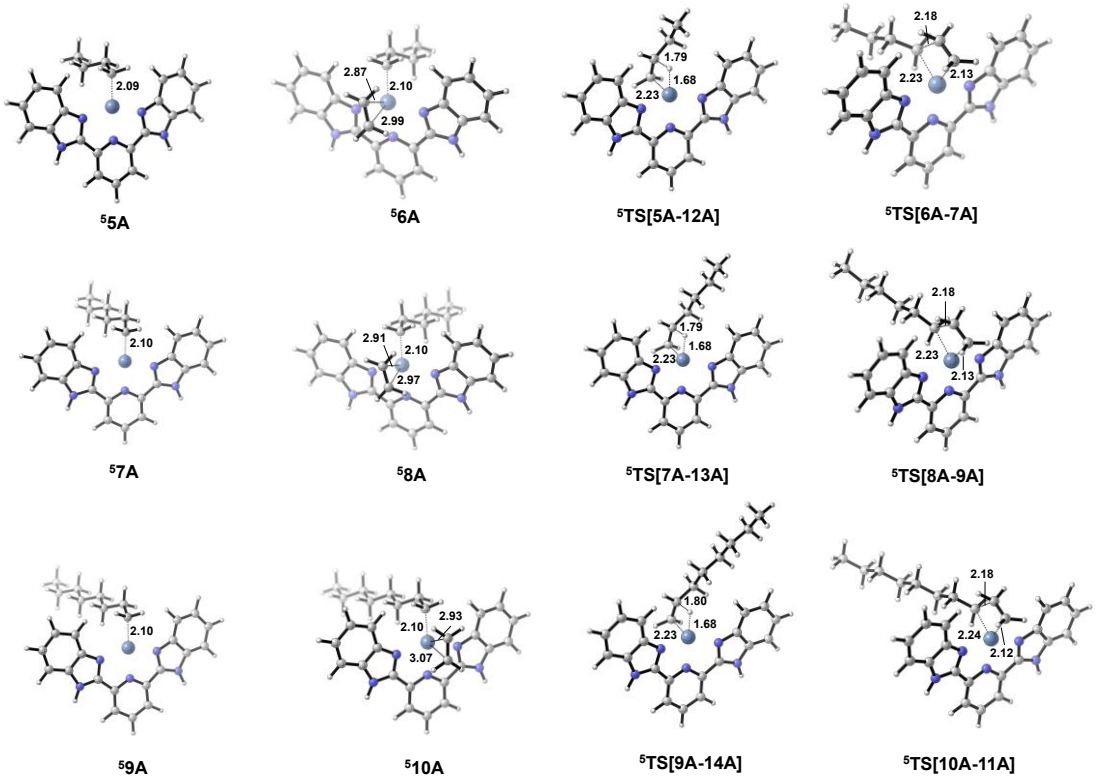


Figure S5. Lowest energy conformers of key intermediates and transition states for the catalytic cycle involving a Cossee-Arlman mechanism.

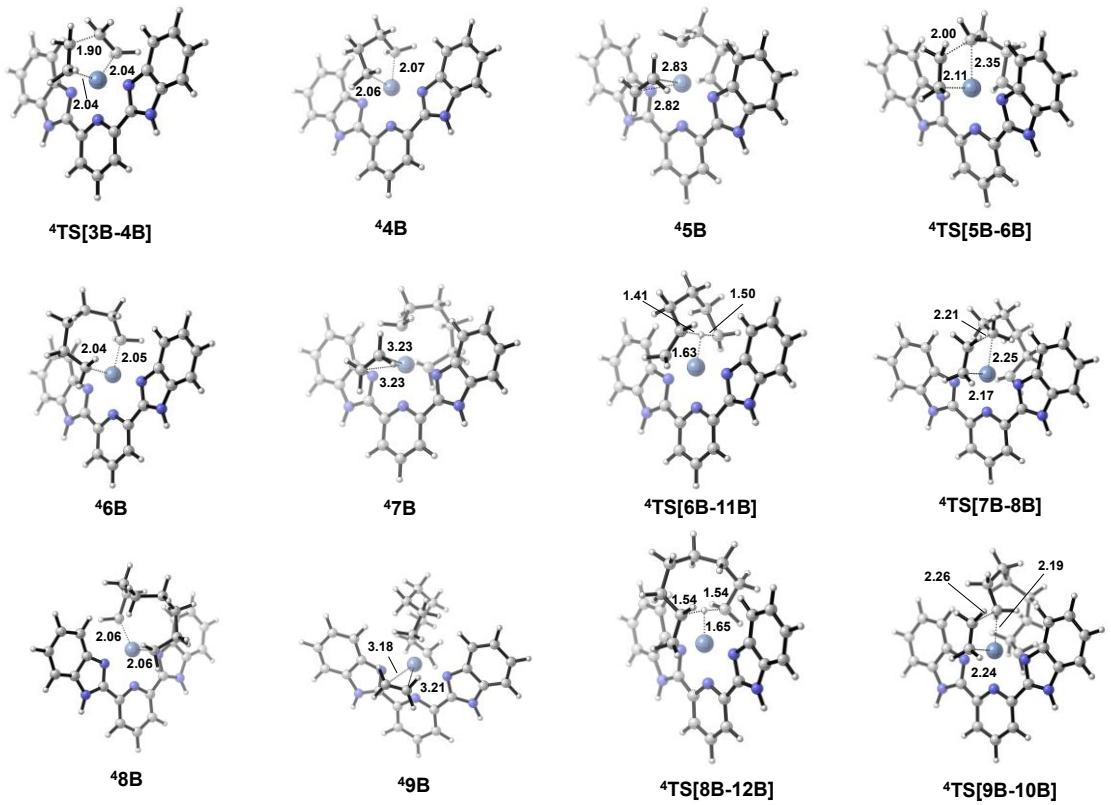


Figure S6. Lowest energy conformers of key intermediates and transition states for the catalytic cycle involving a metallacycle mechanism.

S6. *Kinetic Isotope Effect on the 3,7-H shift process*

Isotope effect on the 3,7-H shift process of Cr/NNN system was further examined and DFT calculation results (Figure S7) revealed a relatively small KIE value (1.9) compared to β-H elimination step (4.4). It is reasonable to speculate that two types of hydrogen transform mode will lead to different KIE. The presence of KIE causes a deviation of isotopic products distribution from the ideal. However, no matter how large the kinetic isotope effect is, metallacycle routes always deliver even-numbered isotopomers since concerted H-shift process occurs inside the chromacycle.

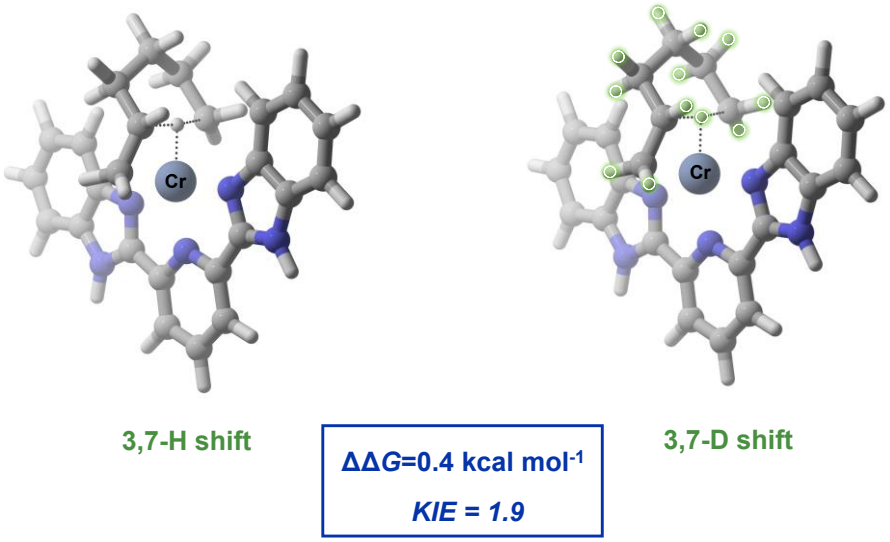


Figure S7. KIE on the 3,7-H shift process of metallacycle mechanism.

S7. *The formation of isotopic metallacycloheptane via a metallacycle mechanism and theoretical distribution of 1-hexene*

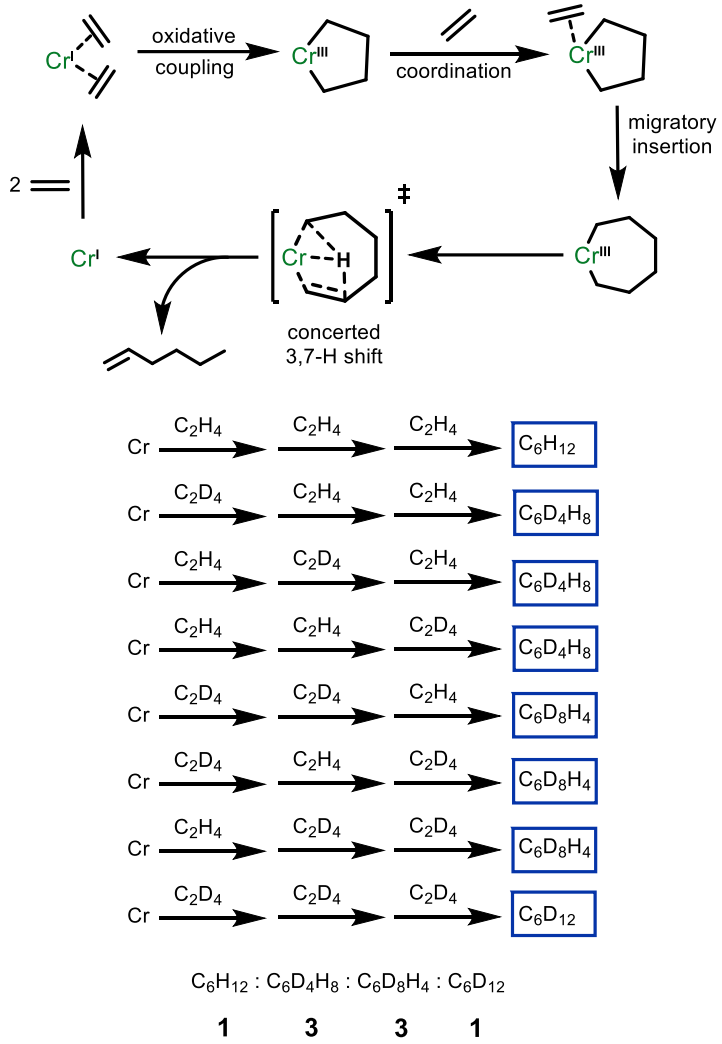


Figure S8. Proposed metallacycle mechanism for 1-hexene formation (top) and expected isotopomers distribution from a 1:1 C_2D_4 / C_2H_4 mixture with negligible KIE (bottom).

S8. *Expected isotopomeric 1-hexene via a Cossee-Arlman mechanism in this case*

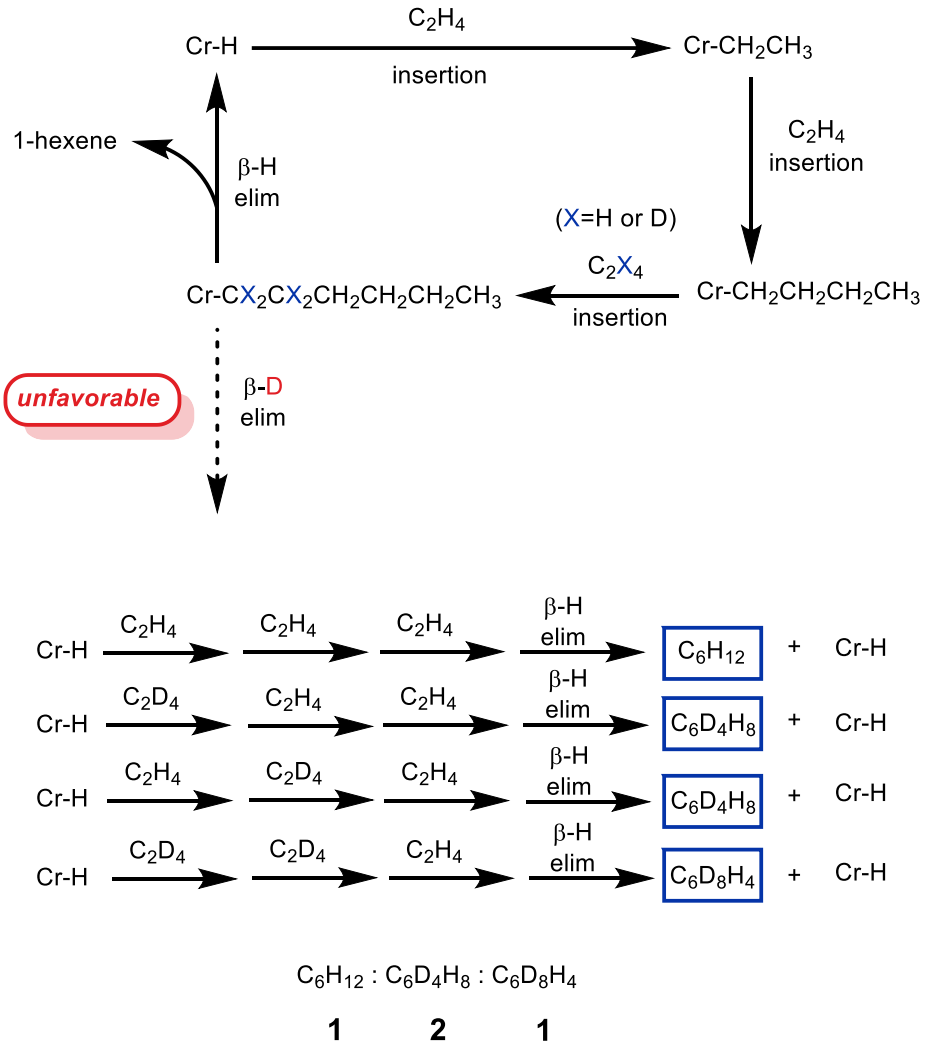


Figure S9. Proposed Cossee-Arlman mechanism for 1-hexene formation (top) and expected isotopomers distribution from a 1:1 C_2D_4 / C_2H_4 mixture when KIE is considered (bottom).

S9. *Explanation of the gas chromatography data in Cr/NNN system*

As for 1-C_{10} products, metallacycle mechanism with negligible KIE is supposed to form isotopic $C_{10}D_{20}$, $C_{10}D_{16}H_4$, $C_{10}D_{12}H_8$, $C_{10}D_8H_{12}$, $C_{10}D_4H_{16}$, $C_{10}H_{20}$ products in a ratio of 1:5:10:10:5:1. And this distribution will transform to a ratio of 2:7:9:5:1 of $C_{10}D_{16}H_4$, $C_{10}D_{12}H_8$, $C_{10}D_8H_{12}$, $C_{10}D_4H_{16}$, $C_{10}H_{20}$ when KIE is included. It can be seen that Cossee-type isotopomers distribution are quite similar to metallacycle routes when KIE is both considered in these two proposals. However, the $C_{10}D_{16}H_4$, $C_{10}D_{12}H_8$, $C_{10}D_8H_{12}$, $C_{10}D_4H_{16}$, $C_{10}H_{20}$ products delivered by a Cossee-Arlman mechanism (KIE included) in a ratio of 1:4:6:4:1 (Figure S10) are in great agreement of original data in the literature.[6] In addition, the peaks of isotopic 1-C_{12} and 1-C_{14} from an oligomerization of 1:1 C_2H_4 / C_2D_4 also give a best fit to the Cossee-Arlman mechanism when an isotope effect was considered (Figure S11).

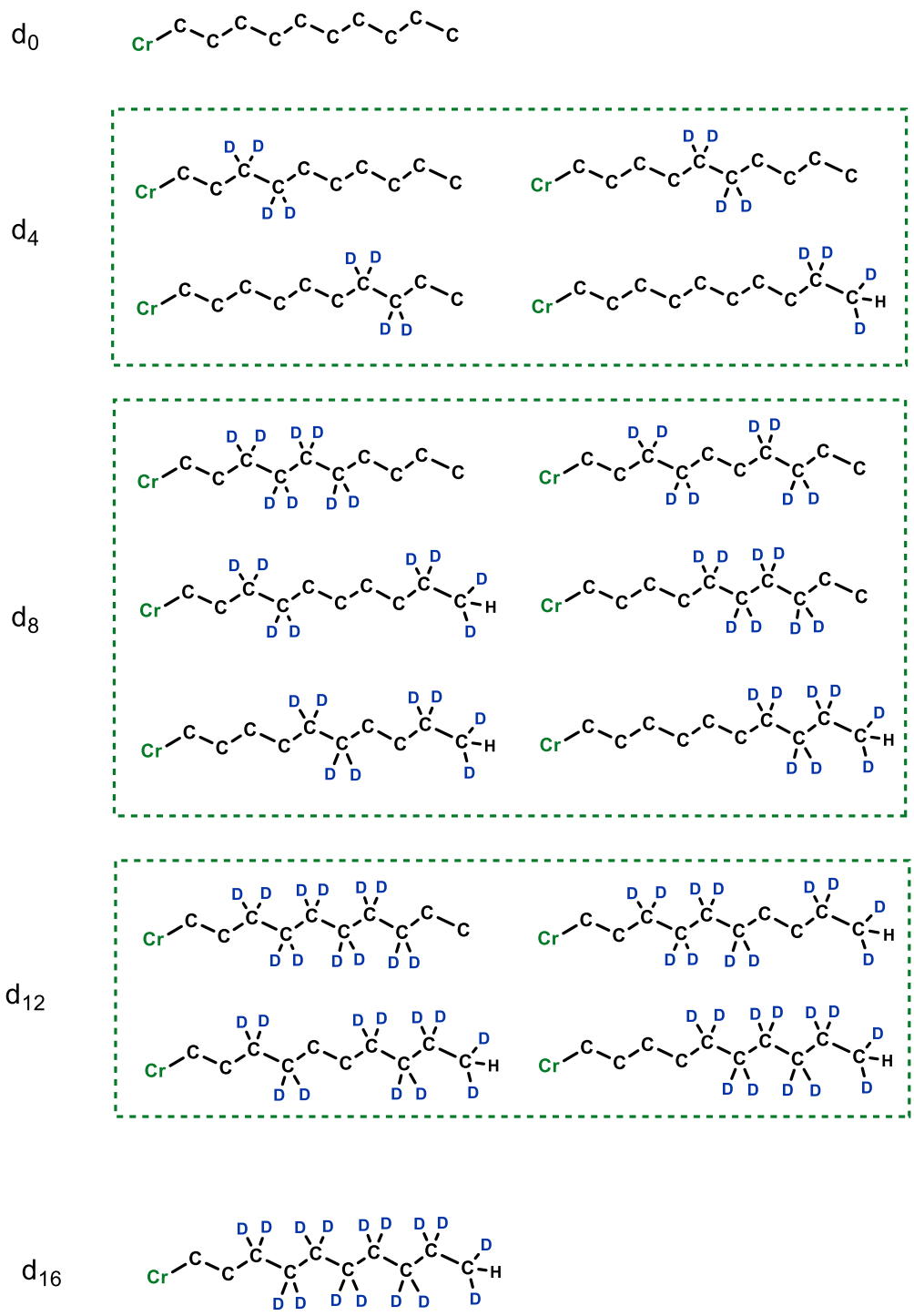


Figure S10. All expected isotopomers of 1-C_{10} and their statistical distribution for a Cossee-Arlman mechanism when KIE is considered.

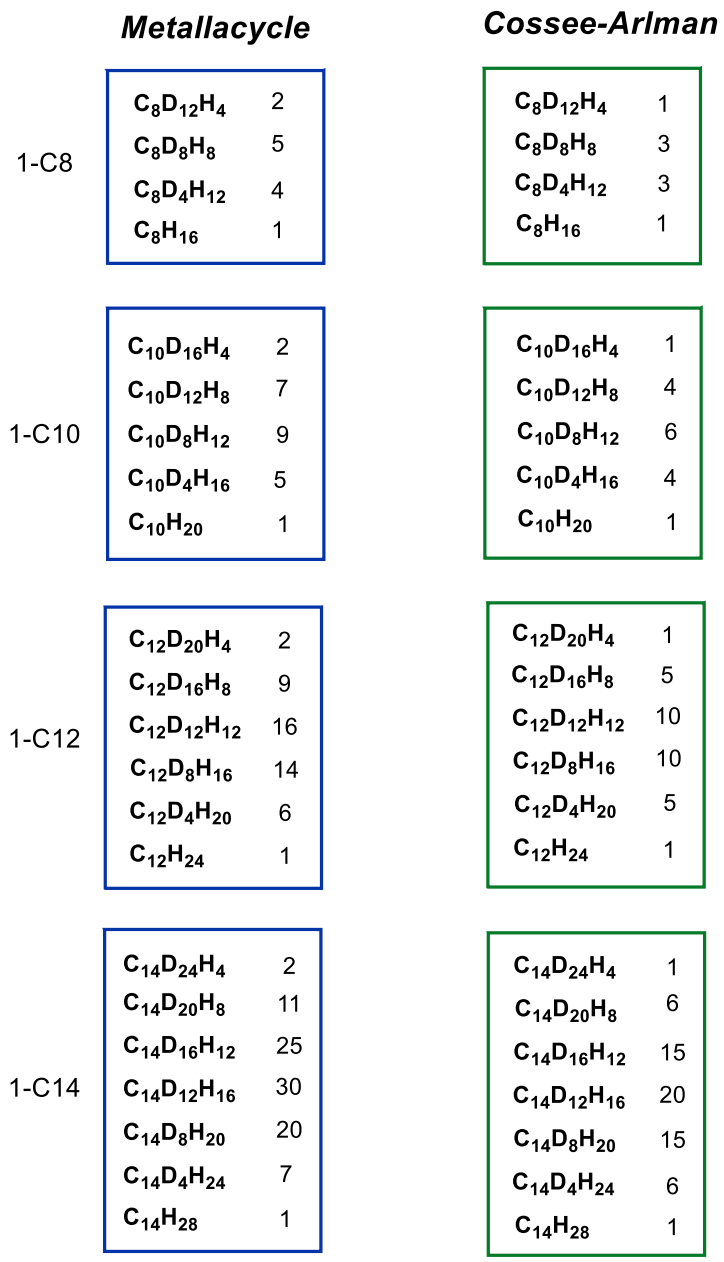


Figure S11. All expected isotopomers of 1-C_8, 1-C_{10}, 1-C_{12}, 1-C_{14} and their statistical distribution for a metallacycle mechanism (left) and a Cossee-Arlman mechanism (right) involving strong KIE.

References

1. R. Robinson, D. S. Mcguinness and B. F. Yates, *ACS Catal.*, 2013, **3**, 3006-3015.
2. V. Tognetti, A. Buchard, A. Auffrant, I. Ciofini, P. Le Floch and C. Adamo, *J. Mol. Model.*, 2013, **19**, 2107-2118.
3. J. Zhang, P. Qiu, Z. Liu, B. Liu, R. J. Batrice, M. Botoshansky and M. S. Eisen, *ACS Catal.*, 2015, **5**, 3562-3574.
4. L. Liu, Z. Liu, R. Cheng, X. He and B. Liu, *Organometallics*, 2021, **40**, 1682-1691.
5. J. N. Harvey, F. Himo, F. Maseras and L. Perrin, *ACS Catal.*, 2019, **9**, 6803-6813.
6. A. K. Tomov, J. J. Chirinos, D. J. Jones, R. J. Long and V. C. Gibson, *J. Am. Chem. Soc.*, 2005, **127**, 10166-10167.

S9. *List of Cartesian Coordinates*

^{3}1A
Geometry with 39 atoms:
Total energy: -2049.813599870

C	-4.865876	-2.726193	-0.000117
C	-3.521136	-2.364557	-0.000227
C	-3.225042	-0.994813	-0.000016
C	-4.263304	-0.029317	0.000272
C	-5.613694	-0.391302	0.000400
C	-5.893937	-1.756851	0.000199
H	-5.135441	-3.784755	-0.000243
H	-2.719378	-3.105120	-0.000482
H	-6.408744	0.356655	0.000628
H	-6.935459	-2.086178	0.000317
N	-3.627631	1.204147	0.000476
H	-4.082058	2.111716	0.000789
N	-2.010273	-0.325760	0.000033
C	-2.289533	0.991331	0.000107
C	1.184853	1.928915	-0.000061
C	1.214161	3.322090	-0.000312
C	0.000004	4.027192	-0.000434
C	-1.214153	3.322102	-0.000314
C	-1.184858	1.928922	-0.000062
N	-0.000003	1.242653	0.000031
H	0.000010	5.118104	-0.000490
H	2.167045	3.855259	-0.000370
H	-2.167034	3.855276	-0.000374
C	2.289526	0.991316	0.000113
C	3.521150	-2.364560	-0.000235
C	4.865893	-2.726186	-0.000129
C	5.893948	-1.756837	0.000192
C	5.613696	-0.391290	0.000403
C	4.263303	-0.029316	0.000278
C	3.225046	-0.994818	-0.000014
H	2.719398	-3.105128	-0.000496
H	5.135466	-3.784746	-0.000265
H	6.935472	-2.086157	0.000304
H	6.408740	0.356673	0.000635
N	3.627620	1.204143	0.000491
H	4.082041	2.111715	0.000810
N	2.010273	-0.325774	0.000041
Cr	-0.000011	-0.762973	-0.000315
H	0.000009	-2.412797	-0.000964

^{3}2A
Geometry with 45 atoms:
Total energy: -2128.397355920

C	-4.908137	-2.589245	-0.334534
C	-3.561042	-2.244344	-0.312241
C	-3.250858	-0.878962	-0.222687
C	-4.278991	0.097011	-0.164341
C	-5.634444	-0.249764	-0.188632
C	-5.926786	-1.608811	-0.273011
H	-5.191190	-3.641963	-0.404367
H	-2.766064	-2.989736	-0.368123
H	-6.422394	0.504333	-0.144686
H	-6.971432	-1.927479	-0.294655
N	-3.626816	1.317306	-0.087709
H	-4.069005	2.229625	-0.037942
N	-2.030724	-0.231103	-0.176125
C	-2.291476	1.079200	-0.099886
C	1.176016	2.017167	-0.037905
C	1.213426	3.413824	0.000640
C	-0.000006	4.112670	0.027816
C	-1.213428	3.413804	0.000580
C	-1.175996	2.017146	-0.037959
N	0.000013	1.349109	-0.032590
H	-0.000016	5.203647	0.060101
H	2.165875	3.946857	0.003112
H	-2.165883	3.946826	0.003004
C	2.291502	1.079234	-0.099800
C	3.560994	-2.244347	-0.312153
C	4.908081	-2.589273	-0.334509
C	5.926751	-1.608856	-0.273057
C	5.634439	-0.249802	-0.188686
C	4.278993	0.096999	-0.164332
C	3.250842	-0.878958	-0.222612
H	2.765987	-2.989711	-0.367980
H	5.191110	-3.641998	-0.404339
H	6.971390	-1.927544	-0.294753
H	6.422406	0.504280	-0.144793
N	3.626846	1.317312	-0.087688
H	4.069055	2.229623	-0.037976
N	2.030724	-0.231068	-0.176002
Cr	0.000096	-0.699449	-0.137729
H	0.000803	-2.220919	-0.729001
C	-0.000212	-1.914773	1.610565
H	0.922824	-2.501838	1.613015
H	-0.923427	-2.501565	1.612684
C	-0.000086	-0.584121	2.033516
H	-0.924832	-0.100549	2.361051
H	0.924725	-0.100828	2.361280

^{3}TS[2A-3A]
Geometry with 45 atoms:
Total energy: -2128.392994380

C	4.904634	-2.568444	-0.347965
C	3.557232	-2.217678	-0.326442
C	3.247921	-0.853767	-0.226640
C	4.279414	0.117822	-0.157738
C	5.632795	-0.233070	-0.181135
C	5.924472	-1.592949	-0.275668
H	5.183287	-3.621870	-0.424889

H	2.764906	-2.965383	-0.390864
H	6.422067	0.519209	-0.128953
H	6.968689	-1.913005	-0.296236
N	3.632551	1.341178	-0.072766
H	4.078344	2.251038	-0.016516
N	2.028409	-0.200366	-0.177758
C	2.294679	1.112721	-0.090806
C	-1.183108	2.041847	-0.022447
C	-1.213335	3.432978	0.059728
C	0.000006	4.136953	0.104468
C	1.213341	3.432979	0.059791
C	1.183118	2.041842	-0.022388
N	0.000003	1.357279	-0.051008
H	0.000005	5.225945	0.169244
H	-2.167097	3.963844	0.084563
H	2.167104	3.963841	0.084676
C	-2.294674	1.112724	-0.090900
C	-3.557229	-2.217674	-0.326479
C	-4.904631	-2.568441	-0.347929
C	-5.924469	-1.592947	-0.275592
C	-5.632789	-0.233067	-0.181087
C	-4.279408	0.117827	-0.157762
C	-3.247917	-0.853760	-0.226707
H	-2.764903	-2.965376	-0.390928
H	-5.183287	-3.621869	-0.424823
H	-6.968685	-1.913005	-0.296100
H	-6.422061	0.519210	-0.128870
N	-3.632542	1.341183	-0.072812
H	-4.078334	2.251041	-0.016527
N	-2.028405	-0.200358	-0.177878
Cr	0.000005	-0.637322	-0.144368
C	-0.000068	-0.918678	1.986382
H	0.927592	-0.481978	2.366075
H	-0.927799	-0.482088	2.366029
C	0.000012	-2.207980	1.441236
H	-0.000142	-2.243152	-0.428725
H	-0.919843	-2.799315	1.419858
H	0.919944	-2.799197	1.419851

^{3}3A
Geometry with 45 atoms:
Total energy: -2128.406344480

C	-5.011496	-2.380973	-0.053899
C	-3.656115	-2.072632	-0.093151
C	-3.302198	-0.713987	-0.060417
C	-4.305882	0.286728	0.016650
C	-5.670252	-0.022218	0.055494
C	-6.002348	-1.373481	0.017137
H	-5.322509	-3.427780	-0.077624
H	-2.891137	-2.847257	-0.142812
H	-6.434447	0.755053	0.113508
H	-7.054911	-1.664489	0.045202
N	-3.623831	1.490245	0.044958
H	-4.043611	2.412943	0.097509
N	-2.062908	-0.096423	-0.078858
C	-2.295778	1.219875	-0.013332
C	1.174845	2.156905	0.017023
C	1.215635	3.552639	0.105219
C	0.000680	4.247823	0.146541
C	-1.214446	3.552942	0.105443
C	-1.173998	2.157200	0.017216
N	0.000341	1.499125	-0.027617
H	0.000822	5.337226	0.216657
H	2.166400	4.087198	0.144787
H	-2.165096	4.087702	0.145198
C	2.296434	1.219326	-0.013566
C	3.656236	-2.073411	-0.092648
C	5.011565	-2.381972	-0.053293
C	6.002585	-1.374627	0.017485
C	5.670715	-0.023299	0.055504
C	4.306399	0.285867	0.016561
C	3.302547	-0.714695	-0.060306
H	2.891138	-2.847950	-0.142075
H	5.322400	-3.428838	-0.076707
H	7.055097	-1.665811	0.045648
H	6.435032	0.753864	0.113351
N	3.624541	1.489496	0.044653
H	4.044465	2.412138	0.097044
N	2.063364	-0.096959	-0.078876
Cr	0.000070	-0.591623	-0.254765
C	-0.001032	-2.660079	-0.388370
H	-0.878664	-2.968570	-0.991675
H	0.878335	-2.970241	-0.988226
C	-0.004186	-3.395824	0.957245
H	-0.005236	-4.499134	0.857587
H	-0.890058	-3.138086	1.566561
H	0.880292	-3.140029	1.569405

^{3}4A
Geometry with 51 atoms:
Total energy: -2206.984166580

C	-5.011003	-2.393998	0.021518
C	-3.655266	-2.078036	0.011783
C	-3.305955	-0.719880	-0.035422
C	-4.315093	0.277565	-0.068332
C	-5.677572	-0.037855	-0.059679
C	-6.005842	-1.391215	-0.014385
H	-5.315803	-3.442275	0.058728
H	-2.888184	-2.851821	0.039921
H	-6.446005	0.737109	-0.084562
H	-7.058084	-1.684441	-0.004732
N	-3.640547	1.486265	-0.100789
H	-4.065452	2.407548	-0.118060
N	-2.069279	-0.094401	-0.047978
C	-2.307807	1.225631	-0.083594
C	1.170479	2.152903	-0.062241
C	1.201046	3.546852	-0.127344
C	-0.011235	4.249852	-0.159828

C	-1.221533	3.542571	-0.145835
C	-1.187364	2.148918	-0.079631
N	-0.007804	1.468172	-0.009949
H	-0.012782	5.339703	-0.210503
H	2.153920	4.079181	-0.161891
H	-2.175652	4.071393	-0.195481
C	2.293624	1.233137	-0.054543
C	3.651649	-2.066789	0.030441
C	5.008406	-2.378634	0.027156
C	5.999904	-1.372809	-0.014563
C	5.667182	-0.020321	-0.052859
C	4.303740	0.290934	-0.049048
C	3.297902	-0.709601	-0.010287
H	2.887141	-2.842809	0.062545
H	5.316644	-3.426100	0.058031
H	7.053062	-1.662878	-0.015912
H	6.432964	0.757072	-0.083156
N	3.625430	1.497559	-0.077046
H	4.047641	2.419944	-0.100432
N	2.059092	-0.087945	-0.016455
Cr	-0.001895	-0.576333	0.020415
C	0.024930	-2.460059	-0.817211
H	-0.899305	-3.034673	-0.669291
H	0.883606	-3.092774	-0.557243
C	0.129725	-1.815367	-2.191274
H	1.073087	-2.040292	-2.712933
H	-0.721929	-2.037520	-2.853244
C	-0.021907	-1.689582	1.961203
H	-0.947225	-2.272189	1.951117
H	0.906808	-2.266482	1.974911
C	-0.029620	-0.347141	2.297847
H	0.894766	0.173368	2.562785
H	-0.962119	0.169035	2.541670
H	0.129767	-0.678103	-2.149942

^{3}TS[4A-5A]

Geometry with 51 atoms:

Total energy: -2206.968771500

C	-4.965138	-2.323744	-0.055370
C	-3.608218	-1.999969	-0.061358
C	-3.260301	-0.642055	-0.020412
C	-4.274707	0.350669	0.014040
C	-5.634020	0.028720	0.020405
C	-5.961686	-1.327297	-0.013176
H	-5.264019	-3.374030	-0.085028
H	-2.846020	-2.777891	-0.100713
H	-6.404233	0.801941	0.048441
H	-7.013331	-1.622567	-0.008757
N	-3.608980	1.565525	0.032963
H	-4.039989	2.483366	0.053620
N	-2.025943	-0.007209	-0.017951
C	-2.271914	1.318157	0.011450
C	1.226941	2.198713	-0.063653
C	1.262358	3.589256	-0.077181
C	0.056790	4.313135	-0.042312
C	-1.162829	3.615945	-0.002144
C	-1.155341	2.224334	0.004635
N	0.029664	1.513262	-0.018214
H	0.068609	5.403625	-0.050330
H	2.220346	4.112676	-0.115512
H	-2.111264	4.158194	0.017161
C	2.327725	1.271618	-0.088085
C	3.647115	-2.051631	0.027100
C	5.001797	-2.381728	0.048331
C	6.003770	-1.390801	0.007037
C	5.681345	-0.034760	-0.048077
C	4.323156	0.291912	-0.066677
C	3.301433	-0.694066	-0.041634
H	2.883716	-2.828095	0.072530
H	5.294205	-3.432888	0.102179
H	7.054049	-1.690451	0.024686
H	6.454080	0.736126	-0.070409
N	3.666368	1.510041	-0.097792
H	4.103582	2.425169	-0.102688
N	2.069044	-0.051869	-0.069174
Cr	0.006719	-0.438016	-0.014808
C	-0.400630	-1.832071	-1.940895
H	-0.097283	-0.752317	-2.039305
H	-1.481373	-1.866418	-2.130250
C	0.003099	-2.552935	-0.655342
H	-0.619009	-3.441270	-0.515478
H	1.054542	-2.856919	-0.692506
C	-0.189907	-2.259666	1.415279
H	0.585132	-3.022339	1.531312
H	-1.205165	-2.657447	1.482153
C	0.037422	-0.964070	1.973594
H	-0.799247	-0.455803	2.461970
H	1.027212	-0.739945	2.383036
H	0.133589	-2.284551	-2.792859

^{3}5A

Geometry with 51 atoms:

Total energy: -2206.982347080

C	5.049562	-2.088608	-0.708796
C	3.694815	-1.780447	-0.656849
C	3.345174	-0.455660	-0.347155
C	4.354433	0.512125	-0.102734
C	5.718484	0.203749	-0.156005
C	6.045379	-1.113796	-0.462870
H	5.356110	-3.109955	-0.945572
H	2.928114	-2.529978	-0.847628
H	6.485603	0.956888	0.032630
H	7.097317	-1.403625	-0.515870
N	3.677190	1.688577	0.164721
H	4.099713	2.585851	0.380516
N	2.106987	0.152952	-0.221758
C	2.348592	1.432070	0.082901
C	-1.104878	2.417060	0.252229

C	-1.120812	3.790913	0.537312
C	0.105467	4.442883	0.691624
C	1.309816	3.736308	0.562989
C	1.239331	2.369136	0.278035
N	0.056117	1.752678	0.134107
H	0.126686	5.512478	0.910272
H	-2.060821	4.338168	0.631690
H	2.270482	4.242099	0.676160
C	-2.240036	1.526449	0.034355
C	-3.680799	-1.648329	-0.702519
C	-5.044031	-1.914090	-0.770035
C	-6.010512	-0.904888	-0.548734
C	-5.644105	0.404185	-0.250062
C	-4.271610	0.668868	-0.180057
C	-3.290984	-0.332890	-0.402976
H	-2.935263	-2.424445	-0.870021
H	-5.380018	-2.927986	-0.998714
H	-7.070717	-1.160440	-0.612952
H	-6.388143	1.184088	-0.078106
N	-3.563294	1.824438	0.092154
H	-3.961097	2.735132	0.296914
N	-2.033463	0.235762	-0.263866
Cr	0.014257	-0.308210	-0.391933
C	-0.761970	-3.179020	1.386119
H	-1.745025	-3.453625	0.963110
H	-0.873033	-2.129322	1.724069
C	0.035438	-2.319874	-0.913385
H	0.825203	-2.456687	-1.680065
H	-0.905472	-2.618680	-1.416123
C	0.302467	-3.251062	0.282356
H	0.390126	-4.309970	-0.037806
H	1.283243	-3.009155	0.737170
C	-0.457431	-4.065470	2.592832
H	0.500133	-3.784249	3.064322
H	-1.242339	-3.991921	3.363703
H	-0.378475	-5.126144	2.299741

^{3}TS[5A-12A]

Geometry with 51 atoms:

Total energy: -2206.977801190

C	4.929410	-2.032583	-0.835993
C	3.570745	-1.750956	-0.710586
C	3.207658	-0.425407	-0.434809
C	4.200479	0.578982	-0.303480
C	5.564352	0.298574	-0.428608
C	5.909767	-1.025780	-0.695158
H	5.246168	-3.055743	-1.050783
H	2.810838	-2.524255	-0.825636
H	6.321581	1.078212	-0.326120
H	6.964376	-1.290248	-0.801091
N	3.509648	1.755737	-0.060024
H	3.919755	2.675228	0.064738
N	1.963316	0.161498	-0.260281
C	2.181707	1.472450	-0.050066
C	-1.327472	2.268473	0.098125
C	-1.403525	3.642343	0.311257
C	-0.214831	4.380118	0.437156
C	1.022161	3.723973	0.334460
C	1.041940	2.347169	0.120062
N	-0.118820	1.625338	0.018862
H	-0.252499	5.457106	0.606196
H	-2.374497	4.137937	0.374691
H	1.955290	4.285857	0.415135
C	-2.404467	1.317040	-0.077980
C	-3.538195	-2.025647	-0.621070
C	-4.871535	-2.420992	-0.704650
C	-5.927654	-1.491412	-0.578513
C	-5.688033	-0.134141	-0.365095
C	-4.349797	0.260890	-0.278753
C	-3.282412	-0.665031	-0.403323
H	-2.716519	-2.735940	-0.727409
H	-5.108992	-3.473662	-0.874551
H	-6.958796	-1.844572	-0.651780
H	-6.505390	0.583331	-0.271309
N	-3.750625	1.495460	-0.076112
H	-4.230949	2.381022	0.044132
N	-2.088891	0.024800	-0.272245
Cr	-0.054909	-0.351572	-0.213236
C	-0.095667	-0.664706	1.932484
H	0.847710	-0.279620	2.332249
H	-1.003308	-0.144754	2.247668
C	-0.160972	-1.971759	1.457062
H	-0.077652	-1.945688	-0.570838
C	0.973222	-2.954630	1.594737
H	0.930966	-3.294241	2.648238
H	1.936320	-2.429555	1.494472
C	0.911422	-4.174512	0.681831
H	-0.035921	-4.722972	0.814456
H	0.978281	-3.887740	-0.379418
H	1.734100	-4.871957	0.903742
H	-1.155254	-2.414574	1.324943

^{3}6A

Geometry with 57 atoms:

Total energy: -2285.560499710

C	4.986475	-2.310359	-0.575786
C	3.635139	-1.980192	-0.553852
C	3.300276	-0.636410	-0.323401
C	4.320225	0.332179	-0.132513
C	5.679398	0.001681	-0.153622
C	5.992303	-1.336792	-0.376780
H	5.280473	-3.347680	-0.751036
H	2.860994	-2.731261	-0.708719
H	6.455215	0.754849	-0.004352
H	7.040752	-1.642453	-0.401035
N	3.658910	1.533930	0.054704
H	4.093051	2.437439	0.212456
N	2.071182	-0.002501	-0.241361

C	2.325830	1.293265	-0.019349
C	-1.133740	2.252083	0.091985
C	-1.158648	3.620857	0.372388
C	0.060279	4.296750	0.512129
C	1.266467	3.594037	0.392056
C	1.216336	2.226753	0.110165
N	0.035800	1.587724	-0.065091
H	0.070257	5.366311	0.728842
H	-2.107098	4.150029	0.487331
H	2.224941	4.101313	0.521704
C	-2.258543	1.340373	-0.054143
C	-3.605515	-1.919567	-0.574732
C	-4.960781	-2.230442	-0.621535
C	-5.955942	-1.238366	-0.463206
C	-5.628878	0.098944	-0.252763
C	-4.265851	0.410284	-0.205422
C	-3.258427	-0.576328	-0.363793
H	-2.835562	-2.681384	-0.692113
H	-5.266758	-3.266453	-0.783402
H	-7.008098	-1.528790	-0.507273
H	-6.397179	0.864733	-0.131037
N	-3.589085	1.603127	-0.013097
H	-4.011680	2.514865	0.127829
N	-2.021777	0.038653	-0.263238
Cr	0.012624	-0.440447	-0.385850
C	0.243237	-1.399694	2.606267
H	0.268635	-0.377581	2.169103
H	1.295804	-1.734995	2.612738
C	-0.075902	-2.404251	0.254696
H	0.944251	-2.827567	0.230345
H	-0.706912	-3.082469	-0.342602
C	-0.578680	-2.337033	1.706823
H	-1.635659	-2.011214	1.727758
H	-0.577789	-3.344307	2.169642
C	-0.285113	-1.302855	4.034973
H	-1.320286	-0.921381	4.053538
H	-0.292827	-2.294826	4.517360
H	0.331514	-0.634416	4.657913
C	0.042854	-1.269414	-2.340252
H	0.967556	-1.848075	-2.428055
H	-0.880521	-1.839208	-2.476898
C	0.049104	0.117040	-2.502446
H	-0.872031	0.656424	-2.740585
H	0.979368	0.657037	-2.699791

^{3}TS[6A-7A]
Geometry with 57 atoms:
Total energy: -2285.549631890

C	4.966477	-2.170312	-0.551376
C	3.614364	-1.829838	-0.508813
C	3.286208	-0.485835	-0.282002
C	4.312818	0.476868	-0.096850
C	5.667511	0.138487	-0.140078
C	5.976339	-1.202793	-0.371640
H	5.250975	-3.210187	-0.727662
H	2.837414	-2.581469	-0.644806
H	6.448262	0.888256	0.001563
H	7.023905	-1.509506	-0.413369
N	3.661991	1.681823	0.115240
H	4.104016	2.579184	0.281500
N	2.060289	0.155516	-0.181134
C	2.321781	1.455702	0.061409
C	-1.167341	2.347016	0.256696
C	-1.191997	3.708159	0.542478
C	0.020192	4.410346	0.668329
C	1.233981	3.719103	0.511769
C	1.214350	2.356577	0.229838
N	0.023018	1.670139	0.091395
H	0.018245	5.478326	0.889034
H	-2.147162	4.224094	0.668160
H	2.187600	4.242857	0.613912
C	-2.276619	1.447561	0.086702
C	-3.646051	-1.766279	-0.682991
C	-5.005819	-2.065132	-0.765200
C	-5.992544	-1.086910	-0.527503
C	-5.648449	0.226105	-0.205993
C	-4.285361	0.521265	-0.126567
C	-3.278052	-0.454382	-0.350438
H	-2.896300	-2.530979	-0.879992
H	-5.313649	-3.081092	-1.022943
H	-7.047408	-1.360949	-0.601056
H	-6.408051	0.989841	-0.028668
N	-3.611106	1.698621	0.145971
H	-4.034606	2.600018	0.336487
N	-2.035078	0.150950	-0.197874
Cr	0.025431	-0.233521	-0.328461
C	0.276098	-2.035411	1.238162
H	0.033392	-0.959397	1.496737
H	1.350121	-2.126176	1.461813
C	-0.005726	-2.441661	-0.208501
H	0.650237	-3.267283	-0.499105
H	-1.046177	-2.763509	-0.322472
C	0.294287	-1.676683	-2.131732
H	-0.450087	-2.403354	-2.468030
H	1.323373	-2.030068	-2.232500
C	0.057526	-0.288919	-2.384097
H	0.898228	0.327460	-2.715926
H	-0.923064	0.009941	-2.767742
C	-0.559746	-2.837458	2.253094
H	-1.629805	-2.701198	2.021696
H	-0.343314	-3.909429	2.108612
C	-0.279214	-2.434440	3.698678
H	0.780841	-2.588161	3.960665
H	-0.515188	-1.370501	3.871598
H	-0.886015	-3.028383	4.400137

^{3}7A
Geometry with 57 atoms:

Total energy: -2285.590403320

C	-4.248165	-3.612767	-0.650133
C	-2.947144	-3.127104	-0.523922
C	-2.763330	-1.945476	0.205607
C	-3.873872	-1.276845	0.781822
C	-5.177836	-1.762815	0.659250
C	-5.344282	-2.942953	-0.066984
H	-4.425131	-4.531966	-1.213184
H	-2.101173	-3.647195	-0.977993
H	-6.026449	-1.243537	1.108476
H	-6.347929	-3.356744	-0.188060
N	-3.351121	-0.156123	1.410548
H	-3.879147	0.546889	1.916301
N	-1.617026	-1.222139	0.499113
C	-2.004760	-0.153111	1.222906
C	1.361294	1.148181	1.486755
C	1.244950	2.327078	2.211291
C	-0.023495	2.750296	2.652488
C	-1.151669	1.963959	2.363278
C	-1.001120	0.788264	1.636900
N	0.245193	0.387660	1.182259
H	-0.128219	3.676734	3.217899
H	2.135463	2.917471	2.437078
H	-2.143827	2.268648	2.703987
C	2.544171	0.536446	0.937377
C	4.115073	-2.052992	-0.958710
C	5.475664	-2.127985	-1.253267
C	6.383403	-1.149165	-0.796081
C	5.961434	-0.060343	-0.032182
C	4.596924	0.013962	0.259080
C	3.676296	-0.967253	-0.189803
H	3.412848	-2.808545	-1.317581
H	5.849563	-2.961176	-1.852657
H	7.441915	-1.244443	-1.048590
H	6.663623	0.698323	0.318523
N	3.841722	0.939408	0.964266
H	4.192996	1.776802	1.416381
N	2.410992	-0.616092	0.254304
Cr	0.407060	-1.176557	0.086419
C	-0.696304	1.760713	-1.885809
H	0.201614	2.155771	-2.395574
H	-0.471911	1.807044	-0.808125
C	0.211042	-0.629012	-1.851921
H	0.060007	-1.671893	-2.219875
H	1.201199	-0.280593	-2.189292
C	-0.907906	0.299219	-2.295198
H	-1.001812	0.251896	-3.398489
H	-1.875384	-0.059853	-1.905188
C	-1.895301	2.663328	-2.179389
H	-2.790214	2.248138	-1.677400
H	-2.122872	2.643685	-3.261225
C	-1.693329	4.111624	-1.725827
H	-0.807481	4.531404	-2.236368
H	-1.449902	4.119577	-0.646877
C	-2.905710	5.004670	-1.985015
H	-2.729672	6.039120	-1.647644
H	-3.152057	5.043104	-3.059676
H	-3.799974	4.630191	-1.457406

^{3}TS[7A-13A]
Geometry with 57 atoms:
Total energy: -2285.557481440

C	-4.985475	0.528504	-0.992613
C	-3.600700	0.556294	-0.841908
C	-2.959980	-0.649617	-0.525988
C	-3.708847	-1.845112	-0.379566
C	-5.098565	-1.875442	-0.530952
C	-5.722233	-0.666612	-0.837903
H	-5.515494	1.451557	-1.238502
H	-3.027626	1.475089	-0.965437
H	-5.667458	-2.799976	-0.416477
H	-6.806896	-0.644101	-0.965357
N	-2.780276	-2.833098	-0.089252
H	-2.981511	-3.815901	0.062784
N	-1.621081	-0.941558	-0.314897
C	-1.548537	-2.261666	-0.063949
C	2.046342	-2.253299	0.169871
C	2.419263	-3.567768	0.440388
C	1.419968	-4.543994	0.584618
C	0.070984	-4.182162	0.437090
C	-0.247623	-2.854358	0.161580
N	0.727205	-1.896929	0.051658
H	1.690034	-5.578564	0.800616
H	3.474176	-3.833651	0.536250
H	-0.717587	-4.931937	0.530293
C	2.889347	-1.094695	-0.036667
C	3.267330	2.391776	-0.713310
C	4.482265	3.065586	-0.818209
C	5.715521	2.395153	-0.659468
C	5.777480	1.028235	-0.389426
C	4.557629	0.353743	-0.282310
C	3.314345	1.017684	-0.441526
H	2.309523	2.899350	-0.841692
H	4.484756	4.137146	-1.030592
H	6.644972	2.961730	-0.751341
H	6.731441	0.511740	-0.267719
N	4.241826	-0.972842	-0.027531
H	4.903761	-1.725071	0.131939
N	2.299959	0.088601	-0.281950
Cr	0.229676	0.010379	-0.225609
C	0.166618	0.341740	1.912117
H	-0.650547	-0.271377	2.304982
H	1.173345	0.075273	2.242893
C	-0.100343	1.620655	1.429602
H	-0.126076	1.560826	-0.595614
C	-1.453519	2.271700	1.541750
H	-1.518594	2.620490	2.591569
H	-2.246142	1.513018	1.435790

C	-1.713998	3.460526	0.618144
H	-0.912917	4.210388	0.751970
H	-1.637864	3.129768	-0.432669
H	0.745521	2.307594	1.310935
C	-3.075862	4.117213	0.855007
C	-3.354193	5.280432	-0.095554
H	-3.135462	4.468696	1.900885
H	-3.868054	3.353485	0.749633
H	-3.341752	4.949360	-1.148237
H	-4.338446	5.736365	0.098393
H	-2.594095	6.073296	0.008212

^{3}8A
Geometry with 63 atoms:
Total energy: -2364.140217630

C	-5.016307	-1.676703	-1.835155
C	-3.665757	-1.542821	-1.528925
C	-3.332262	-0.817864	-0.373974
C	-4.352702	-0.260269	0.440014
C	-5.711171	-0.392277	0.132689
C	-6.022619	-1.109110	-1.019940
H	-5.309347	-2.234258	-2.727628
H	-2.890110	-1.981657	-2.156269
H	-6.487146	0.042976	0.765133
H	-7.070413	-1.238405	-1.300645
N	-3.693050	0.362883	1.485520
H	-4.128532	0.857268	2.257322
N	-2.104275	-0.514833	0.191454
C	-2.359641	0.186639	1.303013
C	1.099983	0.579685	2.183256
C	1.129890	1.347795	3.349694
C	-0.085380	1.758708	3.911331
C	-1.292186	1.413742	3.289920
C	-1.248640	0.637071	2.129179
N	-0.071787	0.207893	1.614823
H	-0.091811	2.359240	4.822453
H	2.080767	1.628008	3.807247
H	-2.246347	1.748352	3.701211
C	2.224105	0.087248	1.401478
C	3.565371	-1.657168	-1.402900
C	4.919821	-1.852951	-1.654050
C	5.916373	-1.350668	-0.785219
C	5.591911	-0.635618	0.365096
C	4.229686	-0.440636	0.617130
C	3.221049	-0.939531	-0.247350
H	2.793604	-2.041037	-2.069575
H	5.224318	-2.408249	-2.544037
H	6.967708	-1.529074	-1.022432
H	6.360671	-0.248707	1.036629
N	3.554828	0.202192	1.641531
H	3.979095	0.667694	2.437255
N	1.985845	-0.588624	0.270173
Cr	-0.052464	-0.845564	-0.149504
C	-0.055848	1.555517	-2.044828
H	-0.001358	1.488162	-0.935417
H	-1.135371	1.550852	-2.281613
C	0.029522	-1.003836	-2.212715
H	-1.009225	-1.108479	-2.575066
H	0.594147	-1.852266	-2.632723
C	0.616099	0.333694	-2.690096
H	1.698717	0.370762	-2.470353
H	0.537522	0.436161	-3.790802
C	0.557963	2.897591	-2.442904
H	1.640772	2.882220	-2.217896
H	0.480854	3.015775	-3.539452
C	-0.102461	-2.970299	-0.181152
H	-1.020781	-3.267341	-0.697221
H	0.826068	-3.315538	-0.644695
C	-0.126045	-2.597263	1.163326
H	0.786205	-2.621286	1.766067
H	-1.064187	-2.571324	1.724644
C	-0.087024	4.100770	-1.750315
C	0.540105	5.437293	-2.143840
H	-0.014875	3.966699	-0.654123
H	-1.168044	4.115258	-1.980712
H	0.056696	6.282335	-1.626989
H	1.614780	5.464275	-1.894634
H	0.450843	5.616104	-3.228667

^{3}TS[8A-9A]
Geometry with 63 atoms:
Total energy: -2364.128433500

C	4.979240	-1.577392	-1.660301
C	3.643698	-1.214688	-1.485477
C	3.363747	-0.156309	-0.610022
C	4.419969	0.500908	0.074029
C	5.758300	0.140822	-0.100748
C	6.019539	-0.909667	-0.981834
H	5.226368	-2.398246	-2.337399
H	2.842736	-1.738011	-2.006849
H	6.562507	0.655633	0.428387
H	7.052892	-1.222858	-1.147171
N	3.812701	1.467676	0.859681
H	4.282592	2.115068	1.482850
N	2.164110	0.427225	-0.229185
C	2.469494	1.395565	0.657587
C	-0.979257	2.306875	1.192763
C	-0.955519	3.315312	2.150544
C	0.278641	3.759897	2.656950
C	1.464948	3.166925	2.191463
C	1.396967	2.156483	1.238085
N	0.184922	1.730329	0.729991
H	0.314516	4.552726	3.404970
H	-1.890569	3.756565	2.503004
H	2.435361	3.490843	2.573973
C	-2.117513	1.708335	0.549919
C	-3.591037	-0.561346	-1.790283
C	-4.957090	-0.685244	-2.042763

C	-5.908463	0.100221	-1.360858
C	-5.521233	1.041236	-0.406729
C	-4.152047	1.162785	-0.157552
C	-3.180481	0.371824	-0.826779
H	-2.868985	-1.170059	-2.332698
H	-5.298438	-1.406343	-2.788880
H	-6.969622	-0.027187	-1.586692
H	-6.253169	1.657406	0.119159
N	-3.439854	1.986824	0.696311
H	-3.830806	2.687905	1.315935
N	-1.920723	0.728409	-0.356793
Cr	0.122854	0.319007	-0.614988
C	0.211369	-2.047873	-0.182907
H	0.005477	-1.249753	0.592406
H	1.267401	-2.309799	-0.017175
C	-0.014500	-1.633368	-1.638790
H	0.618730	-2.234932	-2.297418
H	-1.061277	-1.784356	-1.921648
C	0.413117	-0.019511	-2.895904
H	-0.354170	-0.416080	-3.566305
H	1.423870	-0.345453	-3.152666
C	0.267387	1.316572	-2.406783
H	1.157976	1.950375	-2.359460
H	-0.672074	1.842362	-2.604336
C	-0.708493	-3.203425	0.250058
H	-1.759551	-2.908018	0.087813
H	-0.521619	-4.065384	-0.413338
C	-0.505316	-3.615716	1.709054
H	0.553743	-3.889723	1.868982
H	-0.695062	-2.743827	2.363365
C	-1.401391	-4.778437	2.143546
C	-1.198656	-5.179923	3.603758
H	-1.208325	-5.648120	1.489653
H	-2.458709	-4.503417	1.976468
H	-1.419077	-4.340136	4.284749
H	-1.854259	-6.018893	3.887443
H	-0.157590	-5.492855	3.792397

^{3}9A
Geometry with 63 atoms:
Total energy: -2364.170928590

C	-3.243104	3.764104	-0.369967
C	-2.351614	2.692142	-0.340355
C	-0.983362	2.985739	-0.275954
C	-0.539758	4.332691	-0.248421
C	-1.430605	5.408652	-0.277937
C	-2.790372	5.099765	-0.338073
H	-4.316387	3.566540	-0.418290
H	-2.704467	1.660792	-0.364205
H	-1.079681	6.442078	-0.255555
H	-3.520936	5.911572	-0.361559
N	0.844597	4.270008	-0.191595
H	1.477919	5.061473	-0.155661
N	0.127659	2.156504	-0.229677
C	1.210832	2.960521	-0.182698
C	3.537782	0.186015	-0.156651
C	4.801564	0.761403	-0.132439
C	4.924572	2.163384	-0.105077
C	3.766204	2.959394	-0.112519
C	2.514948	2.352699	-0.141128
N	2.400241	0.973381	-0.155236
H	5.910815	2.627941	-0.082705
H	5.690167	0.126373	-0.136007
H	3.843635	4.048374	-0.100483
C	3.174599	-1.207278	-0.192026
C	0.692000	-3.779062	-0.259179
C	0.949073	-5.149588	-0.267304
C	2.267099	-5.652879	-0.252041
C	3.373794	-4.803112	-0.226888
C	3.113898	-3.430427	-0.217013
C	1.793068	-2.912580	-0.234263
H	-0.328507	-3.391774	-0.270548
H	0.112343	-5.851684	-0.285888
H	2.425659	-6.733600	-0.259721
H	4.393645	-5.192259	-0.214852
N	3.949220	-2.323584	-0.190912
H	4.962838	-2.340506	-0.166540
N	1.866081	-1.527871	-0.220103
Cr	0.670560	0.163502	-0.087886
C	-1.858776	-0.867558	1.035933
H	-1.483347	-1.899176	1.158418
H	-1.586280	-0.576468	-0.014052
C	0.358672	0.037536	1.908775
H	0.856916	0.866482	2.432867
H	0.803571	-0.918715	2.229311
C	-1.159776	0.054609	2.048895
H	-1.457948	-0.261965	3.066810
H	-1.544560	1.081184	1.928294
C	-3.385001	-0.868753	1.120921
H	-3.760771	0.165890	1.027315
H	-3.672930	-1.200499	2.134624
C	-4.059199	-1.759494	0.075898
H	-3.674101	-2.791634	0.173649
H	-3.764252	-1.422529	-0.936454
C	-5.585904	-1.777071	0.176022
H	-5.880243	-2.112167	1.187894
H	-5.970116	-0.744394	0.078426
C	-6.261686	-2.669141	-0.868677
C	-7.785631	-2.681958	-0.758408
H	-5.874488	-3.699810	-0.769190
H	-5.965861	-2.332356	-1.879450
H	-8.242642	-3.332753	-1.521449
H	-8.112304	-3.048021	0.229872
H	-8.205623	-1.670030	-0.889493

^{3}TS[9A-14A]
Geometry with 63 atoms:
Total energy: -2364.136104750

C	4.312119	1.880614	-0.724801
C	3.068571	1.259817	-0.632031
C	1.953277	2.075237	-0.395085
C	2.103937	3.480167	-0.273694
C	3.351321	4.105320	-0.364768
C	4.452056	3.279514	-0.589808
H	5.200780	1.272735	-0.909726
H	2.956810	0.182256	-0.744925
H	3.458149	5.187414	-0.267986
H	5.445901	3.725824	-0.669016
N	0.824382	3.976233	-0.076563
H	0.572472	4.953023	0.031116
N	0.608997	1.763664	-0.256099
C	-0.039945	2.929176	-0.081057
C	-3.292061	1.382298	-0.004688
C	-4.210303	2.419899	0.134875
C	-3.737987	3.738552	0.240799
C	-2.356393	3.986547	0.187284
C	-1.481900	2.911968	0.041805
N	-1.942383	1.623730	-0.033609
H	-4.440446	4.565606	0.352403
H	-5.281427	2.207811	0.152628
H	-1.970287	5.006370	0.250530
C	-3.539913	-0.036583	-0.147158
C	-2.330065	-3.373477	-0.545243
C	-3.123674	-4.516968	-0.603530
C	-4.531448	-4.445437	-0.510736
C	-5.195133	-3.228431	-0.357381
C	-4.397751	-2.081649	-0.297157
C	-2.983668	-2.143618	-0.388386
H	-1.242524	-3.417629	-0.624496
H	-2.649325	-5.493293	-0.726510
H	-5.115526	-5.367209	-0.561115
H	-6.283103	-3.174892	-0.286906
N	-4.703393	-0.736594	-0.147447
H	-5.633791	-0.341704	-0.059985
N	-2.483635	-0.856086	-0.290255
Cr	-0.661482	0.104947	-0.181930
C	-0.553408	-0.139913	1.973477
H	-0.081717	0.766836	2.365211
H	-1.590743	-0.313298	2.269081
C	0.240538	-1.194179	1.532200
H	0.285326	-1.177343	-0.518941
C	1.739942	-1.204926	1.675908
H	1.931081	-1.513657	2.722843
H	2.125797	-0.175428	1.598542
C	2.507065	-2.139401	0.741229
H	2.138048	-3.173257	0.868019
H	2.274355	-1.869393	-0.303314
H	-0.233250	-2.174776	1.408406
C	4.021395	-2.098913	0.956339
C	4.802385	-2.929476	-0.064330
H	4.261878	-2.445209	1.978147
H	4.364496	-1.048921	0.908178
H	4.469693	-3.982920	-0.013490
H	4.546817	-2.584667	-1.084335
C	6.320889	-2.867573	0.119858
C	7.090350	-3.682325	-0.919015
H	6.578471	-3.221529	1.134677
H	6.647309	-1.811820	0.078105
H	8.179187	-3.619265	-0.760342
H	6.810002	-4.748734	-0.879637
H	6.882178	-3.325728	-1.942482

^{3}10A
Geometry with 69 atoms:
Total energy: -2442.718267000

C	-4.427040	-3.059015	-1.656304
C	-3.119290	-2.657030	-1.404605
C	-2.887612	-1.911205	-0.238926
C	-3.957003	-1.589314	0.636141
C	-5.272709	-1.992862	0.383658
C	-5.485924	-2.732144	-0.777395
H	-4.645476	-3.640014	-2.555160
H	-2.299079	-2.900748	-2.079511
H	-6.090628	-1.740564	1.061015
H	-6.497554	-3.068234	-1.016076
N	-3.386538	-0.856365	1.663773
H	-3.874945	-0.470426	2.465019
N	-1.722265	-1.370518	0.274598
C	-2.056216	-0.749886	1.412969
C	1.289908	0.363937	2.095819
C	1.221977	1.140432	3.255039
C	-0.018149	1.288056	3.889569
C	-1.157103	0.682211	3.345325
C	-1.017968	-0.078323	2.181248
N	0.191864	-0.252078	1.596185
H	-0.099340	1.887469	4.797848
H	2.112713	1.630872	3.652301
H	-2.134133	0.809351	3.814817
C	2.450049	0.106802	1.254214
C	3.988930	-1.344908	-1.615858
C	5.344731	-1.276718	-1.920491
C	6.259090	-0.588667	-1.089584
C	5.848059	0.052155	0.076515
C	4.484920	-0.018670	0.382786
C	3.556332	-0.702042	-0.445273
H	3.284130	-1.876320	-2.255334
H	5.715332	-1.767112	-2.823446
H	7.314889	-0.561654	-1.368602
H	6.554289	0.579074	0.720827
N	3.742352	0.477217	1.440932
H	4.102137	1.012682	2.224230
N	2.299995	-0.599295	0.126838
Cr	0.316159	-1.240030	-0.201517
C	-0.202236	1.212567	-1.895605
H	0.823155	1.467431	-2.219191
H	-0.113258	1.027300	-0.801754

C	0.182457	-1.290309	-2.268537
H	-0.226011	-2.201939	-2.734547
H	1.207949	-1.164446	-2.662505
C	-0.668947	-0.059657	-2.620709
H	-0.667244	0.138770	-3.710793
H	-1.726355	-0.245958	-2.359618
C	-1.119770	2.423710	-2.056622
H	-2.147260	2.139208	-1.762959
H	-1.176280	2.696435	-3.126108
C	-0.673230	3.633938	-1.232958
H	0.349120	3.926577	-1.536439
H	-0.595246	3.334853	-0.169373
C	-1.601435	4.844860	-1.343850
H	-1.667442	5.160115	-2.401538
H	-2.627059	4.546038	-1.055997
C	-1.163507	6.035717	-0.486602
C	-2.099665	7.238703	-0.592905
H	-0.140327	6.335739	-0.778463
H	-1.092795	5.714407	0.569493
H	-1.758911	8.076451	0.037203
H	-2.161279	7.607344	-1.630882
H	-3.124129	6.978535	-0.275727
C	0.718019	-3.015100	1.015731
H	1.648505	-2.852230	1.566536
H	-0.162869	-3.231543	1.626518
C	0.733242	-3.317550	-0.347069
H	-0.128806	-3.798831	-0.817644
H	1.679065	-3.418772	-0.888333

^{3}TS[10A-11A]
Geometry with 69 atoms:
Total energy: -2442.707172370

C	-4.502273	2.701386	-2.047045
C	-3.431456	1.841915	-1.800933
C	-3.412819	1.153793	-0.579584
C	-4.456366	1.349098	0.363028
C	-5.530230	2.208332	0.118370
C	-5.535544	2.880765	-1.104563
H	-4.541732	3.249493	-2.991171
H	-2.634200	1.711299	-2.531719
H	-6.327662	2.347795	0.850893
H	-6.357669	3.561895	-1.335603
N	-4.135007	0.550228	1.448655
H	-4.671834	0.460215	2.304238
N	-2.503598	0.251590	-0.046341
C	-2.965016	-0.087270	1.174237
C	-0.161000	-2.243231	1.882636
C	-0.384892	-2.738432	3.163181
C	-1.544558	-2.355902	3.860984
C	-2.453150	-1.474860	3.250621
C	-2.193146	-1.003809	1.967589
N	-1.057843	-1.386256	1.279047
H	-1.733818	-2.735908	4.865442
H	0.336773	-3.418588	3.621307
H	-3.356094	-1.154507	3.775192
C	0.950066	-2.496712	1.004507
C	2.654424	-2.124262	-2.119241
C	3.856089	-2.744076	-2.461183
C	4.530851	-3.594180	-1.561569
C	4.020450	-3.854881	-0.289867
C	2.816227	-3.232770	0.047995
C	2.127392	-2.366794	-0.842155
H	2.142221	-1.476958	-2.829859
H	4.283447	-2.569502	-3.451225
H	5.469551	-4.061539	-1.867544
H	4.534740	-4.517619	0.408775
N	2.043232	-3.282496	1.194607
H	2.241059	-3.829616	2.025199
N	0.971718	-1.915722	-0.213204
Cr	-0.734173	-0.732766	-0.527972
C	0.213975	1.380899	-1.165574
H	0.155881	0.947792	-0.119635
H	-0.529397	2.191792	-1.130452
C	-0.104049	0.416776	-2.310766
H	-0.585446	0.954365	-3.132315
H	0.813091	-0.048155	-2.685853
C	-1.416589	-1.147223	-2.714352
H	-0.752294	-1.410494	-3.541979
H	-2.257240	-0.517676	-3.016723
C	-1.674490	-2.129993	-1.706929
H	-2.698492	-2.235757	-1.336850
H	-1.082701	-3.050526	-1.716963
C	1.643590	1.942872	-1.237861
H	2.356525	1.101198	-1.280321
H	1.756299	2.492481	-2.188239
C	1.994588	2.856061	-0.062263
H	1.271015	3.690303	-0.015086
H	1.871874	2.294033	0.882851
C	3.416229	3.417531	-0.135926
C	3.783692	4.315473	1.047325
H	3.535144	3.985184	-1.077211
H	4.135357	2.579632	-0.197023
H	3.664555	3.746356	1.988548
H	3.062825	5.152147	1.109332
C	5.205475	4.878973	0.974967
C	5.564725	5.770476	2.162826
H	5.321314	5.449369	0.035258
H	5.924281	4.041649	0.909198
H	6.591902	6.161589	2.081321
H	4.884132	6.636122	2.234326
H	5.494046	5.217371	3.115151

^{3}11A
Geometry with 69 atoms:
Total energy: -2442.722045800

C	2.826795	-4.870797	-1.594768
C	2.402884	-3.551459	-1.478197
C	2.991815	-2.769648	-0.470846

C	3.983130	-3.327809	0.378209
C	4.410862	-4.655126	0.262550
C	3.813073	-5.414997	-0.738769
H	2.388480	-5.506044	-2.367743
H	1.645852	-3.132605	-2.139500
H	5.173218	-5.072462	0.922835
H	4.113415	-6.457260	-0.868663
N	4.350256	-2.306711	1.235731
H	5.040171	-2.369389	1.977383
N	2.789529	-1.448251	-0.106026
C	3.618967	-1.209801	0.916661
C	2.630953	2.216431	1.363963
C	3.413689	2.731309	2.401950
C	4.344210	1.880611	3.011172
C	4.474313	0.553847	2.582370
C	3.656807	0.113797	1.535421
N	2.768429	0.941771	0.953368
H	4.970834	2.252950	3.823809
H	3.303835	3.768158	2.725372
H	5.197873	-0.115264	3.051755
C	1.606344	2.908264	0.586929
C	-0.848775	3.067498	-1.988434
C	-1.613179	4.186637	-2.299384
C	-1.473103	5.403404	-1.591347
C	-0.562467	5.540189	-0.547489
C	0.204484	4.412348	-0.235454
C	0.073992	3.185081	-0.936865
H	-0.953446	2.130023	-2.532100
H	-2.340424	4.128068	-3.112368
H	-2.094379	6.256936	-1.872289
H	-0.451929	6.478759	-0.001358
N	1.182549	4.189401	0.716951
H	1.524791	4.864938	1.392540
N	0.964077	2.269356	-0.398039
Cr	1.562290	0.231942	-0.617701
C	-1.793179	-0.624098	-1.328588
H	-2.132868	0.221358	-1.954014
H	-1.425663	-0.162430	-0.389554
C	0.582818	-0.450879	-2.314943
H	1.331520	-1.013211	-2.909187
H	0.282732	0.396935	-2.962125
C	-0.638615	-1.343774	-2.035120
H	-1.035636	-1.785712	-2.972152
H	-0.342604	-2.213290	-1.415921
C	-2.989763	-1.520359	-1.004569
H	-2.655030	-2.361621	-0.368883
H	-3.362069	-1.981338	-1.938059
C	-4.138706	-0.785844	-0.309516
H	-4.476134	0.050640	-0.949649
H	-3.762822	-0.317347	0.619860
C	-5.334703	-1.680209	0.024479
H	-5.708735	-2.150191	-0.903996
H	-4.997739	-2.514864	0.667323
C	-6.483914	-0.942127	0.715319
C	-7.678230	-1.836848	1.054484
H	-6.822969	-0.110407	0.069800
H	-6.108433	-0.468089	1.641736
H	-8.052787	-2.312534	0.128743
H	-7.340013	-2.667754	1.701860
C	-8.829557	-1.098271	1.742535
C	-10.015380	-2.001528	2.079262
H	-9.168304	-0.270133	1.093141
H	-8.453562	-0.621090	2.666361
H	-10.827554	-1.441034	2.570602
H	-10.434885	-2.466811	1.170862
H	-9.716959	-2.818484	2.758413

^{5}1A

Geometry with 39 atoms:

Total energy: -2049.873007040

C	-4.984015	-2.661322	-0.018189
C	-3.631550	-2.343076	0.006948
C	-3.294955	-0.979920	0.006746
C	-4.304678	0.017076	-0.017442
C	-5.667229	-0.303501	-0.041520
C	-5.984268	-1.658734	-0.041580
H	-5.288352	-3.710387	-0.020848
H	-2.849325	-3.103997	0.024026
H	-6.440614	0.466544	-0.060031
H	-7.034494	-1.958846	-0.061150
N	-3.627349	1.224275	-0.016301
H	-4.051385	2.146590	-0.032845
N	-2.062016	-0.358423	0.021647
C	-2.297589	0.955696	0.004361
C	1.173439	1.897401	-0.000142
C	1.216197	3.297142	0.003563
C	-0.000001	3.989910	0.005224
C	-1.216199	3.297142	0.003577
C	-1.173440	1.897400	-0.000132
N	-0.000000	1.246567	-0.004768
H	-0.000002	5.081914	0.011131
H	2.166105	3.834273	0.009858
H	-2.166108	3.834271	0.009887
C	2.297589	0.955697	0.004338
C	3.631551	-2.343075	0.006997
C	4.984017	-2.661322	-0.018128
C	5.984270	-1.658733	-0.041554
C	5.667229	-0.303500	-0.041540
C	4.304678	0.017077	-0.017470
C	3.294956	-0.979920	0.006748
H	2.849328	-3.103996	0.024100
H	5.288355	-3.710386	-0.020754
H	7.034495	-1.958845	-0.061116
H	6.440614	0.466544	-0.060077
N	3.627348	1.224275	-0.016369
H	4.051384	2.146590	-0.032947
N	2.062017	-0.358422	0.021619
Cr	-0.000001	-0.886958	0.053651

```
 H   0.000002  -2.579806   0.077517

5 2A
Geometry with  45 atoms:
Total energy:    -2128.417754180
 C  -4.992673  -2.540284  -0.445379
 C  -3.639524  -2.224215  -0.419663
 C  -3.301091  -0.866299  -0.305332
 C  -4.309568   0.129161  -0.225122
 C  -5.672561  -0.189013  -0.253025
 C  -5.991543  -1.539592  -0.363092
 H  -5.298370  -3.585230  -0.534266
 H  -2.857492  -2.982476  -0.488750
 H  -6.445337   0.579502  -0.192317
 H  -7.042446  -1.836923  -0.388866
 N  -3.630420   1.331047  -0.123943
 H  -4.052327   2.251823  -0.057063
 N  -2.066982  -0.250518  -0.251240
 C  -2.299657   1.059409  -0.143883
 C   1.173075   1.993114  -0.059077
 C   1.215184   3.389849   0.032128
 C  -0.000099   4.082102   0.082775
 C  -1.215375   3.389807   0.032436
 C  -1.173240   1.993076  -0.058749
 N  -0.000073   1.340098  -0.085912
 H  -0.000107   5.171501   0.156440
 H   2.166517   3.923890   0.059978
 H  -2.166722   3.923812   0.060519
 C   2.299506   1.059486  -0.144452
 C   3.639437  -2.224111  -0.420067
 C   4.992590  -2.540198  -0.445334
 C   5.991445  -1.539510  -0.362799
 C   5.672447  -0.188920  -0.252903
 C   4.309449   0.129275  -0.225433
 C   3.300988  -0.866182  -0.305918
 H   2.857417  -2.982371  -0.489282
 H   5.298303  -3.585157  -0.534008
 H   7.042352  -1.836861  -0.388183
 H   6.445216   0.579583  -0.191960
 N   3.630271   1.331148  -0.124295
 H   4.052163   2.251909  -0.057135
 N   2.066877  -0.250424  -0.251995
Cr  -0.000108  -0.791488  -0.249505
 H  -0.000105  -2.429601  -0.669835
 C   0.000864  -1.883231   2.361973
 H   0.931103  -2.436352   2.198358
 H  -0.929345  -2.435840   2.196510
 C   0.000781  -0.613260   2.787744
 H  -0.931528  -0.073658   2.983518
 H   0.932977  -0.074063   2.985200

5 TS[2A-3A]
Geometry with  45 atoms:
Total energy:    -2128.403044410
 C   4.973282  -2.483225  -0.469974
 C   3.621863  -2.152772  -0.460080
 C   3.289806  -0.800222  -0.291079
 C   4.304650   0.180814  -0.147056
 C   5.664264  -0.149992  -0.159067
 C   5.977023  -1.497865  -0.320796
 H   5.270463  -3.526369  -0.599563
 H   2.839918  -2.904407  -0.583258
 H   6.441280   0.608531  -0.047362
 H   7.026042  -1.802345  -0.335899
 N   3.637006   1.385640  -0.008617
 H   4.066659   2.295475   0.121907
 N   2.058092  -0.173760  -0.237243
 C   2.301717   1.131737  -0.064531
 C  -1.180223   2.055433   0.029005
 C  -1.214438   3.451230   0.072543
 C   0.000077   4.149410   0.104576
 C   1.214569   3.451186   0.072592
 C   1.180310   2.055389   0.029047
 N   0.000034   1.385934   0.036013
 H   0.000096   5.240459   0.136602
 H  -2.165906   3.986360   0.069282
 H   2.166053   3.986286   0.069368
 C  -2.301658   1.131819  -0.064606
 C  -3.621793  -2.152685  -0.460239
 C  -4.973207  -2.483157  -0.470079
 C  -5.976951  -1.497816  -0.320796
 C  -5.664201  -0.149946  -0.159009
 C  -4.304591   0.180879  -0.147045
 C  -3.289749  -0.800140  -0.291177
 H  -2.839841  -2.904301  -0.583495
 H  -5.270380  -3.526298  -0.599710
 H  -7.025967  -1.802309  -0.335863
 H  -6.441226   0.608557  -0.047226
 N  -3.636947   1.385708  -0.008591
 H  -4.066599   2.295537   0.121970
 N  -2.058039  -0.173665  -0.237396
Cr  -0.000016  -0.659533  -0.041442
 C  -0.000290  -1.436695   2.093665
 H   0.933709  -1.028646   2.491590
 H  -0.934273  -1.028434   2.491409
 C  -0.000385  -2.621166   1.373271
 H  -0.000187  -2.316558  -0.378073
 H  -0.921913  -3.197395   1.249293
 H   0.920994  -3.197672   1.249476

5 3A
Geometry with  45 atoms:
Total energy:    -2128.449949220
 C  -5.044905  -2.352579  -0.068189
 C  -3.687069  -2.055920  -0.085000
 C  -3.324235  -0.699245  -0.052018
 C  -4.320111   0.310882   0.001258
 C  -5.687868   0.013169   0.017306
```

C	-6.028769	-1.335666	-0.019606
H	-5.365121	-3.396571	-0.093224
H	-2.924921	-2.834693	-0.120632
H	-6.447449	0.796072	0.057139
H	-7.083900	-1.618494	-0.009149
N	-3.625918	1.506882	0.032892
H	-4.037464	2.434166	0.069883
N	-2.080370	-0.095802	-0.055854
C	-2.299691	1.220782	-0.001459
C	1.172758	2.159291	0.025503
C	1.216244	3.558470	0.077896
C	0.000192	4.251105	0.103721
C	-1.215889	3.558514	0.078140
C	-1.172459	2.159335	0.025695
N	0.000136	1.509940	0.001693
H	0.000217	5.342239	0.146111
H	2.165719	4.096052	0.100283
H	-2.165341	4.096127	0.100758
C	2.299935	1.220667	-0.001717
C	3.687055	-2.056163	-0.084773
C	5.044867	-2.352926	-0.067846
C	6.028810	-1.336086	-0.019375
C	5.688009	0.012779	0.017321
C	4.320276	0.310596	0.001165
C	3.324315	-0.699456	-0.052033
H	2.924862	-2.834897	-0.120312
H	5.365000	-3.396948	-0.092693
H	7.083918	-1.618995	-0.008820
H	6.447649	0.795628	0.057087
N	3.626185	1.506659	0.032644
H	4.037806	2.433911	0.069577
N	2.080502	-0.095901	-0.056017
Cr	0.000033	-0.635418	-0.133104
C	-0.000256	-2.704831	-0.438678
H	-0.879347	-2.969505	-1.060350
H	0.879353	-2.970218	-1.059293
C	-0.001324	-3.538808	0.849580
H	-0.001724	-4.632741	0.671170
H	-0.886230	-3.328115	1.478628
H	0.883143	-3.328902	1.479509

^{5}4A

Geometry with 51 atoms:

Total energy: -2206.994682820

C	-5.078539	-2.351419	-0.038145
C	-3.721761	-2.049423	-0.053014
C	-3.361884	-0.692356	-0.096916
C	-4.363551	0.313747	-0.122350
C	-5.730182	0.011450	-0.107918
C	-6.066672	-1.338360	-0.065955
H	-5.393938	-3.396672	-0.005038
H	-2.957953	-2.826832	-0.033665
H	-6.492641	0.792359	-0.128127
H	-7.120910	-1.624444	-0.053912
N	-3.675769	1.512665	-0.158077
H	-4.090462	2.439040	-0.171735
N	-2.119454	-0.084595	-0.118076
C	-2.347133	1.231004	-0.150735
C	1.115042	2.207573	-0.147695
C	1.140379	3.605257	-0.228778
C	-0.082878	4.283400	-0.275430
C	-1.288148	3.572928	-0.251880
C	-1.228145	2.176058	-0.168180
N	-0.048580	1.537927	-0.105513
H	-0.096975	5.373137	-0.341692
H	2.084965	4.151456	-0.263158
H	-2.245073	4.094792	-0.305642
C	2.257831	1.291798	-0.119041
C	3.700209	-1.960417	-0.087796
C	5.062779	-2.234347	-0.055398
C	6.029246	-1.200321	-0.030706
C	5.665738	0.143317	-0.039574
C	4.293495	0.418052	-0.071858
C	3.314435	-0.609714	-0.092351
H	2.951163	-2.751881	-0.113475
H	5.400069	-3.273235	-0.051031
H	7.088897	-1.464820	-0.005697
H	6.412354	0.939464	-0.022727
N	3.579678	1.602693	-0.090877
H	3.974642	2.537594	-0.083658
N	2.060099	-0.028391	-0.120166
Cr	-0.016649	-0.603345	-0.093322
C	0.083684	-2.627994	-0.632754
H	-0.892078	-3.124748	-0.466962
H	0.788469	-3.150537	0.045381
C	0.516227	-2.828074	-2.091235
H	1.500086	-2.368625	-2.300199
H	0.603058	-3.892801	-2.387079
C	0.204268	-1.611585	2.700256
H	-0.587366	-2.357030	2.573373
H	1.233875	-1.973322	2.616744
C	-0.072565	-0.331530	2.973936
H	0.720351	0.408766	3.123583
H	-1.103036	0.022476	3.082181
H	-0.200976	-2.370217	-2.797680

^{5}TS[4A-5A]

Geometry with 51 atoms:

Total energy: -2206.968956550

C	4.986472	-2.302749	-0.266808
C	3.634684	-1.964924	-0.255377
C	3.302880	-0.607191	-0.137660
C	4.327786	0.370071	-0.040260
C	5.684520	0.033832	-0.052607
C	5.995115	-1.320588	-0.166209
H	5.274220	-3.352616	-0.357473
H	2.862713	-2.728912	-0.339001
H	6.463351	0.795049	0.022836

H	7.043025	-1.628629	-0.179310
N	3.674493	1.586888	0.060120
H	4.114847	2.497127	0.140906
N	2.075024	0.037279	-0.093692
C	2.336547	1.350632	0.025710
C	-1.143850	2.294807	0.082259
C	-1.161474	3.685487	0.161233
C	0.057218	4.381194	0.209172
C	1.266961	3.667440	0.170782
C	1.229464	2.278135	0.092657
N	0.037544	1.599922	0.058930
H	0.065047	5.470290	0.270986
H	-2.110894	4.224787	0.183550
H	2.223533	4.193051	0.199588
C	-2.264745	1.386631	0.005054
C	-3.653282	-1.892226	-0.288841
C	-5.014108	-2.190805	-0.319805
C	-5.995336	-1.180380	-0.234908
C	-5.645368	0.163854	-0.118693
C	-4.279630	0.459269	-0.087451
C	-3.279971	-0.545636	-0.166947
H	-2.907206	-2.681283	-0.360977
H	-5.329786	-3.232241	-0.414143
H	-7.051652	-1.457134	-0.263247
H	-6.401288	0.948998	-0.056077
N	-3.596253	1.657618	0.018422
H	-4.013609	2.579423	0.089621
N	-2.033284	0.064909	-0.105478
Cr	0.023891	-0.384476	-0.127580
C	-0.694843	-3.002127	2.110299
H	-0.452492	-4.016375	1.752855
H	-1.767735	-2.823986	1.932156
C	0.169831	-1.942582	1.461372
H	-0.067764	-0.955463	1.916439
H	1.244487	-2.122638	1.603884
C	-0.003415	-2.691962	-0.594243
H	-0.961803	-3.161714	-0.369486
H	0.853035	-3.318656	-0.335061
C	0.075425	-1.818159	-1.697283
H	1.029533	-1.684343	-2.217062
H	-0.827741	-1.608617	-2.280367
H	-0.543155	-3.007124	3.204505

^{5}5A

Geometry with 51 atoms:

Total energy: -2207.029800490

C	5.082185	-2.052194	-0.723750
C	3.725205	-1.754766	-0.675725
C	3.364852	-0.434339	-0.358623
C	4.365140	0.540073	-0.102553
C	5.731881	0.242081	-0.152300
C	6.069446	-1.070887	-0.466873
H	5.398121	-3.069473	-0.965685
H	2.963241	-2.507551	-0.874162
H	6.492910	0.999118	0.045195
H	7.123764	-1.352528	-0.517170
N	3.676479	1.707904	0.171175
H	4.090330	2.606901	0.395980
N	2.122292	0.161497	-0.234099
C	2.349480	1.438901	0.081631
C	-1.110550	2.402089	0.257849
C	-1.135434	3.772176	0.549211
C	0.089146	4.431049	0.706738
C	1.294777	3.732829	0.573949
C	1.231487	2.364744	0.282044
N	0.051651	1.745260	0.136808
H	0.104076	5.499687	0.930721
H	-2.078426	4.313882	0.646911
H	2.253120	4.243019	0.688702
C	-2.253132	1.511036	0.036500
C	-3.723241	-1.642649	-0.712861
C	-5.088480	-1.895189	-0.779453
C	-6.046248	-0.878387	-0.550502
C	-5.669052	0.425710	-0.244760
C	-4.293960	0.677652	-0.175691
C	-3.322373	-0.331592	-0.405950
H	-2.983862	-2.423695	-0.886549
H	-5.434552	-2.904430	-1.013683
H	-7.108579	-1.124899	-0.614758
H	-6.406420	1.210709	-0.067395
N	-3.571862	1.824140	0.100069
H	-3.959361	2.738553	0.308898
N	-2.062545	0.224367	-0.267359
Cr	0.024142	-0.332186	-0.407449
C	-0.733161	-3.210246	1.397031
H	-1.712370	-3.500968	0.975079
H	-0.856975	-2.158237	1.723150
C	0.052249	-2.365433	-0.909789
H	0.831385	-2.514826	-1.684720
H	-0.896173	-2.671241	-1.394634
C	0.332333	-3.281162	0.294464
H	0.431214	-4.342944	-0.013633
H	1.311030	-3.024076	0.746114
C	-0.420830	-4.080316	2.613694
H	0.532524	-3.782892	3.083807
H	-1.207920	-4.007811	3.382524
H	-0.328930	-5.143100	2.332232

^{5}TS[5A-12A]

Geometry with 51 atoms:

Total energy: -2206.987955450

C	5.027684	-1.887211	-0.794144
C	3.660475	-1.641424	-0.708061
C	3.254915	-0.329364	-0.420929
C	4.218827	0.696806	-0.241422
C	5.593592	0.451824	-0.327896
C	5.978541	-0.858065	-0.604854
H	5.377639	-2.897649	-1.017291

H	2.923855	-2.429613	-0.863749
H	6.327781	1.247419	-0.187522
H	7.042078	-1.095461	-0.682338
N	3.491873	1.848534	0.000769
H	3.874218	2.771767	0.175506
N	1.990482	0.218046	-0.282070
C	2.171121	1.523268	-0.031816
C	-1.344883	2.298193	0.119768
C	-1.433258	3.684448	0.257421
C	-0.246940	4.426385	0.340747
C	0.993477	3.779515	0.263281
C	1.014206	2.389316	0.129801
N	-0.138609	1.675313	0.092502
H	-0.289987	5.511819	0.446490
H	-2.404378	4.181109	0.289129
H	1.923105	4.351020	0.291469
C	-2.427026	1.341089	-0.047434
C	-3.604229	-1.964311	-0.659581
C	-4.940701	-2.346682	-0.723199
C	-5.986563	-1.412109	-0.541995
C	-5.732210	-0.064777	-0.293700
C	-4.387793	0.318089	-0.228314
C	-3.330931	-0.612452	-0.403529
H	-2.789979	-2.675613	-0.808843
H	-5.191839	-3.391180	-0.921443
H	-7.021811	-1.755904	-0.601379
H	-6.541713	0.654851	-0.158155
N	-3.772930	1.539014	-0.008213
H	-4.241785	2.422968	0.158420
N	-2.126540	0.057744	-0.286651
Cr	-0.056860	-0.360923	-0.067376
C	-0.144265	-1.168253	2.015784
H	0.779305	-0.813674	2.486940
H	-1.083048	-0.741861	2.380293
C	-0.145439	-2.378648	1.324196
H	-0.071301	-2.005304	-0.426571
C	1.033996	-3.323714	1.332146
H	0.990439	-3.838889	2.310235
H	1.970718	-2.742861	1.342865
C	1.050862	-4.368119	0.220173
H	0.130757	-4.976041	0.230439
H	1.121846	-3.900096	-0.774797
H	1.904044	-5.054379	0.337972
H	-1.115990	-2.853662	1.136349

^{5}6A
Geometry with 57 atoms:
Total energy: -2285.575063440

C	5.086816	-2.015060	-0.778805
C	3.725868	-1.739129	-0.713810
C	3.345931	-0.444805	-0.321980
C	4.333129	0.527439	-0.010975
C	5.703617	0.250666	-0.073673
C	6.060096	-1.037197	-0.462916
H	5.417064	-3.011720	-1.080265
H	2.973324	-2.490073	-0.953551
H	6.453724	1.005719	0.168430
H	7.118340	-1.300694	-0.527247
N	3.629294	1.671218	0.318467
H	4.032545	2.562722	0.587904
N	2.095134	0.126368	-0.171983
C	2.304705	1.390444	0.203581
C	-1.167343	2.302763	0.442321
C	-1.202587	3.638258	0.859409
C	0.014671	4.298238	1.060424
C	1.224608	3.624867	0.860683
C	1.175094	2.289444	0.443817
N	0.000823	1.675631	0.225646
H	0.020179	5.340559	1.385098
H	-2.150721	4.151317	1.028157
H	2.178248	4.128040	1.027947
C	-2.304255	1.410942	0.209064
C	-3.724101	-1.748416	-0.600612
C	-5.084969	-2.024610	-0.667767
C	-6.058970	-1.031749	-0.404829
C	-5.704762	0.270816	-0.064402
C	-4.334464	0.548171	0.002412
C	-3.348296	-0.437947	-0.262847
H	-2.968152	-2.508617	-0.797157
H	-5.414517	-3.033056	-0.927906
H	-7.117023	-1.295893	-0.469825
H	-6.456734	1.035236	0.139391
N	-3.628993	1.700672	0.299568
H	-4.030516	2.603676	0.530520
N	-2.097691	0.134782	-0.123146
Cr	-0.012973	-0.382586	-0.358963
C	0.485072	-2.544466	2.248164
H	0.488537	-1.436349	2.280798
H	1.521813	-2.833646	1.994440
C	-0.067139	-2.484517	-0.261544
H	0.922057	-2.897286	-0.543727
H	-0.769751	-2.877621	-1.023140
C	-0.452388	-3.013620	1.127746
H	-1.484612	-2.699936	1.380743
H	-0.477746	-4.123326	1.147332
C	0.120920	-3.092710	3.626891
H	-0.899432	-2.791328	3.921120
H	0.150803	-4.195625	3.636930
H	0.812558	-2.735350	4.407877
C	-0.186360	-0.792655	-3.193860
H	0.604982	-1.548180	-3.226998
H	-1.215891	-1.163712	-3.185636
C	0.088508	0.517784	-3.211523
H	-0.706446	1.271233	-3.205078
H	1.118341	0.887553	-3.250701

^{5}TS[6A-7A]
Geometry with 57 atoms:

Total energy: -2285.548706310

C	5.050278	-2.328984	-0.897445
C	3.722262	-1.908458	-0.880549
C	3.457238	-0.607463	-0.428854
C	4.522687	0.236195	-0.019424
C	5.856273	-0.183169	-0.036139
C	6.100102	-1.481616	-0.480679
H	5.287398	-3.337834	-1.242675
H	2.917109	-2.564039	-1.210411
H	6.666762	0.474177	0.284466
H	7.127465	-1.851675	-0.509231
N	3.930128	1.431419	0.350926
H	4.410066	2.251778	0.705606
N	2.265915	0.089423	-0.294420
C	2.587488	1.306890	0.176958
C	-0.828051	2.458904	0.269978
C	-0.773867	3.793676	0.665596
C	0.475726	4.367406	0.947890
C	1.642802	3.597576	0.816332
C	1.531020	2.268623	0.413511
N	0.309550	1.708287	0.158770
H	0.541099	5.411689	1.256904
H	-1.687867	4.385388	0.745603
H	2.622688	4.036220	1.015372
C	-1.987426	1.677924	-0.103279
C	-3.484615	-1.293383	-1.398138
C	-4.848994	-1.482967	-1.606766
C	-5.790835	-0.475127	-1.305382
C	-5.398143	0.758697	-0.789050
C	-4.028507	0.946553	-0.580720
C	-3.071653	-0.060686	-0.871177
H	-2.762874	-2.071143	-1.644085
H	-5.199995	-2.432484	-2.017083
H	-6.851389	-0.665327	-1.485348
H	-6.123742	1.541604	-0.560669
N	-3.302244	2.022940	-0.100126
H	-3.683309	2.913647	0.200440
N	-1.810601	0.424053	-0.556321
Cr	0.193887	-0.197392	-0.463321
C	-1.319573	-2.410689	1.592565
H	-1.385801	-3.469796	1.287112
H	-2.173201	-1.900022	1.114250
C	-0.014795	-1.808485	1.101224
H	0.126644	-0.815835	1.583562
H	0.863985	-2.405134	1.380462
C	0.037900	-2.508882	-0.962277
H	-0.937480	-2.972596	-0.803069
H	0.870616	-3.158497	-0.683155
C	0.196795	-1.612231	-2.043553
H	1.171536	-1.529603	-2.535745
H	-0.671902	-1.359313	-2.661027
C	-1.491447	-2.327428	3.117144
H	-0.640782	-2.832310	3.609165
H	-1.437117	-1.267905	3.428194
C	-2.807664	-2.936865	3.598937
H	-2.915344	-2.854066	4.692511
H	-3.673827	-2.431727	3.138206
H	-2.873268	-4.006709	3.338304

^{5}7A

Geometry with 57 atoms:

Total energy: -2285.608682230

C	-5.040126	1.884382	-1.395814
C	-3.714669	1.474546	-1.309812
C	-3.450872	0.285147	-0.609817
C	-4.514012	-0.451290	-0.023984
C	-5.849086	-0.039786	-0.109871
C	-6.090315	1.140922	-0.805822
H	-5.281070	2.804459	-1.933108
H	-2.905483	2.044639	-1.764760
H	-6.658083	-0.614557	0.344619
H	-7.116276	1.504062	-0.900319
N	-3.915244	-1.545118	0.573378
H	-4.390507	-2.284977	1.080547
N	-2.260491	-0.372503	-0.352839
C	-2.579054	-1.461022	0.353123
C	0.789902	-2.665894	0.706346
C	0.721933	-3.855355	1.442479
C	-0.540173	-4.303357	1.848156
C	-1.691033	-3.574032	1.528879
C	-1.535563	-2.391691	0.793827
N	-0.320734	-1.979549	0.404531
H	-0.627936	-5.229592	2.419681
H	1.622529	-4.418278	1.693709
H	-2.677042	-3.921436	1.843260
C	1.986453	-2.001954	0.182174
C	3.665089	0.621807	-1.539005
C	5.041547	0.719735	-1.705413
C	5.925599	-0.257122	-1.187858
C	5.461062	-1.365220	-0.485818
C	4.074610	-1.461831	-0.318778
C	3.176443	-0.489723	-0.832556
H	2.981822	1.372841	-1.933557
H	5.455158	1.572288	-2.248782
H	7.000137	-0.136743	-1.343922
H	6.142236	-2.118649	-0.086026
N	3.277367	-2.399328	0.312186
H	3.602858	-3.230392	0.795478
N	1.884085	-0.858968	-0.502221
Cr	-0.152049	-0.173334	-0.740802
C	0.910577	2.968041	0.228225
H	1.890572	3.055675	-0.276713
H	0.963679	2.020033	0.801775
C	-0.052403	1.652902	-1.764952
H	-0.855408	1.668611	-2.529306
H	0.890210	1.741341	-2.340937
C	-0.196722	2.864693	-0.829029
H	-0.218287	3.818870	-1.395334

H	-1.171897	2.823437	-0.304939
C	0.738985	4.129805	1.208143
H	-0.242007	4.038719	1.712028
H	0.697698	5.080287	0.644325
C	1.842526	4.216856	2.266238
H	2.821030	4.319361	1.762118
H	1.889342	3.260533	2.820307
C	1.650840	5.368951	3.251766
H	2.460114	5.405136	3.999419
H	1.634960	6.341690	2.731341
H	0.696712	5.273872	3.798155

^{5}TS[7A-13A]

Geometry with 57 atoms:

Total energy: -2285.567482870

C	-5.063058	0.307153	-0.730502
C	-3.674869	0.380562	-0.664320
C	-2.975212	-0.805498	-0.396038
C	-3.674173	-2.027577	-0.218059
C	-5.069920	-2.103394	-0.283400
C	-5.749232	-0.914339	-0.539943
H	-5.638247	1.212127	-0.939089
H	-3.140960	1.317984	-0.818664
H	-5.600604	-3.046777	-0.142431
H	-6.839917	-0.926604	-0.600542
N	-2.697747	-2.983196	0.001168
H	-2.855485	-3.971237	0.169753
N	-1.617273	-1.048238	-0.275930
C	-1.487520	-2.361943	-0.041217
C	2.111476	-2.272821	0.067735
C	2.533543	-3.599842	0.167528
C	1.562269	-4.607313	0.243490
C	0.201599	-4.276871	0.196031
C	-0.155772	-2.930095	0.094644
N	0.791111	-1.958346	0.062942
H	1.866300	-5.652783	0.319876
H	3.597015	-3.847371	0.175279
H	-0.560930	-5.057434	0.225583
C	2.931793	-1.080395	-0.077835
C	3.292265	2.425063	-0.594905
C	4.500480	3.114174	-0.639638
C	5.738147	2.448726	-0.479370
C	5.809936	1.072898	-0.271013
C	4.594236	0.381702	-0.224498
C	3.346643	1.039911	-0.379247
H	2.332612	2.927993	-0.727605
H	4.497523	4.193722	-0.806487
H	6.662709	3.029091	-0.522222
H	6.766710	0.561596	-0.149489
N	4.286364	-0.955192	-0.039781
H	4.951071	-1.705275	0.117887
N	2.335276	0.100854	-0.284983
Cr	0.219044	0.007517	-0.069614
C	0.107328	0.769249	2.026303
H	-0.695628	0.191005	2.496757
H	1.126055	0.577890	2.375290
C	-0.192908	1.957953	1.362958
H	-0.210280	1.602234	-0.394936
C	-1.560513	2.595513	1.406441
H	-1.621857	3.094981	2.392229
H	-2.335632	1.811671	1.422478
C	-1.853712	3.624832	0.315301
H	-1.069889	4.404200	0.328880
H	-1.773736	3.141628	-0.674971
H	0.634164	2.653410	1.175907
C	-3.228658	4.281480	0.458329
C	-3.529480	5.292377	-0.646843
H	-3.296262	4.776912	1.443751
H	-4.005995	3.495557	0.464799
H	-3.505997	4.816904	-1.642384
H	-4.524264	5.748923	-0.519061
H	-2.787783	6.109057	-0.655362

^{5}8A

Geometry with 63 atoms:

Total energy: -2364.154317280

C	-4.970111	0.363019	-2.140920
C	-3.608637	0.329524	-1.862075
C	-3.183505	-0.503135	-0.813753
C	-4.126595	-1.270856	-0.081025
C	-5.497822	-1.237741	-0.359863
C	-5.899751	-0.407386	-1.402202
H	-5.335479	1.000014	-2.949569
H	-2.889196	0.923932	-2.424972
H	-6.214840	-1.832194	0.209426
H	-6.960380	-0.347710	-1.657120
N	-3.383590	-1.965991	0.855472
H	-3.748271	-2.622592	1.537480
N	-1.919874	-0.750056	-0.309051
C	-2.078111	-1.629853	0.682809
C	1.411454	-1.868359	1.516849
C	1.503779	-2.693933	2.642603
C	0.321336	-3.237294	3.156584
C	-0.909734	-2.941729	2.560684
C	-0.916681	-2.106563	1.436481
N	0.227828	-1.612334	0.936082
H	0.356839	-3.883431	4.036012
H	2.467069	-2.896670	3.113973
H	-1.837596	-3.342045	2.972187
C	2.501186	-1.158448	0.848972
C	3.783388	1.154367	-1.529056
C	5.126741	1.470001	-1.699166
C	6.137258	0.871440	-0.909223
C	5.838015	-0.061978	0.079303
C	4.485337	-0.378856	0.250060
C	3.462698	0.211293	-0.538787
H	2.999775	1.616103	-2.129949
H	5.413117	2.199773	-2.459736

H	7.179486	1.151501	-1.078947
H	6.617833	-0.521244	0.689647
N	3.830306	-1.237799	1.114729
H	4.264886	-1.830587	1.814442
N	2.240833	-0.299432	-0.138586
Cr	0.152213	-0.205153	-0.679270
C	-0.876268	2.962558	0.197932
H	-0.883555	2.051260	0.829300
H	-1.864326	2.980635	-0.299012
C	0.065799	1.595063	-1.763653
H	-0.889529	1.664729	-2.321593
H	0.853875	1.593282	-2.542275
C	0.219571	2.833869	-0.867718
H	1.203597	2.812058	-0.358782
H	0.226940	3.769676	-1.464445
C	-0.740919	4.190621	1.099470
H	0.246532	4.171045	1.598571
H	-0.741794	5.103641	0.475406
C	0.585418	-1.386289	-3.308256
H	-0.222071	-0.848857	-3.815181
H	1.598085	-0.997306	-3.453172
C	0.350533	-2.483265	-2.577207
H	1.162519	-3.034779	-2.091486
H	-0.660227	-2.887299	-2.458836
C	-1.840586	4.303470	2.158958
C	-1.698163	5.531641	3.056987
H	-1.840184	3.388094	2.780302
H	-2.825350	4.324473	1.656888
H	-2.504093	5.584635	3.807319
H	-0.737499	5.522179	3.600131
H	-1.731578	6.463553	2.467216

^{5}TS[8A-9A]
Geometry with 63 atoms:
Total energy: -2364.127486900

C	-4.667434	2.659652	-1.699682
C	-3.484551	1.941290	-1.537257
C	-3.475649	0.908498	-0.588404
C	-4.643768	0.621989	0.165368
C	-5.831338	1.341674	0.004524
C	-5.821630	2.365514	-0.941840
H	-4.705121	3.469279	-2.432076
H	-2.598083	2.172331	-2.126741
H	-6.723883	1.110261	0.589056
H	-6.729017	2.952144	-1.102322
N	-4.305560	-0.439491	0.987974
H	-4.915112	-0.891682	1.660945
N	-2.477405	0.024913	-0.206475
C	-3.010599	-0.768301	0.738785
C	-0.000050	-2.707170	1.164835
C	-0.305770	-3.685244	2.109307
C	-1.594966	-3.717154	2.664088
C	-2.551542	-2.772233	2.257671
C	-2.193441	-1.814084	1.313483
N	-0.931985	-1.779705	0.780682
H	-1.854742	-4.477129	3.402292
H	0.444773	-4.417834	2.412069
H	-3.561847	-2.790294	2.670976
C	1.240914	-2.501233	0.451024
C	3.218548	-0.811799	-1.997684
C	4.547155	-1.102896	-2.300729
C	5.250508	-2.129345	-1.634360
C	4.644696	-2.902339	-0.645046
C	3.311729	-2.608086	-0.343964
C	2.593916	-1.573521	-0.999117
H	2.682776	-0.023190	-2.523680
H	5.057051	-0.525057	-3.074884
H	6.291513	-2.324279	-1.901892
H	5.183515	-3.700289	-0.130429
N	2.422386	-3.165418	0.557919
H	2.616738	-3.936447	1.187397
N	1.307811	-1.529817	-0.478310
Cr	-0.471305	-0.413905	-0.605487
C	1.592624	2.395825	-0.169455
H	1.559171	3.122394	-1.000294
H	2.423580	1.703345	-0.394685
C	0.287876	1.624803	-0.094371
H	0.325252	0.972515	0.806015
H	-0.587404	2.281191	0.013785
C	0.086117	1.206051	-2.230361
H	1.160532	1.329504	-2.374321
H	-0.463878	2.149366	-2.274804
C	-0.523810	0.019602	-2.688250
H	-1.578442	0.029944	-2.981689
H	0.096330	-0.759426	-3.144773
C	1.911951	3.152363	1.128886
H	1.072582	3.829815	1.370542
H	1.969949	2.431883	1.965555
C	3.212677	3.956209	1.059153
H	4.049410	3.276658	0.811012
H	3.152156	4.676980	0.222483
C	3.538556	4.709893	2.351525
C	4.835080	5.514692	2.271884
H	3.600818	3.987936	3.186384
H	2.698618	5.384608	2.598762
H	5.042805	6.044548	3.215730
H	5.699446	4.862593	2.059050
H	4.788326	6.270775	1.469613

^{5}9A
Geometry with 63 atoms:
Total energy: -2364.187155250

C	-4.045500	3.640827	-1.648433
C	-3.100485	2.627087	-1.540515
C	-3.335693	1.624177	-0.584975
C	-4.501487	1.666150	0.224386
C	-5.453036	2.687069	0.117889
C	-5.202191	3.671512	-0.833145

H	-3.894264	4.436582	-2.381305
H	-2.210145	2.602133	-2.167464
H	-6.345094	2.709392	0.746510
H	-5.916060	4.489544	-0.954488
N	-4.423626	0.549813	1.036449
H	-5.101583	0.274765	1.739830
N	-2.597087	0.505218	-0.241656
C	-3.279068	-0.110089	0.728042
C	-0.940576	-2.803846	1.190925
C	-1.471879	-3.634656	2.185536
C	-2.701439	-3.277386	2.750161
C	-3.370438	-2.123327	2.327197
C	-2.770364	-1.346830	1.328105
N	-1.592348	-1.701240	0.795296
H	-3.143371	-3.905025	3.526758
H	-0.947792	-4.533704	2.513890
H	-4.331298	-1.843187	2.762526
C	0.317746	-2.971671	0.458525
C	2.731216	-1.993070	-1.965991
C	3.927160	-2.654298	-2.219554
C	4.297063	-3.822194	-1.510250
C	3.482098	-4.367068	-0.522460
C	2.278961	-3.699399	-0.267749
C	1.895500	-2.527736	-0.971733
H	2.442408	-1.092800	-2.507446
H	4.602136	-2.264709	-2.984907
H	5.247279	-4.307606	-1.744519
H	3.767356	-5.267056	0.025357
N	1.251201	-3.942865	0.624518
H	1.203803	-4.709961	1.287883
N	0.668762	-2.102909	-0.493359
Cr	-0.759364	-0.498332	-0.773472
C	1.897705	1.742936	-0.895034
H	2.653994	1.190074	-1.482632
H	1.621233	1.061835	-0.064444
C	-0.000824	0.723407	-2.301061
H	-0.840772	0.985474	-2.976024
H	0.716388	0.170229	-2.940051
C	0.667516	2.003998	-1.772278
H	0.975034	2.676006	-2.600191
H	-0.059079	2.596089	-1.181479
C	2.534355	3.004176	-0.308689
H	1.777684	3.550960	0.285077
H	2.818289	3.686131	-1.131414
C	3.759580	2.728097	0.566052
H	4.522634	2.196593	-0.032848
H	3.478070	2.030758	1.378026
C	4.381363	3.986186	1.176239
H	4.659687	4.685681	0.365889
H	3.618623	4.514820	1.778644
C	5.609537	3.710602	2.047990
C	6.215919	4.973708	2.658179
H	6.373269	3.188248	1.442954
H	5.331688	3.006813	2.854357
H	7.099009	4.744270	3.276781
H	6.533631	5.683328	1.875166
H	5.487223	5.498031	3.300004

^{5}TS[9A-14A]
Geometry with 63 atoms:
Total energy: -2364.146126080

C	4.296384	1.859355	-0.672575
C	3.050084	1.245052	-0.599148
C	1.935481	2.065999	-0.372140
C	2.090173	3.470412	-0.243263
C	3.342919	4.090116	-0.316095
C	4.440436	3.258898	-0.529926
H	5.185234	1.249086	-0.848523
H	2.930830	0.168751	-0.717245
H	3.455330	5.171023	-0.212865
H	5.437779	3.699842	-0.594778
N	0.811679	3.967545	-0.060125
H	0.562610	4.943093	0.062718
N	0.591923	1.753684	-0.257168
C	-0.051911	2.915865	-0.074695
C	-3.325558	1.416603	-0.026059
C	-4.239944	2.469732	0.038755
C	-3.746295	3.779268	0.118114
C	-2.364540	4.013795	0.102892
C	-1.502928	2.916053	0.032993
N	-1.989905	1.650459	0.008772
H	-4.440516	4.620059	0.170151
H	-5.313719	2.274530	0.017703
H	-1.970921	5.031660	0.132280
C	-3.600241	-0.004910	-0.167372
C	-2.512168	-3.371078	-0.578460
C	-3.341824	-4.486914	-0.630551
C	-4.747473	-4.368836	-0.527542
C	-5.370581	-3.132583	-0.370659
C	-4.535293	-2.011380	-0.315871
C	-3.123948	-2.119285	-0.414833
H	-1.426694	-3.449559	-0.663450
H	-2.901600	-5.478718	-0.756449
H	-5.360956	-5.271653	-0.573253
H	-6.455725	-3.044286	-0.291835
N	-4.793442	-0.659432	-0.164928
H	-5.707881	-0.233866	-0.056264
N	-2.575088	-0.853181	-0.323223
Cr	-0.688226	0.068588	-0.021741
C	-0.438043	-0.455623	2.133880
H	0.000990	0.443886	2.579241
H	-1.459034	-0.708566	2.433402
C	0.394866	-1.431443	1.588731
H	0.328279	-1.261465	-0.198755
C	1.899453	-1.368007	1.707013
H	2.134056	-1.699327	2.736577
H	2.227163	-0.316596	1.651338
C	2.689098	-2.226527	0.719008

H	2.395241	-3.285615	0.833871
H	2.401589	-1.950366	-0.310868
H	-0.020130	-2.437068	1.452358
C	4.204355	-2.089988	0.881519
C	5.003542	-2.862033	-0.170205
H	4.500867	-2.426291	1.891961
H	4.477614	-1.019771	0.831552
H	4.744292	-3.935667	-0.113786
H	4.690396	-2.531833	-1.178954
C	6.519741	-2.698639	-0.036407
C	7.307707	-3.465692	-1.097394
H	6.833420	-3.029558	0.970451
H	6.773914	-1.623698	-0.091700
H	8.394364	-3.325850	-0.977358
H	7.103848	-4.548693	-1.042528
H	7.039654	-3.132384	-2.114758

^{5}10A
Geometry with 69 atoms:
Total energy: -2442.732847910

C	-4.390460	3.301029	-1.747769
C	-3.377239	2.361725	-1.593182
C	-3.408166	1.563096	-0.438008
C	-4.440763	1.729871	0.522196
C	-5.461361	2.675098	0.367680
C	-5.416014	3.454901	-0.784402
H	-4.396726	3.940239	-2.633539
H	-2.581783	2.243695	-2.328822
H	-6.251594	2.794870	1.111201
H	-6.190928	4.207171	-0.948988
N	-4.166719	0.809434	1.517382
H	-4.711197	0.661776	2.360811
N	-2.554832	0.564474	-0.004623
C	-3.038716	0.140242	1.165167
C	-0.447544	-2.276378	1.781662
C	-0.713776	-2.837596	3.036949
C	-1.854164	-2.406423	3.723704
C	-2.687484	-1.428806	3.169358
C	-2.347665	-0.911909	1.913223
N	-1.266473	-1.354061	1.251655
H	-2.089600	-2.829572	4.702345
H	-0.052344	-3.588206	3.473046
H	-3.572239	-1.076677	3.702891
C	0.687344	-2.553006	0.897804
C	2.586758	-2.041164	-2.066864
C	3.768191	-2.699444	-2.388040
C	4.336793	-3.668871	-1.527662
C	3.741496	-4.012206	-0.317314
C	2.551693	-3.349260	0.004427
C	1.971034	-2.374635	-0.849026
H	2.147022	-1.290774	-2.723287
H	4.274402	-2.463745	-3.326871
H	5.267248	-4.159972	-1.821785
H	4.180745	-4.759156	0.346424
N	1.706161	-3.430352	1.095578
H	1.828859	-4.033440	1.902648
N	0.813439	-1.899461	-0.259995
Cr	-0.784960	-0.487326	-0.649081
C	1.857474	1.744425	-0.941927
H	2.549390	1.077408	-1.489367
H	1.568722	1.180668	-0.032289
C	-0.097653	0.701783	-2.243926
H	-0.955857	0.950675	-2.898912
H	0.585222	0.111070	-2.887433
C	0.613637	1.991378	-1.804454
H	0.920185	2.603123	-2.678408
H	-0.086043	2.636398	-1.236677
C	2.605607	3.011685	-0.524700
H	1.917213	3.679998	0.026200
H	2.905927	3.571892	-1.429462
C	3.842857	2.738218	0.333720
H	4.524356	2.063323	-0.217416
H	3.540927	2.181351	1.241332
C	4.606646	3.998543	0.745940
H	4.906139	4.556063	-0.161183
H	3.927923	4.673255	1.301036
C	5.847889	3.719427	1.597691
C	6.605039	4.984259	2.000712
H	6.524470	3.045007	1.041170
H	5.547912	3.162716	2.504940
H	7.492727	4.750968	2.611312
H	6.949188	5.544004	1.114283
H	5.965365	5.663775	2.589741
C	-2.496691	-2.758885	-1.815626
H	-1.875173	-3.615574	-1.534721
H	-3.428727	-2.621984	-1.257503
C	-2.146146	-1.933689	-2.809370
H	-2.778239	-1.091391	-3.107854
H	-1.227170	-2.083796	-3.384690

^{5}TS[10A-11A]
Geometry with 69 atoms:
Total energy: -2442.706082570

C	4.815368	-3.266814	-1.919940
C	3.831230	-2.296621	-1.743278
C	3.811838	-1.603569	-0.524329
C	4.778245	-1.891077	0.474871
C	5.766826	-2.863587	0.299982
C	5.766827	-3.547046	-0.915016
H	4.855102	-3.823586	-2.858907
H	3.104532	-2.078587	-2.525014
H	6.503169	-3.076744	1.077147
H	6.521713	-4.316022	-1.094393
N	4.491026	-1.038487	1.526993
H	4.988712	-0.987363	2.409360
N	2.976915	-0.600442	-0.055344
C	3.414291	-0.287232	1.176245
C	0.912937	2.253448	1.712859

C	1.202338	2.818109	2.953933
C	2.290563	2.322917	3.689440
C	3.071196	1.280665	3.163896
C	2.738731	0.755302	1.917883
N	1.668842	1.229516	1.210576
H	2.534998	2.754304	4.661274
H	0.598358	3.639036	3.345196
H	3.928981	0.892164	3.716509
C	-0.127641	2.619186	0.775675
C	-1.728696	2.331267	-2.403566
C	-2.833234	3.071660	-2.819328
C	-3.438096	4.032979	-1.980717
C	-2.953273	4.290510	-0.699327
C	-1.844514	3.546647	-0.284736
C	-1.233561	2.568983	-1.112735
H	-1.261219	1.599994	-3.061191
H	-3.240513	2.908115	-3.819618
H	-4.303291	4.590713	-2.346248
H	-3.415997	5.037259	-0.051457
N	-1.115451	3.546465	0.892060
H	-1.286954	4.134105	1.700972
N	-0.172221	2.004500	-0.420065
Cr	1.244973	0.464278	-0.597996
C	-1.657093	-1.286523	-0.992469
H	-1.854225	-1.773643	-1.963444
H	-2.024780	-0.249961	-1.087291
C	-0.165801	-1.277998	-0.708608
H	-0.010963	-0.950907	0.343009
H	0.293709	-2.272266	-0.792431
C	0.596436	-0.579906	-2.625168
H	-0.432295	-0.411932	-2.949257
H	0.944211	-1.597730	-2.816836
C	1.515190	0.491540	-2.704526
H	2.574892	0.281975	-2.884235
H	1.160326	1.475540	-3.029082
C	-2.475065	-2.001959	0.092575
H	-2.108446	-3.038587	0.205680
H	-2.295735	-1.509769	1.066701
C	-3.978097	-2.016707	-0.197229
H	-4.333051	-0.977141	-0.326407
H	-4.157673	-2.517514	-1.166511
C	-4.808276	-2.703987	0.889236
C	-6.311117	-2.713979	0.600678
H	-4.626121	-2.203783	1.858979
H	-4.453366	-3.743582	1.016798
H	-6.664808	-1.673860	0.469784
H	-6.493480	-3.216045	-0.367958
C	-7.145963	-3.396754	1.687413
C	-8.644461	-3.399618	1.388016
H	-6.962673	-2.894107	2.655013
H	-6.792227	-4.436041	1.816857
H	-9.218292	-3.896459	2.187291
H	-9.035090	-2.372378	1.287498
H	-8.863392	-3.927740	0.444184

^{5}11A
Geometry with 69 atoms:
Total energy: -2442.765742210

C	3.189372	-4.726264	-1.655164
C	2.691049	-3.433298	-1.545013
C	3.168452	-2.645853	-0.483653
C	4.121850	-3.173229	0.426520
C	4.624729	-4.474963	0.316498
C	4.139992	-5.239496	-0.740416
H	2.839495	-5.366193	-2.468333
H	1.958739	-3.037055	-2.247511
H	5.356971	-4.869823	1.023140
H	4.501682	-6.262383	-0.867904
N	4.366118	-2.156112	1.330727
H	5.003689	-2.201197	2.119250
N	2.867903	-1.348149	-0.109192
C	3.601144	-1.091520	0.977718
C	2.381898	2.258155	1.462890
C	3.032037	2.768519	2.592658
C	3.950622	1.942394	3.248898
C	4.201914	0.647534	2.781867
C	3.510393	0.212512	1.643666
N	2.634865	1.017267	1.023716
H	4.475986	2.310286	4.132666
H	2.832320	3.779973	2.950194
H	4.918312	0.002583	3.293221
C	1.384933	2.930531	0.626281
C	-0.875800	3.076949	-2.116685
C	-1.681609	4.163772	-2.434991
C	-1.668590	5.351286	-1.664530
C	-0.849051	5.490554	-0.548322
C	-0.038995	4.394827	-0.228651
C	-0.040994	3.198852	-0.993825
H	-0.883544	2.159386	-2.704085
H	-2.343875	4.103301	-3.301546
H	-2.319406	6.179464	-1.954308
H	-0.839482	6.405694	0.046536
N	0.876765	4.178867	0.784846
H	1.123609	4.836554	1.517537
N	0.857835	2.309654	-0.431998
Cr	1.614916	0.301179	-0.723194
C	-1.698370	-0.717634	-1.380922
H	-2.064157	0.112889	-2.012677
H	-1.335072	-0.236140	-0.450758
C	0.644997	-0.472588	-2.411420
H	1.408007	-1.013097	-3.007906
H	0.291992	0.343215	-3.073928
C	-0.529756	-1.411219	-2.090731
H	-0.927141	-1.892207	-3.008530
H	-0.185192	-2.251783	-1.456348
C	-2.868304	-1.641447	-1.037616
H	-2.507065	-2.465040	-0.393338
H	-3.234684	-2.124551	-1.962243

C	-4.032219	-0.928798	-0.344725
H	-4.396235	-0.110979	-0.994349
H	-3.663236	-0.436878	0.575320
C	-5.201476	-1.850117	0.010102
H	-5.566208	-2.346245	-0.908422
H	-4.838943	-2.663969	0.665585
C	-6.367997	-1.132152	0.693050
C	-7.535136	-2.053630	1.054478
H	-6.733136	-0.322389	0.033987
H	-6.002005	-0.630599	1.608745
H	-7.899015	-2.558186	0.139838
H	-7.171289	-2.861495	1.716941
C	-8.704835	-1.334298	1.731868
C	-9.862833	-2.264221	2.092074
H	-9.069374	-0.529950	1.066750
H	-8.339475	-0.827378	2.644052
H	-10.689348	-1.717514	2.574967
H	-10.271598	-2.760440	1.195230
H	-9.538215	-3.057784	2.786771

^{5}12A

Geometry with 51 atoms:

Total energy: -2207.005527920

C	4.951189	-1.865294	-1.307687
C	3.586880	-1.640972	-1.167817
C	3.187712	-0.364032	-0.742618
C	4.149099	0.643978	-0.471998
C	5.523637	0.418434	-0.612739
C	5.903081	-0.852714	-1.034400
H	5.303027	-2.845358	-1.637761
H	2.841378	-2.409928	-1.376337
H	6.258926	1.197430	-0.403462
H	6.965095	-1.076356	-1.159515
N	3.417800	1.752429	-0.080415
H	3.797712	2.658411	0.174412
N	1.928331	0.150308	-0.504500
C	2.102516	1.415742	-0.116477
C	-1.404942	2.141483	0.210967
C	-1.507252	3.489097	0.576813
C	-0.322954	4.213733	0.751505
C	0.920186	3.603020	0.552355
C	0.937856	2.252896	0.182763
N	-0.205261	1.564864	0.036284
H	-0.369415	5.266447	1.037729
H	-2.479682	3.964586	0.714946
H	1.846086	4.167142	0.674582
C	-2.492057	1.191812	-0.041644
C	-3.699861	-2.025921	-0.956230
C	-5.037417	-2.401965	-0.991579
C	-6.073645	-1.495923	-0.657620
C	-5.808750	-0.183422	-0.276802
C	-4.461286	0.194765	-0.239638
C	-3.415640	-0.705712	-0.572256
H	-2.889817	-2.710480	-1.213750
H	-5.301116	-3.420737	-1.284567
H	-7.110296	-1.837900	-0.700596
H	-6.609517	0.512300	-0.019674
N	-3.830824	1.382621	0.088445
H	-4.287796	2.239233	0.384496
N	-2.208341	-0.050652	-0.437447
Cr	-0.112457	-0.478405	-0.577022
C	-0.199593	-1.119337	2.404402
H	0.672259	-0.547127	2.734760
H	-1.173558	-0.632176	2.503371
C	-0.103719	-2.381893	1.958865
H	-0.033102	-1.995075	-1.327932
C	1.153462	-3.190592	1.807586
H	1.231285	-3.482614	0.743628
H	1.009450	-4.144005	2.349627
C	2.443437	-2.518137	2.265635
H	2.628484	-1.583125	1.714423
H	2.412664	-2.276370	3.340798
H	3.308985	-3.176268	2.093606
H	-1.025653	-2.897565	1.660858

^{5}13A

Geometry with 57 atoms:

Total energy: -2285.586167870

C	4.725314	-0.801924	-1.884488
C	3.353108	-0.777974	-1.666997
C	2.821451	0.366543	-1.052313
C	3.662839	1.446885	-0.678965
C	5.045538	1.423130	-0.897818
C	5.557246	0.279595	-1.505065
H	5.178728	-1.676147	-2.356771
H	2.699139	-1.602669	-1.953649
H	5.688858	2.255729	-0.607604
H	6.631029	0.213460	-1.694668
N	2.820859	2.388293	-0.111620
H	3.097781	3.289202	0.265151
N	1.522601	0.674223	-0.697119
C	1.558483	1.889088	-0.145104
C	-1.982867	2.085109	0.456060
C	-2.229740	3.349979	1.003362
C	-1.139020	4.202286	1.208041
C	0.154914	3.796603	0.861684
C	0.318785	2.517520	0.317781
N	-0.734561	1.703854	0.143047
H	-1.299312	5.194895	1.633954
H	-3.243755	3.663979	1.256803
H	1.006848	4.462053	1.007691
C	-2.953731	1.034025	0.140262
C	-3.802663	-2.194086	-1.088455
C	-5.086790	-2.723902	-1.133823
C	-6.210088	-1.991367	-0.678119
C	-6.088616	-0.704696	-0.160755
C	-4.794944	-0.171986	-0.113194
C	-3.662529	-0.897789	-0.567432

H	-2.927760	-2.742887	-1.441311
H	-5.238698	-3.729365	-1.532803
H	-7.200204	-2.449381	-0.735874
H	-6.956755	-0.142671	0.188438
N	-4.299341	1.043773	0.325028
H	-4.844007	1.805357	0.716716
N	-2.537814	-0.116492	-0.394507
Cr	-0.422657	-0.222811	-0.704256
C	-0.199966	-1.183951	2.136481
H	0.644141	-0.570608	2.464181
H	-1.200120	-0.802226	2.358770
C	-0.035106	-2.384521	1.558177
H	-0.202159	-1.608498	-1.657973
C	1.264594	-3.063046	1.235169
H	1.263586	-3.283774	0.151065
H	1.258293	-4.056992	1.722201
C	2.538816	-2.309233	1.611567
H	2.530905	-1.316614	1.129626
H	2.550410	-2.122209	2.700705
H	-0.934110	-2.949272	1.279473
C	3.818066	-3.046778	1.208830
C	5.089840	-2.278472	1.563468
H	3.795740	-3.239584	0.121311
H	3.834765	-4.039797	1.693150
H	5.994577	-2.831217	1.262388
H	5.117959	-1.299046	1.057584
H	5.158089	-2.096045	2.649665

^{5}14A
Geometry with 63 atoms:
Total energy: -2364.166386560

C	-4.257422	-0.345709	2.195644
C	-2.901500	-0.426033	1.902299
C	-2.330368	0.653503	1.210623
C	-3.118117	1.771519	0.832975
C	-4.485019	1.851271	1.124830
C	-5.035982	0.773181	1.812130
H	-4.739812	-1.164929	2.732990
H	-2.288178	-1.281088	2.190048
H	-5.087742	2.712178	0.830353
H	-6.099051	0.788896	2.061908
N	-2.246280	2.632906	0.188476
H	-2.483268	3.537154	-0.207038
N	-1.032825	0.862759	0.784883
C	-1.016193	2.056776	0.187354
C	2.509769	2.005439	-0.520865
C	2.820262	3.226448	-1.131923
C	1.779530	4.137353	-1.343003
C	0.473304	3.831298	-0.944170
C	0.244569	2.588931	-0.339344
N	1.250419	1.718779	-0.155966
H	1.989014	5.097902	-1.818367
H	3.842116	3.462373	-1.433039
H	-0.335836	4.546785	-1.096223
C	3.421129	0.906905	-0.192145
C	4.098923	-2.325897	1.126176
C	5.341827	-2.947903	1.128244
C	6.489988	-2.317700	0.588914
C	6.435297	-1.044403	0.028955
C	5.182997	-0.418736	0.025482
C	4.026247	-1.041680	0.562987
H	3.205640	-2.796698	1.540352
H	5.441058	-3.947844	1.556676
H	7.445310	-2.847034	0.613684
H	7.321688	-0.560607	-0.385397
N	4.753311	0.812027	-0.439308
H	5.330913	1.516505	-0.886943
N	2.952883	-0.187705	0.410114
Cr	0.841553	-0.161036	0.772114
C	0.712507	-1.182983	-2.121296
H	-0.062994	-0.488602	-2.457940
H	1.746358	-0.914737	-2.354718
C	0.425677	-2.341699	-1.507324
H	0.555896	-1.540270	1.724194
C	-0.937335	-2.862659	-1.151320
H	-0.933376	-3.083721	-0.067638
H	-1.067954	-3.847733	-1.639143
C	-2.115330	-1.950810	-1.486610
H	-1.944886	-0.963370	-1.025420
H	-2.154378	-1.776686	-2.576954
H	1.261020	-2.993191	-1.220430
C	-3.462792	-2.490588	-1.004949
C	-4.620832	-1.521249	-1.247553
H	-3.398497	-2.709233	0.076115
H	-3.675178	-3.456682	-1.498396
H	-4.387395	-0.556288	-0.761912
H	-4.702580	-1.308220	-2.330013
C	-5.968449	-2.024257	-0.725578
C	-7.112531	-1.039231	-0.960305
H	-5.877690	-2.233404	0.355839
H	-6.207396	-2.992525	-1.201549
H	-8.068102	-1.421681	-0.565784
H	-6.911105	-0.072184	-0.468761
H	-7.254369	-0.838113	-2.036000

^{5}15A
Geometry with 57 atoms:
Total energy: -2285.548422970

C	-4.936251	-1.921189	1.282675
C	-3.578012	-1.702394	1.085685
C	-3.196600	-0.442050	0.598673
C	-4.168391	0.554208	0.322381
C	-5.536639	0.334329	0.521377
C	-5.898697	-0.919688	1.005413
H	-5.274902	-2.888305	1.661176
H	-2.823944	-2.463157	1.293948
H	-6.280523	1.103976	0.307829
H	-6.955261	-1.138588	1.176646

N	-3.452842	1.645393	-0.140545
H	-3.846017	2.537859	-0.420067
N	-1.947961	0.062852	0.297285
C	-2.135962	1.310245	-0.138573
C	1.362784	2.016595	-0.582022
C	1.453023	3.307168	-1.118908
C	0.262499	4.002957	-1.355925
C	-0.974446	3.418872	-1.060419
C	-0.979772	2.125664	-0.522897
N	0.169776	1.467045	-0.305446
H	0.298162	5.009296	-1.778160
H	2.420671	3.755653	-1.352955
H	-1.904843	3.956291	-1.252876
C	2.457789	1.095915	-0.264632
C	3.695660	-2.052240	0.832753
C	5.038149	-2.401188	0.921411
C	6.067288	-1.493858	0.569516
C	5.790198	-0.206491	0.117896
C	4.438028	0.144792	0.028099
C	3.399457	-0.757368	0.377590
H	2.890582	-2.739022	1.099820
H	5.311482	-3.399585	1.270424
H	7.108140	-1.814573	0.654878
H	6.585562	0.490171	-0.153136
N	3.795994	1.304263	-0.371247
H	4.246658	2.155826	-0.690222
N	2.185467	-0.130661	0.183544
Cr	0.094092	-0.552666	0.382865
C	0.120147	-0.950199	-2.799371
H	-0.796432	-0.440415	-3.110183
H	1.053241	-0.390726	-2.909096
C	0.121503	-2.213625	-2.349766
H	0.023110	-2.137115	0.986927
C	-1.070995	-3.112890	-2.180084
H	-1.079027	-3.457179	-1.129657
H	-0.890579	-4.028218	-2.775054
C	-2.424113	-2.510612	-2.544130
H	-2.643595	-1.621015	-1.932986
H	-2.464405	-2.211955	-3.604588
H	-3.233625	-3.236350	-2.370262
H	1.083038	-2.663343	-2.070263
C	0.323959	0.138459	3.466387
H	-0.521590	-0.529638	3.658375
H	1.317785	-0.321039	3.471677
C	0.153558	1.446407	3.253008
H	1.001129	2.116910	3.073910
H	-0.841063	1.905075	3.263154

^{5}16A
Geometry with 57 atoms:
Total energy: -2285.582975940

C	-5.033853	-1.908162	-0.907706
C	-3.667804	-1.671407	-0.808241
C	-3.256147	-0.347325	-0.584950
C	-4.216131	0.691499	-0.465506
C	-5.592115	0.455016	-0.565600
C	-5.980822	-0.862708	-0.788527
H	-5.389390	-2.926246	-1.081665
H	-2.934191	-2.472411	-0.896799
H	-6.322438	1.260971	-0.472210
H	-7.044407	-1.097313	-0.873475
N	-3.482273	1.842973	-0.247053
H	-3.857621	2.777441	-0.122797
N	-1.991994	0.193983	-0.432583
C	-2.167375	1.503470	-0.237334
C	1.325765	2.315752	0.038215
C	1.404506	3.700807	0.230981
C	0.208886	4.425979	0.281559
C	-1.021726	3.776576	0.133975
C	-1.014279	2.387625	-0.048958
N	0.138510	1.701942	-0.079620
H	0.236525	5.507117	0.431924
H	2.368093	4.202290	0.337773
H	-1.956249	4.340702	0.156561
C	2.433019	1.362298	-0.068762
C	3.760138	-1.907605	-0.520638
C	5.112087	-2.231152	-0.530409
C	6.114147	-1.247308	-0.352724
C	5.797559	0.094473	-0.161016
C	4.436113	0.419340	-0.150922
C	3.421430	-0.558287	-0.324857
H	2.984778	-2.660338	-0.662166
H	5.412643	-3.270406	-0.681416
H	7.163746	-1.549734	-0.368900
H	6.570863	0.853086	-0.026866
N	3.765060	1.618241	0.008075
H	4.191828	2.528972	0.143834
N	2.188438	0.064848	-0.266898
Cr	0.084634	-0.428421	-0.352002
C	0.102548	-2.429909	-0.971639
H	-0.874690	-2.914734	-0.780638
H	0.826381	-2.990055	-0.345853
C	0.467047	-2.581739	-2.455471
H	0.520704	-3.635095	-2.796665
H	-0.270948	-2.083377	-3.111378
H	1.449305	-2.131588	-2.690625
C	0.102357	-0.292864	2.722120
H	-0.862573	0.184881	2.913908
H	0.981435	0.357026	2.727620
C	0.223073	-1.617691	2.545243
C	-0.883148	-2.635383	2.562626
H	-0.647227	-3.373087	3.352791
H	-0.826928	-3.209526	1.620355
C	-2.293604	-2.089513	2.760244
H	-2.397297	-1.573533	3.728808
H	-2.561548	-1.375193	1.966150
H	-3.034108	-2.903791	2.734532
H	1.227892	-2.028533	2.381564

^{5}TS[6A-16A]
Geometry with 57 atoms:
Total energy: -2285.524667480

C	-5.432688	-1.974653	-0.564463
C	-4.062143	-1.754657	-0.480911
C	-3.627499	-0.442625	-0.227452
C	-4.572509	0.605436	-0.063650
C	-5.952893	0.386993	-0.147538
C	-6.362437	-0.920064	-0.400410
H	-5.805622	-2.982638	-0.760446
H	-3.341572	-2.565195	-0.606384
H	-6.673452	1.197554	-0.021953
H	-7.430391	-1.138549	-0.474222
N	-3.814034	1.736424	0.166897
H	-4.174623	2.673439	0.309162
N	-2.354579	0.070247	-0.096815
C	-2.497938	1.364504	0.135459
C	0.982945	2.356724	0.309460
C	0.962759	3.726082	0.614291
C	-0.271719	4.355518	0.776474
C	-1.445579	3.616142	0.628903
C	-1.343712	2.250982	0.324093
N	-0.151087	1.644428	0.176839
H	-0.318702	5.419522	1.017113
H	1.886813	4.295381	0.725745
H	-2.417914	4.095373	0.755937
C	2.210412	1.580594	0.094547
C	4.052128	-1.353821	-0.655256
C	5.435801	-1.438514	-0.766507
C	6.264353	-0.307149	-0.575719
C	5.736299	0.945033	-0.271475
C	4.343192	1.027265	-0.160229
C	3.498512	-0.100123	-0.343153
H	3.411305	-2.223960	-0.804918
H	5.898710	-2.398242	-1.007482
H	7.346758	-0.419806	-0.672390
H	6.377423	1.817050	-0.128143
N	3.486525	2.073886	0.116793
H	3.761795	3.035942	0.281042
N	2.184771	0.284496	-0.172276
Cr	-0.057423	-0.580822	-0.212722
C	1.230621	-3.447095	1.096092
H	2.123634	-2.801695	1.081602
H	1.262934	-4.058436	0.178206
C	-0.058703	-1.377799	1.840475
H	-1.007745	-1.020407	2.249846
H	0.857159	-0.998893	2.307335
C	-0.013802	-2.573229	1.103590
H	-0.957004	-3.129057	1.005473
H	-0.039185	-2.276565	-0.458902
C	1.275132	-4.365231	2.322192
H	0.396397	-5.030540	2.357150
H	2.175658	-5.000011	2.304058
H	1.288454	-3.779376	3.255128
C	-0.018628	-2.059962	-2.056685
H	-0.907596	-2.694317	-2.151557
H	0.930754	-2.601439	-2.141784
C	-0.083751	-0.715176	-2.430065
H	0.824244	-0.181491	-2.725318
H	-1.040173	-0.271337	-2.721431

^{5}TS[15A-16A]
Geometry with 57 atoms:
Total energy: -2285.532499550

C	5.011851	-2.491266	0.576328
C	3.657003	-2.191811	0.472920
C	3.312100	-0.919526	-0.007215
C	4.318414	0.017063	-0.360038
C	5.681216	-0.283096	-0.257125
C	6.006718	-1.552770	0.215398
H	5.318773	-3.471859	0.947210
H	2.881525	-2.905681	0.756485
H	6.451224	0.439924	-0.532494
H	7.058805	-1.830528	0.312649
N	3.638857	1.150588	-0.772459
H	4.060076	2.009381	-1.110441
N	2.074570	-0.339525	-0.213321
C	2.305462	0.897007	-0.669811
C	-1.180191	1.760398	-0.968833
C	-1.219841	3.115975	-1.302466
C	-0.008066	3.796991	-1.478761
C	1.208280	3.125382	-1.297355
C	1.178675	1.769255	-0.964864
N	0.001579	1.109431	-0.830687
H	-0.011585	4.858461	-1.732583
H	-2.173519	3.636820	-1.407220
H	2.157887	3.654163	-1.399142
C	-2.300361	0.880453	-0.673138
C	-3.630229	-2.216046	0.475436
C	-4.982808	-2.529841	0.565976
C	-5.983882	-1.604531	0.188797
C	-5.667179	-0.334132	-0.287754
C	-4.306739	-0.019672	-0.378146
C	-3.294247	-0.943050	-0.009037
H	-2.849994	-2.919286	0.772214
H	-5.282914	-3.511511	0.939544
H	-7.033854	-1.893235	0.276420
H	-6.441969	0.378840	-0.575638
N	-3.635217	1.118639	-0.790712
H	-4.061892	1.970323	-1.139828
N	-2.060276	-0.350559	-0.205241
C	0.029277	-0.529222	2.953123
H	-1.029273	-0.793908	2.854293
H	0.749113	-1.350620	2.900968
C	0.420169	0.732659	3.170971
C	-0.490082	1.921057	3.304888
H	-0.505597	2.232760	4.366570

H	-1.524557	1.628230	3.054414
C	-0.051198	3.116417	2.453276
H	-0.726260	3.976140	2.591820
H	0.966439	3.446182	2.722407
H	-0.043768	2.861788	1.383192
H	1.493940	0.941146	3.278565
Cr	0.008647	-0.868860	-0.259543
C	0.006525	-2.098348	-2.205397
H	-0.927709	-1.780616	-2.678292
H	0.940208	-1.779771	-2.678847
C	0.007187	-3.099165	-1.250444
H	0.007614	-2.421536	0.415148
H	0.929535	-3.631858	-1.001396
H	-0.914679	-3.632223	-1.000405

^{4}1B

Geometry with 38 atoms:

Total energy: -2049.275756130

C	2.707912	-0.000076	4.973257
C	2.371639	-0.000161	3.619527
C	1.011001	-0.000026	3.285672
C	0.024952	0.000248	4.305554
C	0.358241	0.000411	5.662038
C	1.718018	0.000219	5.977550
H	3.760919	-0.000243	5.263962
H	3.143553	-0.000391	2.846696
H	-0.408146	0.000601	6.439537
H	2.021990	0.000264	7.026721
N	-1.193713	0.000215	3.645138
H	-2.109603	0.000172	4.081009
N	0.372424	-0.000215	2.054126
C	-0.955065	-0.000067	2.306140
C	-1.874091	-0.000109	-1.198514
C	-3.264331	-0.000084	-1.215926
C	-3.973498	-0.000125	-0.000000
C	-3.264331	-0.000084	1.215926
C	-1.874091	-0.000109	1.198514
N	-1.180390	-0.000198	-0.000000
H	-5.064035	-0.000169	-0.000000
H	-3.799631	-0.000033	-2.168325
H	-3.799631	-0.000033	2.168325
C	-0.955065	-0.000067	-2.306140
C	2.371639	-0.000161	-3.619527
C	2.707912	-0.000076	-4.973257
C	1.718018	0.000219	-5.977550
C	0.358241	0.000411	-5.662038
C	0.024952	0.000248	-4.305554
C	1.011001	-0.000026	-3.285672
H	3.143553	-0.000391	-2.846696
H	3.760919	-0.000243	-5.263962
H	2.021990	0.000264	-7.026721
H	-0.408146	0.000601	-6.439537
N	-1.193713	0.000215	-3.645138
H	-2.109603	0.000172	-4.081009
N	0.372424	-0.000215	-2.054126
Cr	0.761181	-0.000112	0.000000

^{4}2B

Geometry with 44 atoms:

Total energy: -2127.837213370

C	-4.998826	-2.443478	-0.024408
C	-3.641679	-2.119967	-0.026000
C	-3.291343	-0.762001	-0.025070
C	-4.306578	0.230221	-0.013297
C	-5.666105	-0.090195	-0.010826
C	-5.995173	-1.446368	-0.018569
H	-5.297400	-3.494278	-0.027261
H	-2.883164	-2.902936	-0.023840
H	-6.435581	0.684254	-0.003086
H	-7.047019	-1.740951	-0.018455
N	-3.640546	1.444666	-0.005464
H	-4.071852	2.362652	0.001270
N	-2.054867	-0.129105	-0.029800
C	-2.303334	1.199004	-0.015340
C	1.195201	2.118982	-0.007269
C	1.215763	3.508499	0.041350
C	-0.000007	4.217828	0.063520
C	-1.215777	3.508500	0.041366
C	-1.195216	2.118983	-0.007255
N	-0.000008	1.424960	-0.038192
H	-0.000006	5.307561	0.105935
H	2.168267	4.042910	0.069300
H	-2.168281	4.042911	0.069329
C	2.303319	1.199004	-0.015367
C	3.641699	-2.119963	-0.025953
C	4.998849	-2.443456	-0.024349
C	5.995184	-1.446335	-0.018550
C	5.666099	-0.090168	-0.010853
C	4.306569	0.230234	-0.013328
C	3.291341	-0.761999	-0.025071
H	2.883207	-2.902953	-0.023750
H	5.297437	-3.494253	-0.027159
H	7.047033	-1.740906	-0.018421
H	6.435567	0.684291	-0.003135
N	3.640529	1.444674	-0.005511
H	4.071830	2.362663	0.001209
N	2.054858	-0.129108	-0.029824
Cr	-0.000010	-0.531471	-0.041336
C	0.000047	-2.935580	-0.520268
C	0.000019	-2.855128	0.827654
H	-0.930092	-3.013249	-1.093459
H	0.930209	-3.013500	-1.093385
H	0.932653	-2.860762	1.402939
H	-0.932651	-2.860443	1.402882

^{4}3B

Geometry with 50 atoms:

Total energy: -2206.385660230

C	-4.952031	-2.402465	0.010342
C	-3.599839	-2.058843	0.005742
C	-3.272839	-0.695947	-0.007718
C	-4.297996	0.285644	-0.011897
C	-5.652556	-0.055966	-0.007752
C	-5.961087	-1.417715	0.002684
H	-5.237157	-3.456939	0.020809
H	-2.821583	-2.824351	0.015555
H	-6.434600	0.705833	-0.011542
H	-7.008793	-1.726770	0.006285
N	-3.643870	1.507460	-0.018348
H	-4.083757	2.421158	-0.019145
N	-2.045440	-0.051644	-0.014251
C	-2.301711	1.273753	-0.017717
C	1.194677	2.190802	-0.009828
C	1.215207	3.582028	-0.014361
C	0.000781	4.292184	-0.015128
C	-1.213776	3.582175	-0.016802
C	-1.193431	2.190972	-0.011979
N	0.000562	1.493034	-0.000625
H	0.000853	5.382801	-0.017978
H	2.168322	4.116287	-0.019111
H	-2.166804	4.116574	-0.023407
C	2.302725	1.273379	-0.014721
C	3.599933	-2.059591	0.001778
C	4.952025	-2.403626	0.006253
C	5.961357	-1.419153	0.001881
C	5.653209	-0.057290	-0.005485
C	4.298751	0.284717	-0.009645
C	3.273320	-0.696597	-0.007993
H	2.821477	-2.824916	0.008337
H	5.236831	-3.458211	0.013900
H	7.008974	-1.728512	0.005385
H	6.435470	0.704294	-0.007134
N	3.644962	1.506720	-0.013986
H	4.085088	2.420300	-0.013433
N	2.046096	-0.051975	-0.013419
Cr	0.000494	-0.479957	-0.015588
C	-0.001965	-2.455391	-1.705614
C	0.000377	-1.290610	-2.389190
H	0.931291	-2.972063	-1.458186
H	-0.937349	-2.967926	-1.457637
H	-0.931775	-0.819145	-2.716877
H	0.934392	-0.823019	-2.717129
C	-0.001675	-1.090121	2.442039
C	-0.005683	-2.303440	1.849537
H	-0.932736	-0.592347	2.730857
H	0.932480	-0.600692	2.735169
H	0.925647	-2.840421	1.641273
H	-0.940938	-2.831523	1.635975

^{4}TS[3B-4B]
Geometry with 50 atoms:
Total energy: -2206.365309560

C	4.968732	-2.324722	-0.253992
C	3.614239	-2.007645	-0.220479
C	3.268390	-0.648852	-0.153858
C	4.279665	0.347430	-0.129906
C	5.641676	0.029814	-0.164294
C	5.966067	-1.323156	-0.225161
H	5.271788	-3.372802	-0.306561
H	2.847974	-2.781210	-0.249329
H	6.411770	0.803228	-0.144907
H	7.017397	-1.618356	-0.253739
N	3.608959	1.556415	-0.073068
H	4.035782	2.476672	-0.047882
N	2.034729	-0.021983	-0.110222
C	2.276483	1.293010	-0.064410
C	-1.208416	2.192400	-0.014312
C	-1.250663	3.588163	-0.011024
C	-0.043109	4.297662	-0.009748
C	1.174741	3.605486	-0.022376
C	1.151351	2.209787	-0.024469
N	-0.024146	1.527232	-0.005252
H	-0.051096	5.389012	-0.008063
H	-2.206541	4.114972	-0.015686
H	2.123893	4.144770	-0.034717
C	-2.320751	1.260426	-0.048825
C	-3.639251	-2.046603	-0.223201
C	-4.991590	-2.372489	-0.246892
C	-5.995030	-1.378158	-0.197423
C	-5.677486	-0.024294	-0.126027
C	-4.317080	0.301037	-0.101707
C	-3.298188	-0.687330	-0.144466
H	-2.870234	-2.816354	-0.270027
H	-5.287592	-3.422119	-0.308291
H	-7.044753	-1.679640	-0.218738
H	-6.451389	0.744783	-0.091823
N	-3.655412	1.513801	-0.041565
H	-4.088743	2.430543	-0.004633
N	-2.067135	-0.052545	-0.107717
H	-0.207861	-2.913650	2.116502
H	1.446967	-2.327206	1.712177
H	-0.967460	-0.607127	2.488365
H	0.807679	-0.149060	2.498022
C	0.373472	-2.119973	1.635285
C	0.019510	-0.750712	2.031624
Cr	-0.006597	-0.465396	0.011273
C	0.034713	-1.992055	-1.339963
C	0.003398	-2.794461	-0.103533
H	-0.873867	-2.000050	-1.954166
H	0.959421	-2.027003	-1.928496
H	0.789972	-3.552996	-0.024415
H	-0.968978	-3.255932	0.095547

^{4}4B
Geometry with 50 atoms:
Total energy: -2206.399872380

C	-5.035170	-2.249444	-0.430060
C	-3.679340	-1.943784	-0.415096
C	-3.325028	-0.591334	-0.280396
C	-4.328854	0.405409	-0.161754
C	-5.694367	0.098986	-0.179326
C	-6.026479	-1.245536	-0.315581
H	-5.347251	-3.291292	-0.531414
H	-2.913191	-2.713792	-0.497999
H	-6.458727	0.872914	-0.088610
H	-7.079683	-1.534978	-0.332896
N	-3.644901	1.601322	-0.033318
H	-4.062500	2.520594	0.071755
N	-2.086158	0.021021	-0.223251
C	-2.317617	1.327939	-0.072483
C	1.145721	2.267900	0.026822
C	1.189682	3.657113	0.202143
C	-0.026782	4.342402	0.300209
C	-1.242726	3.653351	0.218082
C	-1.196190	2.264980	0.042367
N	-0.024451	1.622869	-0.037853
H	-0.027466	5.425207	0.441131
H	2.140121	4.191035	0.259102
H	-2.194574	4.183080	0.288179
C	2.270810	1.337122	-0.100783
C	3.679548	-1.915617	-0.446464
C	5.039844	-2.200712	-0.463363
C	6.016560	-1.182680	-0.350806
C	5.663305	0.156215	-0.216033
C	4.293180	0.441411	-0.197103
C	3.301843	-0.568713	-0.311685
H	2.929580	-2.701240	-0.528847
H	5.366656	-3.238053	-0.564371
H	7.073997	-1.456175	-0.368494
H	6.415058	0.942597	-0.126779
N	3.594709	1.627718	-0.068064
H	4.000671	2.552078	0.037500
N	2.053494	0.026991	-0.249318
H	0.193500	-4.322873	0.703074
H	-1.240311	-3.345556	1.025548
H	0.917636	-2.782688	-1.097612
H	-0.833028	-2.853915	-1.334724
C	-0.174671	-3.278959	0.736422
C	-0.050897	-2.551108	-0.612860
Cr	-0.025163	-0.519052	-0.220335
C	0.052391	-1.026477	1.769957
C	0.562132	-2.467492	1.812086
H	0.674546	-0.315196	2.339909
H	-0.989553	-0.955639	2.129459
H	0.440421	-2.918298	2.817201
H	1.647786	-2.485837	1.603807

^{4}5B
Geometry with 56 atoms:
Total energy: -2284.950074190

C	5.036302	-2.234906	0.223241
C	3.679463	-1.932992	0.208076
C	3.321120	-0.579479	0.093620
C	4.322218	0.422801	-0.005236
C	5.688454	0.119490	0.011244
C	6.024489	-1.226140	0.127590
H	5.351383	-3.277256	0.308988
H	2.915607	-2.706642	0.275464
H	6.451086	0.896776	-0.064365
H	7.078621	-1.512304	0.143772
N	3.634955	1.618541	-0.111101
H	4.049202	2.540823	-0.199515
N	2.080749	0.029354	0.050566
C	2.306866	1.338916	-0.075983
C	-1.160006	2.270319	-0.141424
C	-1.206185	3.658237	-0.328201
C	0.007748	4.346646	-0.430859
C	1.224234	3.658658	-0.352956
C	1.181682	2.271461	-0.165687
N	0.011583	1.627637	-0.060634
H	0.005965	5.428306	-0.579985
H	-2.158314	4.188096	-0.395145
H	2.175453	4.187396	-0.439568
C	-2.285598	1.339859	-0.034588
C	-3.692571	-1.918670	0.246160
C	-5.052345	-2.206958	0.250956
C	-6.029890	-1.188732	0.147759
C	-5.678543	0.153028	0.036025
C	-4.309001	0.441786	0.029675
C	-3.317148	-0.569388	0.132773
H	-2.940268	-2.703168	0.321247
H	-5.378046	-3.246227	0.334102
H	-7.086943	-1.464248	0.154245
H	-6.431771	0.938884	-0.045258
N	-3.611188	1.630810	-0.072380
H	-4.017034	2.556347	-0.165384
N	-2.069749	0.027900	0.091920
H	0.001262	-4.138688	-1.486750
H	1.363745	-3.018679	-1.596187
H	-0.916767	-2.917610	0.469131
H	0.815169	-2.989934	0.810778
C	0.289048	-3.079013	-1.339285
C	0.071428	-2.586280	0.097763
Cr	0.012271	-0.508492	0.061763
C	-0.061769	-0.711348	-1.997699
C	-0.485832	-2.153123	-2.284338
H	-0.727658	0.039979	-2.457115
H	0.967164	-0.527477	-2.355532
H	-0.332125	-2.430612	-3.346398
H	-1.569622	-2.269653	-2.094339
C	0.606541	-0.135875	2.791153
H	1.576751	-0.640202	2.768710
H	0.618076	0.957565	2.845082
C	-0.541587	-0.827808	2.814916

H	-1.512738	-0.329126	2.885320
H	-0.551853	-1.921156	2.809610

^{4}TS[5B-6B]
Geometry with 56 atoms:
Total energy: -2284.913482980

C	5.066358	-2.252654	-0.341313
C	3.710840	-1.947465	-0.289635
C	3.348547	-0.593778	-0.184430
C	4.356962	0.406925	-0.150172
C	5.721698	0.102026	-0.201715
C	6.057441	-1.245076	-0.294373
H	5.375807	-3.297023	-0.422762
H	2.956733	-2.732075	-0.336131
H	6.484167	0.882640	-0.172515
H	7.110723	-1.531571	-0.336627
N	3.682981	1.609562	-0.068094
H	4.104810	2.531907	-0.038296
N	2.111108	0.025976	-0.113941
C	2.351912	1.338615	-0.054470
C	-1.110182	2.301538	0.023644
C	-1.129572	3.693449	0.157269
C	0.091115	4.374144	0.215770
C	1.293974	3.663757	0.148426
C	1.239134	2.272521	0.013624
N	0.056158	1.628164	-0.054572
H	0.104897	5.460309	0.323028
H	-2.075866	4.234529	0.215799
H	2.253693	4.180548	0.204306
C	-2.248435	1.397618	-0.040598
C	-3.694876	-1.851264	-0.280731
C	-5.057659	-2.118030	-0.353204
C	-6.020700	-1.082741	-0.327440
C	-5.648995	0.254795	-0.233681
C	-4.277074	0.521811	-0.162628
C	-3.296909	-0.506843	-0.178558
H	-2.961790	-2.655881	-0.302231
H	-5.395356	-3.153768	-0.432436
H	-7.080832	-1.339721	-0.385452
H	-6.389924	1.056311	-0.218686
N	-3.570884	1.705807	-0.075327
H	-3.968091	2.639186	-0.054743
N	-2.043965	0.078461	-0.091668
C	-0.689735	-2.679872	1.572464
C	0.045751	-1.770655	2.561383
C	0.029869	-0.323617	2.081759
H	-1.739162	-2.355952	1.487688
H	1.087049	-2.131469	2.653702
H	-0.909487	0.179721	2.370525
H	-0.731915	-3.715923	1.959896
H	-0.403177	-1.887937	3.567053
H	0.869138	0.268086	2.484712
Cr	0.028385	-0.394484	-0.050400
C	0.015963	-2.734549	0.194794
H	-0.212347	-3.709624	-0.244890
H	1.105828	-2.725169	0.344930
C	-0.276845	-2.117704	-1.690533
H	-1.294115	-2.505971	-1.797303
H	0.475923	-2.847701	-2.004032
C	-0.059622	-0.760975	-2.130924
H	0.903474	-0.539727	-2.603044
H	-0.912952	-0.223757	-2.556046

^{4}6B
Geometry with 56 atoms:
Total energy: -2284.978124120

C	5.055499	-1.750476	-0.833813
C	3.689045	-1.520487	-0.723638
C	3.271998	-0.203109	-0.471497
C	4.231234	0.834132	-0.333805
C	5.607417	0.605406	-0.446018
C	6.000212	-0.705370	-0.698462
H	5.412460	-2.764288	-1.028492
H	2.962168	-2.324848	-0.822985
H	6.334261	1.412828	-0.339423
H	7.064082	-0.934601	-0.793419
N	3.497381	1.979992	-0.089357
H	3.872289	2.912360	0.053106
N	2.007056	0.336310	-0.308572
C	2.184499	1.641275	-0.084146
C	-1.303663	2.455317	0.160950
C	-1.388021	3.833500	0.395016
C	-0.192459	4.554270	0.491677
C	1.041598	3.910003	0.349247
C	1.034637	2.527777	0.118565
N	-0.116325	1.850916	0.043935
H	-0.222852	5.630384	0.674669
H	-2.352678	4.334195	0.495543
H	1.975412	4.471986	0.414380
C	-2.403663	1.501446	-0.006443
C	-3.719720	-1.741677	-0.653572
C	-5.071292	-2.061051	-0.712400
C	-6.076753	-1.086146	-0.509260
C	-5.762363	0.242844	-0.242114
C	-4.401103	0.562802	-0.182938
C	-3.381996	-0.405730	-0.381011
H	-2.946585	-2.491754	-0.810307
H	-5.367789	-3.091500	-0.920830
H	-7.125970	-1.385209	-0.564802
H	-6.536799	0.996352	-0.087776
N	-3.735267	1.752429	0.050129
H	-4.166000	2.654033	0.228437
N	-2.150677	0.215018	-0.260425
Cr	-0.058181	-0.299991	-0.251793
C	-0.044753	-0.797943	1.721964
C	1.026079	-1.780837	2.195086
C	0.688140	-3.272171	2.059530
C	0.711152	-3.902712	0.659854

C	-0.071092	-2.161819	-1.109105
C	-0.369252	-3.452507	-0.338091
H	-1.060618	-1.168010	1.947801
H	1.991937	-1.579635	1.696399
H	-0.304569	-3.452316	2.514084
H	1.710038	-3.759040	0.208294
H	0.890578	-2.269545	-1.650609
H	0.072500	0.181406	2.222219
H	1.219219	-1.589951	3.269196
H	1.405683	-3.834008	2.683612
H	0.610826	-4.993099	0.800534
H	-0.839255	-2.014383	-1.900105
H	-0.523650	-4.278882	-1.059761
H	-1.325797	-3.365759	0.209853

^{4}TS[6B-11B]
Geometry with 56 atoms:
Total energy: -2284.940365660

C	5.087035	-1.932915	-0.155057
C	3.721025	-1.666238	-0.151354
C	3.310839	-0.324343	-0.132294
C	4.288649	0.705512	-0.109853
C	5.662668	0.443523	-0.115409
C	6.044876	-0.895125	-0.139283
H	5.427547	-2.970616	-0.170739
H	2.992731	-2.472935	-0.164671
H	6.398292	1.249975	-0.100207
H	7.107518	-1.148208	-0.144335
N	3.577964	1.889074	-0.080806
H	3.972651	2.823542	-0.056892
N	2.048276	0.258053	-0.121673
C	2.255196	1.582231	-0.086918
C	-1.229411	2.477439	-0.015688
C	-1.269341	3.871578	0.011106
C	-0.061138	4.581586	0.009406
C	1.153416	3.884410	-0.022738
C	1.126891	2.488832	-0.045751
N	-0.045676	1.801663	-0.033808
H	-0.066657	5.672640	0.028086
H	-2.225227	4.398507	0.027863
H	2.103298	4.422356	-0.031518
C	-2.344095	1.551678	-0.044015
C	-3.658131	-1.761684	-0.219310
C	-5.010987	-2.089633	-0.233788
C	-6.015052	-1.097555	-0.173850
C	-5.698078	0.256930	-0.101164
C	-4.338443	0.584412	-0.085599
C	-3.318670	-0.401913	-0.137714
H	-2.888154	-2.530308	-0.273012
H	-5.305676	-3.139629	-0.295526
H	-7.064596	-1.399965	-0.187556
H	-6.472629	1.025015	-0.059305
N	-3.679081	1.799945	-0.026753
H	-4.114578	2.715525	0.012295
N	-2.088243	0.238169	-0.105822
Cr	-0.047384	-0.202041	0.007803
H	-1.474792	-2.097572	1.539535
H	-0.422505	-1.789967	0.004981
H	1.064620	-0.597766	2.420151
H	-0.689023	-0.074330	2.627359
C	-0.406454	-1.874912	1.411000
C	0.036014	-0.652542	2.045152
C	-0.150148	-1.870201	-1.470405
C	0.443455	-3.144986	1.326693
C	0.134010	-3.966690	0.058655
C	0.496991	-3.256226	-1.264548
H	-1.187611	-1.959795	-1.828819
H	0.410187	-1.286969	-2.220304
H	1.512039	-2.878014	1.359853
H	0.254197	-3.759252	2.223644
H	0.669506	-4.928789	0.105322
H	-0.943042	-4.220176	0.057773
H	1.591695	-3.152872	-1.316704
H	0.228052	-3.918753	-2.106156

^{4}7B
Geometry with 62 atoms:
Total energy: -2363.525890600

C	5.051171	-1.770752	-0.712444
C	3.685302	-1.539327	-0.598105
C	3.274377	-0.233813	-0.282730
C	4.236726	0.791968	-0.090359
C	5.612300	0.561133	-0.205967
C	5.999764	-0.738011	-0.520323
H	5.404795	-2.775369	-0.955000
H	2.953246	-2.332782	-0.740979
H	6.342809	1.358311	-0.056369
H	7.063078	-0.967718	-0.620367
N	3.505829	1.928609	0.202987
H	3.884680	2.850788	0.392855
N	2.011210	0.301974	-0.104216
C	2.190504	1.593182	0.184734
C	-1.298044	2.398454	0.451664
C	-1.381285	3.763071	0.755463
C	-0.185343	4.477319	0.889873
C	1.047523	3.837667	0.721074
C	1.039860	2.470022	0.416416
N	-0.111565	1.801609	0.292849
H	-0.214651	5.542693	1.127566
H	-2.345866	4.257829	0.882615
H	1.983035	4.390022	0.826071
C	-2.399502	1.453722	0.252018
C	-3.717282	-1.754501	-0.547191
C	-5.068942	-2.073022	-0.609544
C	-6.073825	-1.112233	-0.345131
C	-5.759130	0.201478	-0.010643
C	-4.397924	0.521248	0.051095
C	-3.379302	-0.433523	-0.208903

H	-2.943847	-2.493483	-0.748620
H	-5.366027	-3.091790	-0.868457
H	-7.123070	-1.410213	-0.405848
H	-6.533328	0.943583	0.192276
N	-3.731603	1.698611	0.338381
H	-4.162199	2.586866	0.573996
N	-2.148243	0.183321	-0.072077
Cr	-0.058599	-0.326376	-0.111494
C	-0.058068	-0.842107	1.867304
C	1.024613	-1.804598	2.361908
C	0.697397	-3.300088	2.258822
C	0.684061	-3.943149	0.865859
C	-0.101434	-2.222421	-0.918288
C	-0.413910	-3.486185	-0.110204
H	-1.067523	-1.238691	2.076841
H	1.987273	-1.609286	1.854687
H	-0.281288	-3.481211	2.742650
H	1.673292	-3.808418	0.390172
H	0.855852	-2.363008	-1.458963
H	0.025941	0.130994	2.386061
H	1.221079	-1.590778	3.430931
H	1.436503	-3.849026	2.869510
H	0.578862	-5.031813	1.016640
H	-0.866315	-2.092706	-1.712801
H	-0.608692	-4.323693	-0.809326
H	-1.354005	-3.362290	0.458597
C	0.593476	0.248065	-3.226891
H	1.564056	0.752759	-3.194314
H	0.607785	-0.826272	-3.430849
C	-0.552664	0.913853	-3.051744
H	-1.523131	0.411206	-3.110030
H	-0.567878	1.992954	-2.865749

^{4}TS[7B-8B]
Geometry with 62 atoms:
Total energy: -2363.486297180

C	5.101463	-1.931015	-0.841325
C	3.742503	-1.666166	-0.711023
C	3.359173	-0.345576	-0.418214
C	4.351527	0.660521	-0.268265
C	5.719282	0.395376	-0.398085
C	6.075839	-0.918288	-0.686596
H	5.426387	-2.948605	-1.069637
H	3.003295	-2.455422	-0.832809
H	6.467676	1.181296	-0.280673
H	7.132140	-1.173440	-0.798076
N	3.660584	1.826552	-0.001884
H	4.069955	2.743763	0.142639
N	2.112962	0.236079	-0.238047
C	2.335175	1.531429	-0.000148
C	-1.126239	2.433393	0.310916
C	-1.148778	3.789272	0.655689
C	0.067582	4.469271	0.766362
C	1.268814	3.787931	0.549629
C	1.213269	2.429775	0.219781
N	0.034361	1.791407	0.084725
H	0.079863	5.528292	1.030641
H	-2.095866	4.300499	0.835838
H	2.228094	4.299275	0.644496
C	-2.271361	1.555347	0.124428
C	-3.784511	-1.518914	-0.840625
C	-5.151075	-1.726748	-0.991692
C	-6.093292	-0.705837	-0.728108
C	-5.693793	0.563308	-0.321800
C	-4.317629	0.771746	-0.176878
C	-3.357744	-0.250673	-0.408662
H	-3.069371	-2.308223	-1.061794
H	-5.507964	-2.702912	-1.327720
H	-7.157515	-0.915955	-0.857222
H	-6.415130	1.360804	-0.134034
N	-3.587074	1.893800	0.158593
H	-3.961966	2.816253	0.353965
N	-2.090977	0.270228	-0.186587
C	-0.875846	-3.066313	0.311632
C	-0.430860	-3.769963	1.606165
C	-0.266378	-2.831581	2.811319
C	0.114768	-0.385369	1.941196
C	0.673742	-1.618439	2.672224
H	-1.621129	-2.307680	0.591851
H	0.511509	-4.317088	1.420469
H	-1.265774	-2.458114	3.103906
H	-0.919468	-0.192770	2.283871
H	-1.400163	-3.776450	-0.349684
H	-1.177767	-4.537908	1.873927
H	0.081295	-3.445409	3.660724
H	0.707452	0.494668	2.249754
H	0.944773	-1.313020	3.701501
H	1.632684	-1.947346	2.224274
Cr	0.043097	-0.239601	-0.213333
C	0.308027	-2.462532	-0.448435
H	0.743553	-3.220736	-1.105716
H	1.124289	-2.184101	0.232410
C	0.031966	-1.456034	-2.295610
H	-0.855765	-2.063425	-2.500524
H	0.956857	-1.905214	-2.664479
C	-0.072362	-0.042244	-2.374863
H	0.799738	0.518244	-2.723381
H	-1.044558	0.404634	-2.596180

^{4}8B
Geometry with 62 atoms:
Total energy: -2363.550451590

C	5.115254	-1.671622	-0.643612
C	3.752716	-1.399747	-0.599990
C	3.364773	-0.066907	-0.383008
C	4.348603	0.942607	-0.211645
C	5.720784	0.671241	-0.258314
C	6.084367	-0.653869	-0.477817

H	5.449155	-2.698431	-0.808904
H	3.010048	-2.185246	-0.723570
H	6.466413	1.457455	-0.126556
H	7.143936	-0.916169	-0.521167
N	3.640794	2.112332	-0.005340
H	4.038380	3.031857	0.157301
N	2.111803	0.513847	-0.281214
C	2.319294	1.812416	-0.051648
C	-1.150356	2.706625	0.145065
C	-1.206249	4.087771	0.372020
C	0.004512	4.781998	0.475406
C	1.224598	4.108672	0.346510
C	1.188010	2.725684	0.125929
N	0.022959	2.074087	0.045297
H	-0.002879	5.859758	0.650776
H	-2.160840	4.610615	0.457946
H	2.171609	4.648369	0.410320
C	-2.269480	1.781173	-0.044572
C	-3.670313	-1.395346	-0.823605
C	-5.029117	-1.669767	-0.925181
C	-6.008535	-0.671950	-0.706624
C	-5.659071	0.636412	-0.386553
C	-4.290227	0.909875	-0.286089
C	-3.297258	-0.083619	-0.490571
H	-2.916712	-2.159530	-1.003714
H	-5.351836	-2.681062	-1.182496
H	-7.064970	-0.935111	-0.796372
H	-6.412301	1.409676	-0.225188
N	-3.593111	2.071023	-0.008144
H	-3.999033	2.981798	0.181320
N	-2.049288	0.492412	-0.320775
Cr	0.034604	-0.072554	-0.280361
C	0.107721	-0.470110	1.741896
C	-1.003087	-1.289084	2.395137
C	-1.283336	-2.692324	1.838922
C	0.717674	-4.045213	-0.533672
C	0.131122	-1.716354	-1.525689
C	-0.251728	-3.190941	-1.367445
H	0.147717	0.535430	2.199528
H	-0.773123	-1.389941	3.476384
H	-1.636565	-2.604998	0.803745
H	1.678966	-4.093448	-1.079914
H	1.156441	-1.649479	-1.941810
H	1.099001	-0.926018	1.894795
H	-1.947399	-0.716821	2.353491
H	-2.137910	-3.101449	2.406270
H	0.340712	-5.084414	-0.517214
H	-0.529419	-1.252777	-2.297360
H	-0.312344	-3.664076	-2.367188
H	-1.269030	-3.286130	-0.954874
C	1.018534	-3.608886	0.908069
C	-0.135826	-3.714509	1.921154
H	1.431304	-2.590880	0.902489
H	1.836725	-4.253431	1.275908
H	-0.567631	-4.728146	1.830414
H	0.288729	-3.667389	2.941099

^{4}TS[8B-12B]

Geometry with 62 atoms:

Total energy: -2363.518217640

C	5.069866	-1.670684	-0.352796
C	3.705038	-1.400602	-0.310847
C	3.303966	-0.060161	-0.189756
C	4.285912	0.964516	-0.135311
C	5.658157	0.697081	-0.175747
C	6.032795	-0.639775	-0.282178
H	5.405542	-2.705950	-0.445596
H	2.974319	-2.203804	-0.375026
H	6.398350	1.498128	-0.129096
H	7.093990	-0.896508	-0.317191
N	3.580872	2.150017	-0.049235
H	3.980623	3.081627	-0.006887
N	2.046608	0.527741	-0.123527
C	2.256888	1.849443	-0.051539
C	-1.231592	2.725644	-0.046402
C	-1.280836	4.120129	-0.014825
C	-0.077599	4.836788	0.026500
C	1.141668	4.147297	0.027661
C	1.123987	2.752012	-0.011264
N	-0.045509	2.059208	-0.037254
H	-0.090492	5.927591	0.054135
H	-2.239359	4.642205	-0.022374
H	2.088615	4.690137	0.054048
C	-2.340958	1.792969	-0.081813
C	-3.666957	-1.515496	-0.071422
C	-5.019950	-1.840934	-0.061418
C	-6.021482	-0.844343	-0.063089
C	-5.700215	0.510880	-0.069255
C	-4.339325	0.834375	-0.076609
C	-3.322522	-0.156036	-0.084255
H	-2.898527	-2.284691	-0.065287
H	-5.316328	-2.892168	-0.051339
H	-7.071937	-1.143895	-0.056381
H	-6.472255	1.282631	-0.065676
N	-3.675232	2.047402	-0.074504
H	-4.106440	2.965848	-0.065683
N	-2.088157	0.476794	-0.095348
H	-0.118692	-1.597039	-0.021825
H	-1.206250	-1.980406	1.570190
H	-0.939379	0.247871	2.508300
H	0.890285	0.045164	2.529515
C	-0.191280	-1.563072	1.514474
C	-0.061831	-0.226215	2.056765
Cr	-0.027726	0.054635	0.016684
C	-0.748388	-3.858224	-0.859175
C	0.903045	-2.589393	1.815538
C	0.707975	-4.022702	1.297235
C	0.609901	-4.246331	-0.223014

H	-1.448096	-3.591152	-0.050423
H	-1.199441	-4.744663	-1.334170
H	1.870695	-2.192051	1.472019
H	0.991114	-2.648350	2.914915
H	1.555997	-4.615984	1.680398
H	-0.191921	-4.455254	1.772331
H	1.438109	-3.722701	-0.729942
H	0.796318	-5.315793	-0.410482
H	1.151165	-1.648408	-1.649096
H	-0.183207	-0.666310	-2.259954
H	-0.308591	-3.133413	-2.850297
H	-1.766159	-2.455137	-2.141009
C	0.070881	-1.470163	-1.544398
C	-0.724261	-2.731488	-1.907967

^{4}9B

Geometry with 68 atoms:

Total energy: -2442.097765770

C	5.049507	1.857073	1.059423
C	3.706816	1.509093	0.967082
C	3.401819	0.245248	0.433568
C	4.443591	-0.621557	0.009206
C	5.795713	-0.272835	0.103556
C	6.077692	0.981313	0.636554
H	5.321105	2.833112	1.467715
H	2.917381	2.186630	1.288042
H	6.587121	-0.948080	-0.226964
H	7.118509	1.300058	0.728618
N	3.808050	-1.754042	-0.465684
H	4.262131	-2.573373	-0.856323
N	2.188375	-0.380195	0.210010
C	2.470178	-1.567358	-0.332394
C	-0.948627	-2.600754	-0.710691
C	-0.930188	-3.865141	-1.313470
C	0.315489	-4.431289	-1.606930
C	1.497750	-3.744968	-1.308936
C	1.389539	-2.479905	-0.715808
N	0.190432	-1.954550	-0.438229
H	0.365119	-5.416332	-2.075413
H	-1.854123	-4.393160	-1.556082
H	2.471284	-4.181972	-1.539277
C	-2.114386	-1.814016	-0.300241
C	-3.659707	1.072258	1.098971
C	-5.028748	1.246687	1.266532
C	-5.959332	0.252649	0.880910
C	-5.549611	-0.951469	0.316121
C	-4.171062	-1.125068	0.148018
C	-3.226575	-0.135260	0.526463
H	-2.944976	1.837821	1.395835
H	-5.398618	2.175032	1.707482
H	-7.025724	0.435902	1.031442
H	-6.265267	-1.720185	0.019027
N	-3.422752	-2.168387	-0.365849
H	-3.792629	-3.037977	-0.735248
N	-1.956470	-0.598756	0.231643
Cr	0.090548	0.049053	0.328795
C	0.191423	0.843682	-1.567907
C	-1.087341	1.467503	-2.134513
C	-0.882085	2.771427	-2.938477
C	-0.977943	3.736488	0.227258
C	0.099486	1.774612	1.488790
C	0.306814	3.158478	0.855025
H	0.602223	0.073092	-2.243931
H	-1.591611	0.736922	-2.791824
H	-1.873195	3.139143	-3.263433
H	-1.507470	4.339622	0.986062
H	0.925320	1.547411	2.193919
H	0.984184	1.591743	-1.416260
H	-1.815599	1.664184	-1.333912
H	-0.332200	2.523116	-3.864812
H	-1.662586	2.911742	-0.006783
H	-0.817748	1.779533	2.111199
H	1.098779	3.096555	0.089502
H	0.691552	3.883963	1.598793
C	-0.792483	4.594729	-1.035027
C	-0.126999	3.923151	-2.249526
H	-0.193308	5.486251	-0.772660
H	-1.781967	4.979663	-1.343397
H	0.034787	4.706633	-3.010486
H	0.886387	3.584670	-1.974601
C	-0.600155	-1.340174	3.103076
H	-1.278663	-2.162381	2.855770
H	-1.063882	-0.394755	3.400241
C	0.727780	-1.492266	3.075327
H	1.405841	-0.677913	3.348067
H	1.191128	-2.446392	2.803614

^{4}TS[9B-10B]

Geometry with 68 atoms:

Total energy: -2442.062303030

C	5.006273	-2.090472	-0.704528
C	3.677737	-1.684254	-0.648131
C	3.418963	-0.343668	-0.313595
C	4.498531	0.543105	-0.055291
C	5.836200	0.135853	-0.111132
C	6.069406	-1.196358	-0.438438
H	5.237321	-3.126718	-0.961332
H	2.866906	-2.380102	-0.859940
H	6.654618	0.829228	0.091095
H	7.097710	-1.560759	-0.493767
N	3.915293	1.764268	0.222255
H	4.407412	2.621916	0.449386
N	2.232128	0.357218	-0.180217
C	2.567922	1.610998	0.134906
C	-0.807883	2.838158	0.248569
C	-0.733856	4.180517	0.633722
C	0.529706	4.734357	0.863002
C	1.677956	3.948697	0.717426

C	1.525650	2.613123	0.325892
N	0.305152	2.097605	0.087785
H	0.619943	5.778945	1.166898
H	-1.640526	4.774742	0.760715
H	2.666379	4.370217	0.908349
C	-2.005188	2.049477	-0.003691
C	-3.641710	-1.005281	-0.815125
C	-5.016868	-1.175563	-0.928751
C	-5.916908	-0.103796	-0.720263
C	-5.470615	1.173604	-0.393147
C	-4.085908	1.343367	-0.278548
C	-3.172516	0.275915	-0.484348
H	-2.947814	-1.828281	-0.976542
H	-5.415328	-2.159905	-1.184348
H	-6.989683	-0.284388	-0.819670
H	-6.165146	2.000512	-0.233823
N	-3.304546	2.443659	0.023044
H	-3.641039	3.380937	0.217457
N	-1.888316	0.752808	-0.299657
C	-0.571959	-3.344257	-1.257546
C	-0.667706	-4.490714	-0.217660
C	-0.934350	-2.373926	3.060956
C	0.040134	-0.280651	1.811696
C	-1.200812	-1.023969	2.358948
H	-1.577801	-3.174996	-1.683524
H	0.345058	-4.882479	-0.012267
H	-1.877027	-2.724408	3.521002
H	0.199635	0.665984	2.355946
H	0.059616	-3.670757	-2.102740
H	-1.224120	-5.323801	-0.680207
H	-0.233504	-2.199935	3.897108
H	0.956570	-0.879091	1.962559
H	-1.952917	-1.201432	1.567697
H	-1.728439	-0.371749	3.077006
Cr	0.117773	0.089117	-0.312051
C	-0.056399	-2.067697	-0.625503
H	0.941286	-2.231956	-0.197267
H	-0.743157	-1.843017	0.195495
C	0.081738	-0.871153	-2.533570
H	-0.889092	-1.285870	-2.815393
H	0.933718	-1.514887	-2.767938
C	0.249759	0.516732	-2.508522
H	1.242644	0.946271	-2.662152
H	-0.602337	1.166867	-2.721887
C	-1.331550	-4.096036	1.121873
C	-0.364849	-3.500577	2.179981
H	-2.158634	-3.391983	0.918280
H	-1.819376	-4.984627	1.555334
H	0.552401	-3.136685	1.691847
H	-0.025208	-4.318689	2.838266

^{4}10B
Geometry with 68 atoms:
Total energy: -2442.128847120

C	4.947085	1.728606	-0.217468
C	3.614737	1.336448	-0.272805
C	3.339809	-0.038551	-0.187646
C	4.400931	-0.968503	-0.030740
C	5.743566	-0.576252	0.020218
C	5.995728	0.788497	-0.079234
H	5.193184	2.791030	-0.278485
H	2.811422	2.063587	-0.366343
H	6.549791	-1.302595	0.137768
H	7.027725	1.144629	-0.042137
N	3.792506	-2.206192	0.066308
H	4.264780	-3.092425	0.210840
N	2.140580	-0.730854	-0.195055
C	2.452389	-2.019190	-0.023293
C	-0.934006	-3.214246	0.087882
C	-0.870153	-4.609662	0.181771
C	0.395356	-5.205832	0.233050
C	1.553730	-4.423254	0.171014
C	1.401257	-3.033901	0.083072
N	0.184145	-2.476207	0.075116
H	0.479559	-6.292021	0.306198
H	-1.776998	-5.216570	0.204711
H	2.542877	-4.884175	0.179080
C	-2.126031	-2.369871	-0.030658
C	-3.738865	0.787518	-0.352261
C	-5.113959	0.989170	-0.350926
C	-6.024258	-0.088879	-0.237426
C	-5.588582	-1.404580	-0.111121
C	-4.203348	-1.606204	-0.109565
C	-3.279622	-0.535444	-0.238328
H	-3.036728	1.617448	-0.423698
H	-5.505167	2.005441	-0.435569
H	-7.096674	0.119096	-0.242454
H	-6.290457	-2.234814	-0.012967
N	-3.429033	-2.745868	0.016803
H	-3.774099	-3.691702	0.145206
N	-1.997747	-1.051910	-0.197170
Cr	0.026507	-0.360021	-0.233504
C	-0.257986	1.052505	-1.688846
C	0.642910	2.186787	-2.178486
C	0.647780	3.434010	-1.283218
C	-0.724561	2.551549	1.716448
C	0.009698	0.103871	1.775673
C	0.354846	1.546871	2.125085
H	-1.313793	1.371471	-1.674420
H	1.677181	1.817930	-2.288259
H	1.447634	4.118699	-1.618867
H	-1.663399	2.319260	2.251839
H	0.733906	-0.601067	2.220820
H	-0.228664	0.213504	-2.435373
H	0.339740	2.498811	-3.198652
H	0.919430	3.136472	-0.259702
H	-0.953234	2.395715	0.652723
H	-0.994448	-0.162810	2.150514

H	1.315089	1.831752	1.655090
H	0.535894	1.638789	3.215593
C	-0.350069	4.019281	1.965846
C	-0.673530	4.218395	-1.271541
H	0.715843	4.180343	1.723133
H	-0.436202	4.224331	3.047235
H	-1.524238	3.536738	-1.098870
H	-0.828074	4.626185	-2.286066
C	-1.202780	5.030692	1.179045
C	-0.736627	5.369930	-0.249880
H	-1.240414	5.979885	1.740804
H	-2.247462	4.667609	1.143025
H	0.255919	5.855246	-0.196896
H	-1.421910	6.143366	-0.637734

^{4}11B
Geometry with 56 atoms:
Total energy: -2285.002031810

C	4.890732	2.276458	-1.162872
C	3.589324	1.784121	-1.054383
C	3.413251	0.505337	-0.504352
C	4.547065	-0.241072	-0.086770
C	5.850757	0.248013	-0.194234
C	6.003969	1.523278	-0.739708
H	5.050446	3.269919	-1.588255
H	2.744515	2.382840	-1.393511
H	6.709745	-0.341219	0.132785
H	7.006673	1.944390	-0.842111
N	4.048616	-1.439252	0.394822
H	4.595632	-2.207499	0.767380
N	2.271148	-0.251835	-0.262760
C	2.694333	-1.416644	0.275982
C	-0.622858	-2.819888	0.605141
C	-0.438785	-4.075354	1.172492
C	0.863434	-4.514321	1.477387
C	1.955220	-3.671633	1.199636
C	1.729751	-2.422016	0.632693
N	0.450107	-1.991336	0.334301
H	1.023896	-5.496923	1.922319
H	-1.299750	-4.715227	1.378439
H	2.974997	-3.991897	1.426243
C	-1.854629	-2.192183	0.207815
C	-3.702596	0.496394	-1.254347
C	-5.085042	0.521675	-1.440291
C	-5.901983	-0.555335	-1.041119
C	-5.360247	-1.694918	-0.444672
C	-3.975663	-1.715117	-0.260945
C	-3.138985	-0.636895	-0.652096
H	-3.080282	1.331636	-1.572358
H	-5.545297	1.394521	-1.909021
H	-6.980494	-0.498813	-1.205132
H	-5.988528	-2.533715	-0.138779
N	-3.126970	-2.667879	0.276207
H	-3.399690	-3.571408	0.647110
N	-1.823203	-0.959066	-0.341523
Cr	0.162358	-0.206167	-0.417051
C	-0.106423	1.904418	-1.663664
C	-2.038657	6.188310	2.154687
C	0.005792	2.307797	-0.375310
H	0.776385	1.724639	-2.286444
H	-1.076493	1.854784	-2.168602
C	-2.129175	4.701606	1.814809
H	-2.107772	6.811830	1.247227
H	-1.082461	6.429379	2.649318
C	-1.115931	2.739075	0.524403
H	1.012828	2.423318	0.048561
C	-1.017442	4.236596	0.870679
H	-3.109969	4.483666	1.354837
H	-2.089530	4.103186	2.742998
H	-2.091567	2.525797	0.061735
H	-1.073329	2.159083	1.464623
H	-1.051894	4.824457	-0.063766
H	-0.033010	4.444305	1.327975
H	-2.850803	6.496320	2.832546

^{4}12B
Geometry with 62 atoms:
Total energy: -2363.579680140

C	3.548436	-4.347986	1.149989
C	2.716684	-3.229759	1.078966
C	3.205280	-2.087193	0.429231
C	4.514627	-2.095172	-0.120164
C	5.350044	-3.212182	-0.051341
C	4.842885	-4.341808	0.592653
H	3.188951	-5.249562	1.651370
H	1.720805	-3.250217	1.521223
H	6.353630	-3.200829	-0.480998
H	5.462896	-5.238006	0.668030
N	4.694758	-0.838216	-0.672331
H	5.528355	-0.506538	-1.144960
N	2.632889	-0.843056	0.191777
C	3.559654	-0.116969	-0.469847
C	1.476234	2.824844	-0.733718
C	2.240719	3.759791	-1.422031
C	3.544839	3.423058	-1.831451
C	4.047399	2.141685	-1.540157
C	3.249964	1.233849	-0.852497
N	1.972126	1.569198	-0.442724
H	4.157527	4.146446	-2.370427
H	1.829380	4.746548	-1.645795
H	5.055214	1.856815	-1.851763
C	0.137592	2.970166	-0.227357
C	-2.754748	1.786264	1.518679
C	-3.909751	2.530347	1.762734
C	-4.039589	3.860966	1.318342
C	-3.012109	4.490797	0.615682
C	-1.858552	3.741545	0.373600
C	-1.709692	2.397737	0.808696

H	-2.681358	0.760124	1.875362
H	-4.732462	2.069592	2.314296
H	-4.959516	4.410446	1.530504
H	-3.102041	5.523027	0.271571
N	-0.676587	4.057637	-0.271992
H	-0.447254	4.951168	-0.692453
N	-0.455863	1.937851	0.412411
Cr	0.845950	0.249278	0.470516
C	-7.728410	-3.791492	-1.453097
C	-6.589349	-2.783965	-1.602242
H	-7.418619	-4.798491	-1.780956
H	-8.606980	-3.502473	-2.052491
C	-0.425011	-1.261229	1.898393
C	-5.347411	-3.147648	-0.783717
H	-6.308764	-2.696160	-2.667790
H	-6.940919	-1.780456	-1.299466
C	-0.679295	-1.759058	0.662878
H	0.393786	-1.650382	2.512546
H	-1.092796	-0.540627	2.380322
C	-4.206956	-2.136583	-0.919953
H	-5.628010	-3.239100	0.282249
H	-4.988736	-4.148748	-1.087443
C	-1.865455	-1.424211	-0.196964
H	-8.055399	-3.873813	-0.402402
H	-0.023525	-2.550943	0.277753
C	-2.977448	-2.486467	-0.078831
H	-4.570352	-1.134093	-0.626893
H	-3.912682	-2.052835	-1.982233
H	-2.279996	-0.443634	0.076279
H	-1.547418	-1.357099	-1.251778
H	-3.267288	-2.578474	0.982864
H	-2.583978	-3.474211	-0.377739

^{6}1B
Geometry with 38 atoms:
Total energy: -2049.268256970

C	4.988796	-2.698250	-0.060374
C	3.633562	-2.369077	-0.041768
C	3.292987	-1.010264	-0.009645
C	4.308297	-0.019324	-0.001413
C	5.666514	-0.345583	-0.020788
C	5.988463	-1.703493	-0.049717
H	5.284708	-3.749533	-0.085008
H	2.863845	-3.143973	-0.052911
H	6.440223	0.424579	-0.012685
H	7.039017	-2.002275	-0.065534
N	3.642197	1.195391	0.028401
H	4.073650	2.112894	0.057055
N	2.058113	-0.379480	0.012916
C	2.303633	0.949938	0.040921
C	-1.196457	1.875515	0.059312
C	-1.218691	3.259221	-0.078451
C	0.000000	3.964328	-0.123131
C	1.218691	3.259221	-0.078451
C	1.196457	1.875515	0.059312
N	-0.000000	1.205187	0.199660
H	0.000000	5.049411	-0.233907
H	-2.170026	3.788307	-0.169813
H	2.170027	3.788307	-0.169813
C	-2.303633	0.949938	0.040922
C	-3.633562	-2.369077	-0.041767
C	-4.988796	-2.698250	-0.060373
C	-5.988463	-1.703493	-0.049717
C	-5.666514	-0.345583	-0.020789
C	-4.308297	-0.019324	-0.001413
C	-3.292987	-1.010263	-0.009644
H	-2.863845	-3.143972	-0.052909
H	-5.284708	-3.749533	-0.085007
H	-7.039017	-2.002276	-0.065534
H	-6.440223	0.424579	-0.012687
N	-3.642197	1.195391	0.028400
H	-4.073650	2.112894	0.057055
N	-2.058113	-0.379480	0.012916
Cr	-0.000000	-0.784110	0.066562

^{6}2B
Geometry with 44 atoms:
Total energy: -2127.832537370

C	-4.988373	-2.450495	-0.023625
C	-3.631812	-2.124113	-0.029069
C	-3.284156	-0.765507	-0.025977
C	-4.301618	0.224465	-0.008572
C	-5.660475	-0.099027	-0.002126
C	-5.986899	-1.455850	-0.011929
H	-5.284338	-3.502027	-0.028050
H	-2.872224	-2.905696	-0.031813
H	-6.431348	0.673966	0.010065
H	-7.038110	-1.752666	-0.008843
N	-3.640095	1.441023	-0.000416
H	-4.074873	2.357227	0.010988
N	-2.048535	-0.129942	-0.033721
C	-2.301076	1.200026	-0.014738
C	1.197053	2.126827	-0.007411
C	1.219747	3.516764	0.036382
C	0.000016	4.221167	0.056500
C	-1.219716	3.516768	0.036357
C	-1.197027	2.126830	-0.007432
N	0.000012	1.447645	-0.034818
H	0.000017	5.311312	0.095031
H	2.169990	4.054809	0.061806
H	-2.169959	4.054816	0.061763
C	2.301100	1.200018	-0.014710
C	3.631802	-2.124126	-0.029164
C	4.988359	-2.450527	-0.023711
C	5.986895	-1.455893	-0.011933
C	5.660489	-0.099065	-0.002067
C	4.301635	0.224444	-0.008528
C	3.284166	-0.765517	-0.025996

H	2.872188	-2.905684	-0.032003
H	5.284311	-3.502063	-0.028198
H	7.038103	-1.752721	-0.008841
H	6.431371	0.673917	0.010173
N	3.640120	1.441006	-0.000342
H	4.074904	2.357208	0.011091
N	2.048551	-0.129947	-0.033733
Cr	0.000008	-0.539247	-0.047617
C	-0.000066	-2.916219	-0.523956
C	-0.000095	-2.822366	0.829018
H	-0.929581	-3.008472	-1.095499
H	0.929485	-3.008424	-1.095450
H	0.932563	-2.831801	1.403973
H	-0.932766	-2.831890	1.403950

^{6}3B

Geometry with 50 atoms:

Total energy: -2206.374235110

C	-4.991234	-2.360806	0.037428
C	-3.636254	-2.026569	0.020725
C	-3.297674	-0.667084	-0.014340
C	-4.317897	0.320306	-0.016804
C	-5.674475	-0.010813	-0.001336
C	-5.993651	-1.370436	0.023497
H	-5.282706	-3.413279	0.065048
H	-2.865365	-2.798160	0.043689
H	-6.450411	0.757184	-0.006717
H	-7.043477	-1.671856	0.036714
N	-3.656800	1.537864	-0.033198
H	-4.091877	2.453935	-0.038590
N	-2.065370	-0.031689	-0.035640
C	-2.315651	1.297840	-0.038881
C	1.180582	2.231210	-0.030881
C	1.199381	3.621302	0.009138
C	-0.022531	4.323195	0.027537
C	-1.239763	3.612759	0.010416
C	-1.211251	2.222941	-0.028984
N	-0.013140	1.545909	-0.056556
H	-0.026370	5.413485	0.059861
H	2.148417	4.162013	0.026228
H	-2.192408	4.146902	0.030179
C	2.290810	1.313532	-0.049092
C	3.633044	-2.003023	-0.050493
C	4.990243	-2.328610	-0.030021
C	5.986037	-1.331735	-0.015330
C	5.657689	0.025950	-0.017856
C	4.299043	0.348249	-0.038249
C	3.284878	-0.645325	-0.057807
H	2.867266	-2.779685	-0.054531
H	5.288431	-3.379521	-0.023428
H	7.037762	-1.626308	0.000839
H	6.428298	0.799186	-0.003548
N	3.630463	1.561673	-0.033670
H	4.060477	2.480202	-0.023659

N	2.048864	-0.017714	-0.066331
Cr	-0.006474	-0.474016	-0.102674
C	0.049188	-1.217871	2.463997
C	0.323726	-2.436446	1.968436
H	0.846589	-0.515514	2.727461
H	-0.976590	-0.909378	2.691041
H	-0.468045	-3.164846	1.764573
H	1.354458	-2.765054	1.799310
C	-0.125172	-1.674177	-2.276534
C	-0.030780	-2.747371	-1.463573
H	0.764840	-1.219302	-2.724916
H	-1.097157	-1.281946	-2.593452
H	-0.920835	-3.265921	-1.094936
H	0.936215	-3.200147	-1.225185

^{6}4B

Geometry with 50 atoms:

Total energy: -2206.360595610

C	-5.095645	-2.142279	-0.538562
C	-3.736102	-1.851986	-0.546965
C	-3.359929	-0.516560	-0.327624
C	-4.347416	0.481520	-0.117767
C	-5.716498	0.190708	-0.109586
C	-6.069912	-1.138619	-0.322048
H	-5.423966	-3.170974	-0.703429
H	-2.982659	-2.620736	-0.715076
H	-6.467651	0.965354	0.055008
H	-7.126743	-1.415209	-0.323172
N	-3.644910	1.659763	0.058604
H	-4.046435	2.575755	0.230917
N	-2.110400	0.074502	-0.267322
C	-2.321397	1.372614	-0.035288
C	1.150764	2.299132	0.067028
C	1.193707	3.681298	0.289635
C	-0.021003	4.364197	0.417630
C	-1.235353	3.674870	0.324305
C	-1.191022	2.293992	0.096413
N	-0.019765	1.650690	-0.025151
H	-0.021304	5.441956	0.592837
H	2.144868	4.212730	0.360252
H	-2.187526	4.199955	0.422736
C	2.283617	1.382954	-0.079351
C	3.725488	-1.837841	-0.533992
C	5.088263	-2.112169	-0.550175
C	6.055052	-1.091385	-0.388252
C	5.689628	0.238552	-0.202254
C	4.317129	0.512565	-0.184539
C	3.335924	-0.500634	-0.348897
H	2.979791	-2.622949	-0.656135
H	5.424825	-3.141693	-0.691563
H	7.114974	-1.355050	-0.409382
H	6.434576	1.026384	-0.076092
N	3.605732	1.686310	-0.018240
H	4.000335	2.609953	0.126724

N	2.081047	0.078963	-0.281095
H	-0.319629	-4.478354	0.361054
H	-1.436916	-3.229436	0.898439
H	0.901938	-2.859106	-1.083928
H	-0.810044	-2.769014	-1.469610
C	-0.390644	-3.393539	0.576027
C	-0.076540	-2.545429	-0.668662
Cr	-0.025630	-0.467500	-0.344260
C	0.314090	-1.723261	2.354711
C	0.524966	-3.077635	1.773337
H	1.118326	-1.192219	2.873444
H	-0.705014	-1.336517	2.479256
H	0.354398	-3.837424	2.569448
H	1.584043	-3.201385	1.482213

^{6}5B

Geometry with 56 atoms:

Total energy: -2284.898421770

C	5.007279	-2.226959	0.145949
C	3.653373	-1.895964	0.130764
C	3.314900	-0.538137	0.047015
C	4.333524	0.447717	-0.026500
C	5.691699	0.118833	-0.008881
C	6.010063	-1.236420	0.079392
H	5.300968	-3.277216	0.209577
H	2.881146	-2.663645	0.174565
H	6.466890	0.885596	-0.063162
H	7.059908	-1.537767	0.095128
N	3.671663	1.661587	-0.111327
H	4.105129	2.576702	-0.168428
N	2.083296	0.097684	0.013211
C	2.334047	1.416002	-0.086107
C	-1.155293	2.339228	-0.149639
C	-1.180011	3.711901	-0.377909
C	0.036342	4.408356	-0.491632
C	1.250742	3.705772	-0.398097
C	1.222817	2.333770	-0.168100
N	0.032236	1.664540	-0.008952
H	0.037510	5.483846	-0.673921
H	-2.132614	4.238159	-0.474848
H	2.204981	4.225872	-0.510552
C	-2.272707	1.429329	-0.060978
C	-3.673832	-1.853790	0.130810
C	-5.036169	-2.148671	0.151520
C	-6.013445	-1.133129	0.096858
C	-5.657772	0.212729	0.017462
C	-4.291263	0.504292	-0.003953
C	-3.293917	-0.505109	0.054086
H	-2.932822	-2.651346	0.164834
H	-5.355401	-3.191722	0.209421
H	-7.070844	-1.406551	0.115107
H	-6.410792	1.001931	-0.026734
N	-3.604313	1.702895	-0.078080
H	-4.018496	2.627487	-0.124859
N	-2.045178	0.104353	0.022245
H	-0.232582	-4.472660	-1.153161
H	1.243706	-3.527140	-1.367065
H	-0.949612	-2.671062	0.678764
H	0.792042	-3.176570	1.057242
C	0.176068	-3.439284	-1.101108
C	0.039565	-2.946681	0.295940
Cr	0.029248	-0.330457	-0.064419
C	0.021536	-1.103882	-2.003785
C	-0.543588	-2.519060	-2.096073
H	-0.543142	-0.383362	-2.620424
H	1.079559	-1.077430	-2.318342
H	-0.446694	-2.930263	-3.118952
H	-1.625777	-2.519511	-1.875256
C	0.467025	-0.135007	3.108919
H	1.485107	-0.509857	3.257476
H	0.353002	0.949006	3.007483
C	-0.586671	-0.956133	3.063771
H	-1.605001	-0.578565	2.928045
H	-0.477910	-2.038572	3.186111

^{6}6B

Geometry with 56 atoms:

Total energy: -2284.932789700

C	5.089781	-1.613636	-0.863076
C	3.718530	-1.391435	-0.806860
C	3.285936	-0.091950	-0.496581
C	4.230964	0.939823	-0.256252
C	5.611959	0.718481	-0.313796
C	6.021449	-0.576090	-0.620881
H	5.460810	-2.613058	-1.101269
H	2.996185	-2.184871	-0.994399
H	6.330436	1.518974	-0.128091
H	7.089707	-0.797699	-0.677430
N	3.478628	2.067807	0.014779
H	3.840716	2.990508	0.231649
N	2.011432	0.430625	-0.365299
C	2.166824	1.721175	-0.059662
C	-1.341750	2.474928	0.199375
C	-1.438526	3.849238	0.448453
C	-0.253937	4.588235	0.538803
C	0.985651	3.958862	0.382563
C	0.998656	2.578127	0.148940
N	-0.145402	1.877335	0.070593
H	-0.297513	5.663610	0.722834
H	-2.409089	4.336002	0.559572
H	1.913198	4.532508	0.428194
C	-2.439092	1.522852	0.022918
C	-3.743524	-1.708379	-0.692087
C	-5.092249	-2.045478	-0.705040
C	-6.100321	-1.091454	-0.428277
C	-5.792446	0.232661	-0.129230
C	-4.434218	0.570686	-0.115759
C	-3.412894	-0.377156	-0.389265

H	-2.965143	-2.439839	-0.904626
H	-5.384609	-3.072616	-0.934639
H	-7.147110	-1.403182	-0.450019
H	-6.569922	0.968490	0.084057
N	-3.772747	1.758459	0.136928
H	-4.205941	2.646408	0.368130
N	-2.184234	0.251770	-0.295565
Cr	-0.059569	-0.212612	-0.402720
C	-0.068489	-1.308862	2.149598
C	1.114156	-2.198166	2.282966
C	0.890158	-3.667079	1.898964
C	0.828299	-3.995691	0.399444
C	-0.077917	-2.147104	-1.228041
C	-0.355537	-3.432511	-0.422351
H	-1.084354	-1.708963	2.222641
H	1.970453	-1.780810	1.718873
H	-0.033842	-4.025226	2.389848
H	1.779475	-3.693191	-0.073915
H	0.844905	-2.296619	-1.825144
H	0.048706	-0.224701	2.269457
H	1.445119	-2.161984	3.345938
H	1.710352	-4.259520	2.339452
H	0.808797	-5.096499	0.325728
H	-0.880942	-2.032160	-1.987613
H	-0.674543	-4.232598	-1.118588
H	-1.218710	-3.292719	0.255400

^{6}TS[6B-11B]
Geometry with 56 atoms:
Total energy: -2284.913298060

C	5.051633	-1.699948	-0.097491
C	3.683144	-1.435767	-0.066241
C	3.272876	-0.096562	-0.072972
C	4.240721	0.940462	-0.116297
C	5.613674	0.681217	-0.147837
C	6.002312	-0.658554	-0.136525
H	5.396715	-2.736354	-0.092184
H	2.952205	-2.241563	-0.039343
H	6.347309	1.489039	-0.180473
H	7.066038	-0.905996	-0.159710
N	3.519274	2.121591	-0.123476
H	3.906223	3.058739	-0.151797
N	2.008063	0.475819	-0.054439
C	2.195960	1.810096	-0.087840
C	-1.334522	2.581490	-0.041016
C	-1.414081	3.970612	-0.022686
C	-0.229269	4.726992	-0.040957
C	1.015742	4.071319	-0.065874
C	1.047724	2.681599	-0.081723
N	-0.114444	1.946071	-0.085315
H	-0.274613	5.816722	-0.027858
H	-2.385959	4.467049	0.007012
H	1.944884	4.646044	-0.065792
C	-2.408377	1.620318	-0.032553
C	-3.644335	1.734529	-0.147779
C	-4.989875	2.097096	-0.194319
C	-6.016407	1.130538	-0.180052
C	-5.727544	-0.232978	-0.128913
C	-4.377904	-0.592079	-0.083480
C	-3.332501	0.368817	-0.078957
H	-2.861085	2.490534	-0.177317
H	-5.255616	3.155341	-0.247674
H	-7.058584	1.455571	-0.216989
H	-6.518305	-0.985671	-0.129384
N	-3.752646	-1.826411	-0.051250
H	-4.212577	-2.730145	-0.067543
N	-2.115093	-0.302132	-0.033034
Cr	-0.043772	0.013401	0.170175
H	-1.303806	2.570052	1.150937
H	-0.159123	2.059834	-0.143674
H	1.017722	1.012630	2.405726
H	-0.793379	0.725527	2.586448
C	-0.246210	2.273185	1.128806
C	0.022543	1.086426	1.948097
C	-0.029062	2.705909	-1.648837
C	0.663553	3.498652	1.221467
C	0.460542	4.498749	0.078622
C	0.800327	3.908388	-1.304950
H	-1.100489	2.859741	-1.826141
H	0.420132	1.909608	-2.256080
H	1.716342	3.178096	1.273007
H	0.449941	3.989149	2.186852
H	1.081748	5.391129	0.255572
H	-0.589033	4.845620	0.080602
H	1.871720	3.650972	-1.341935
H	0.652067	4.694461	-2.072020

^{6}7B
Geometry with 62 atoms:
Total energy: -2363.480065010

C	-5.153638	-2.098891	0.837639
C	-3.803664	-1.770283	0.811421
C	-3.458186	-0.500768	0.322141
C	-4.465557	0.396701	-0.119234
C	-5.825604	0.067901	-0.092855
C	-6.148998	-1.195840	0.391296
H	-5.457392	-3.079399	1.210987
H	-3.033292	-2.462107	1.151577
H	-6.591891	0.764890	-0.437422
H	-7.197706	-1.499463	0.429481
N	-3.792066	1.535475	-0.519938
H	-4.218386	2.376354	-0.895942
N	-2.226420	0.108944	0.177376
C	-2.465420	1.324989	-0.321203
C	0.983405	2.348033	-0.441639
C	1.004903	3.606642	-1.055215
C	-0.215391	4.177833	-1.432853
C	-1.414287	3.495353	-1.215180

C	-1.351609	2.239752	-0.597200
N	-0.177902	1.717923	-0.208845
H	-0.228686	5.157432	-1.914843
H	1.945105	4.124798	-1.249946
H	-2.367198	3.922421	-1.533711
C	2.132893	1.531808	-0.024633
C	3.584224	-1.465168	1.239027
C	4.946279	-1.690435	1.398370
C	5.908808	-0.705189	1.070706
C	5.539694	0.541304	0.570456
C	4.168166	0.767588	0.413955
C	3.193797	-0.211128	0.741499
H	2.840902	-2.226300	1.476944
H	5.285907	-2.655774	1.780515
H	6.968499	-0.930513	1.210610
H	6.279031	1.302582	0.315250
N	3.451409	1.856201	-0.057003
H	3.845217	2.731568	-0.385513
N	1.942099	0.294610	0.443997
Cr	-0.140347	-0.269405	0.610999
C	2.677031	-1.715797	-2.725577
C	1.363388	-1.649158	-3.420624
C	0.341768	-2.745794	-3.056754
C	-0.311574	-2.574450	-1.674741
C	-0.002111	-2.340613	0.842069
C	0.597466	-2.859181	-0.476353
H	3.146013	-2.678040	-2.494459
H	0.900661	-0.654051	-3.265228
H	0.819850	-3.740230	-3.130173
H	-0.703963	-1.539781	-1.594916
H	-0.977171	-2.828196	1.040902
H	3.329590	-0.836982	-2.688445
H	1.547032	-1.695609	-4.519278
H	-0.450354	-2.738080	-3.825448
H	-1.208308	-3.218900	-1.607802
H	0.640921	-2.612567	1.697000
H	0.830784	-3.943749	-0.466732
H	1.568380	-2.359034	-0.648274
C	-1.186690	0.151268	3.424839
H	-2.113288	0.694121	3.212266
H	-1.293550	-0.917206	3.645372
C	0.004091	0.764978	3.435074
H	0.928276	0.229080	3.674335
H	0.094399	1.837647	3.233196

^{6}8B
Geometry with 62 atoms:
Total energy: -2363.482087820

C	5.078070	-1.689097	-0.662661
C	3.711672	-1.404089	-0.619700
C	3.324791	-0.072097	-0.412251
C	4.317466	0.931387	-0.244839
C	5.683052	0.649886	-0.289824
C	6.049120	-0.682006	-0.503192
H	5.401452	-2.720705	-0.820380
H	2.973332	-2.196633	-0.730075
H	6.431012	1.434532	-0.160252
H	7.108253	-0.945935	-0.542965
N	3.621659	2.113270	-0.041894
H	4.029464	3.027168	0.122905
N	2.076305	0.522130	-0.317404
C	2.290556	1.840521	-0.083358
C	-1.175051	2.718267	0.138870
C	-1.229301	4.131071	0.384581
C	-0.010043	4.809942	0.480863
C	1.220179	4.160395	0.343919
C	1.191454	2.744774	0.105508
N	0.013798	2.102907	0.027227
H	-0.019765	5.887474	0.666297
H	-2.183151	4.648885	0.483386
H	2.164517	4.700634	0.410704
C	-2.257753	1.794187	-0.051627
C	-3.615640	-1.431920	-0.815533
C	-4.975321	-1.727995	-0.931613
C	-5.965352	-0.745861	-0.736336
C	-5.625673	0.572932	-0.422133
C	-4.266401	0.865818	-0.308259
C	-3.255666	-0.115643	-0.494040
H	-2.861044	-2.200837	-0.972630
H	-5.278524	-2.747631	-1.180644
H	-7.018512	-1.018064	-0.835092
H	-6.388001	1.340539	-0.275743
N	-3.593041	2.045735	-0.029888
H	-4.018140	2.950354	0.142582
N	-2.019154	0.485270	-0.318815
Cr	0.026704	0.103969	-0.280561
C	0.120341	-0.389381	1.727519
C	-0.999951	-1.201939	2.359276
C	-1.263080	-2.618640	1.829323
C	0.813028	-4.180099	-0.393745
C	0.032914	-2.038456	-1.583814
C	-0.224060	-3.467157	-1.274879
H	0.179626	0.613604	2.179537
H	-0.774830	-1.279392	3.443137
H	-1.581066	-2.556304	0.780081
H	1.775260	-4.196645	-0.936004
H	1.058244	-1.728012	-1.823261
H	1.109491	-0.860529	1.825855
H	-1.942093	-0.631797	2.298160
H	-2.144548	-3.004177	2.369347
H	0.506242	-5.235439	-0.298171
H	-0.780313	-1.460558	-2.047916
H	-0.242655	-3.977242	-2.265489
H	-1.244436	-3.600616	-0.884650
C	1.053002	-3.592563	1.004614
C	-0.126661	-3.645128	1.992513
H	1.424306	-2.562224	0.904511
H	1.890712	-4.157418	1.447570

H	-0.560441	-4.660226	1.945747
H	0.273595	-3.545882	3.017229

^{6}TS[8B-12B]
Geometry with 62 atoms:
Total energy: -2363.494030890

C	5.047323	-1.868719	0.947977
C	3.723102	-1.447671	0.911195
C	3.470089	-0.151717	0.432399
C	4.541744	0.676618	0.008504
C	5.875924	0.254834	0.045578
C	6.106863	-1.031673	0.523434
H	5.279267	-2.871491	1.313728
H	2.905356	-2.090632	1.232901
H	6.692146	0.900789	-0.283220
H	7.131916	-1.406203	0.572003
N	3.951127	1.859308	-0.396788
H	4.436039	2.669129	-0.769502
N	2.282868	0.541365	0.274820
C	2.610492	1.737124	-0.224311
C	-0.752852	2.997105	-0.389293
C	-0.674179	4.310307	-0.867586
C	0.592398	4.821293	-1.172723
C	1.738462	4.037454	-0.995018
C	1.572660	2.733833	-0.508367
N	0.351931	2.254968	-0.229811
H	0.687983	5.842329	-1.547755
H	-1.570288	4.919548	-0.996047
H	2.727471	4.438571	-1.224519
C	-1.956024	2.253355	-0.008096
C	-3.644304	-0.653912	1.154725
C	-5.024078	-0.799514	1.241910
C	-5.907541	0.245728	0.880283
C	-5.440188	1.471175	0.414299
C	-4.050782	1.615159	0.322830
C	-3.154217	0.577347	0.689460
H	-2.962369	-1.458432	1.425725
H	-5.440797	-1.744764	1.596822
H	-6.984494	0.083823	0.966337
H	-6.121245	2.275524	0.130427
N	-3.248158	2.656637	-0.108135
H	-3.569996	3.550715	-0.464941
N	-1.858763	1.012047	0.474173
H	-0.963197	-2.193463	-0.241671
H	-1.392163	-3.194120	1.254213
H	-0.812889	-1.237245	2.481303
H	0.884481	-1.711362	2.246951
C	-0.508783	-2.656675	0.865874
C	-0.060440	-1.494538	1.712175
Cr	0.171862	0.284789	0.607749
C	-1.975448	-4.217926	-1.698309
C	0.579222	-3.623941	0.412547
C	0.121902	-4.913306	-0.286069
C	-0.539671	-4.795419	-1.671435
H	-2.397369	-4.242974	-0.679351
H	-2.624026	-4.875918	-2.300587
H	1.287376	-3.085723	-0.246454
H	1.171494	-3.917624	1.301108
H	1.009429	-5.561665	-0.392697
H	-0.564853	-5.459360	0.387556
H	0.117564	-4.211821	-2.341740
H	-0.562810	-5.809930	-2.102962
H	-0.140552	-1.800294	-1.989209
H	-1.569736	-0.742033	-1.588528
H	-1.946831	-2.824712	-3.354908
H	-3.158623	-2.462871	-2.124177
C	-1.183340	-1.768268	-1.641167
C	-2.112669	-2.788553	-2.258583

^{6}9B
Geometry with 68 atoms:
Total energy: -2442.061587670

C	5.060944	1.206748	1.703906
C	3.699975	0.964515	1.556342
C	3.320428	-0.088210	0.707007
C	4.305258	-0.862316	0.038095
C	5.675700	-0.619791	0.187071
C	6.032755	0.428378	1.030606
H	5.392315	2.018688	2.355161
H	2.948227	1.560747	2.072506
H	6.425945	-1.221088	-0.329805
H	7.090959	0.656507	1.177953
N	3.598250	-1.795052	-0.699369
H	3.996577	-2.505082	-1.305149
N	2.068855	-0.563312	0.360003
C	2.274999	-1.581201	-0.478220
C	-1.199740	-2.278027	-1.079286
C	-1.245426	-3.311488	-2.023120
C	-0.032418	-3.840208	-2.478067
C	1.182698	-3.331213	-2.006443
C	1.140939	-2.296896	-1.063880
N	-0.028722	-1.814814	-0.617004
H	-0.033924	-4.646665	-3.214447
H	-2.198105	-3.687246	-2.399860
H	2.134145	-3.722606	-2.369872
C	-2.330380	-1.543451	-0.509199
C	-3.752037	1.022241	1.501969
C	-5.111770	1.278943	1.634324
C	-6.084135	0.506785	0.954525
C	-5.728483	-0.548203	0.119028
C	-4.358996	-0.804901	-0.014183
C	-3.373761	-0.038388	0.662514
H	-2.997599	1.614495	2.019400
H	-5.441859	2.097828	2.277473
H	-7.141537	0.746082	1.089364
H	-6.478999	-1.143668	-0.404185
N	-3.653384	-1.745523	-0.742520
H	-4.052024	-2.454199	-1.349709

N	-2.123042	-0.525606	0.328978
Cr	-0.024484	-0.192782	0.796512
C	0.474995	1.148446	-2.669090
C	-0.363198	2.278045	-3.155551
C	0.320540	3.653575	-3.116828
C	-0.692958	3.191839	0.177063
C	0.042235	1.527203	1.989134
C	0.370466	2.814906	1.218236
H	0.038583	0.155366	-2.531031
H	-0.673453	2.076104	-4.204789
H	-0.368808	4.397970	-3.552846
H	-1.640218	3.405098	0.704370
H	0.801935	1.354744	2.779135
H	1.563047	1.238362	-2.595544
H	-1.319014	2.303969	-2.597709
H	1.196032	3.620840	-3.790742
H	-0.902267	2.314313	-0.459270
H	-0.914214	1.657846	2.535447
H	1.345775	2.703385	0.707947
H	0.502408	3.682748	1.897981
C	-0.326312	4.398026	-0.702446
C	0.786973	4.155797	-1.741063
H	-0.020256	5.222115	-0.033811
H	-1.228573	4.762410	-1.226480
H	1.329167	5.101752	-1.909160
H	1.537343	3.459162	-1.327612
C	-0.629732	-1.799332	3.332803
H	-1.459587	-2.431489	2.999465
H	-0.897472	-0.874325	3.853292
C	0.645709	-2.151139	3.138590
H	1.473267	-1.526405	3.489572
H	0.914488	-3.084946	2.633025

^{6}10B
Geometry with 68 atoms:
Total energy: -2442.091536230

C	4.947101	1.999918	-0.419942
C	3.632397	1.555434	-0.503888
C	3.399395	0.180862	-0.331814
C	4.483731	-0.696929	-0.068455
C	5.808560	-0.252859	0.011885
C	6.019092	1.110758	-0.170578
H	5.160145	3.063662	-0.547386
H	2.809252	2.243268	-0.687522
H	6.632814	-0.939358	0.213963
H	7.035971	1.505918	-0.114364
N	3.912869	-1.946298	0.086385
H	4.406041	-2.804427	0.309791
N	2.223488	-0.551164	-0.337457
C	2.571000	-1.813410	-0.068353
C	-0.773108	-3.125821	0.097241
C	-0.656339	-4.510258	0.268686
C	0.630391	-5.055402	0.350310
C	1.756550	-4.230780	0.247852
C	1.552874	-2.855775	0.078651
N	0.314478	-2.341582	0.028976
H	0.756745	-6.132056	0.481014
H	-1.541078	-5.147589	0.325184
H	2.763514	-4.650077	0.288937
C	-2.001355	-2.342516	-0.049736
C	-3.772286	0.694903	-0.598960
C	-5.155722	0.830656	-0.590925
C	-6.010226	-0.274508	-0.364161
C	-5.508082	-1.551815	-0.132450
C	-4.114980	-1.686210	-0.139175
C	-3.246736	-0.587441	-0.371745
H	-3.112720	1.544797	-0.768835
H	-5.597506	1.814515	-0.763951
H	-7.091518	-0.119370	-0.369140
H	-6.166204	-2.403981	0.047115
N	-3.283571	-2.774117	0.058065
H	-3.579515	-3.723465	0.260624
N	-1.938905	-1.034695	-0.314288
Cr	0.070325	-0.293619	-0.565844
C	-0.253037	1.059091	-2.140259
C	0.516513	2.368900	-2.348696
C	0.357551	3.403719	-1.225290
C	-0.724642	2.136378	2.001823
C	0.111475	-0.134295	2.773775
C	0.318165	1.337923	2.795689
H	-1.342464	1.245654	-2.194173
H	1.591110	2.147139	-2.475698
H	1.023883	4.263868	-1.422036
H	-1.736616	1.827988	2.321649
H	0.923435	-0.816916	3.040764
H	-0.044199	0.384220	-3.000043
H	0.214462	2.855818	-3.299258
H	0.705073	2.967082	-0.272599
H	-0.652107	1.861016	0.932746
H	-0.903748	-0.543895	2.751251
H	1.336846	1.586932	2.442887
H	0.298453	1.690954	3.851969
C	-0.581906	3.650879	2.181265
C	-1.072535	3.933360	-1.065328
H	0.436356	3.967777	1.891181
H	-0.656685	3.859299	3.263253
H	-1.764655	3.095034	-0.878427
H	-1.379183	4.354808	-2.038930
C	-1.624845	4.507680	1.438872
C	-1.268174	5.000086	0.026763
H	-1.832083	5.403516	2.048764
H	-2.581742	3.954042	1.397934
H	-0.363055	5.633038	0.082732
H	-2.080242	5.677458	-0.289258

^{6}11B
Geometry with 56 atoms:
Total energy: -2284.996336860

C	4.808176	2.520809	-1.112042
C	3.532078	1.964776	-1.009811
C	3.418348	0.671157	-0.479237
C	4.586282	-0.025938	-0.070159
C	5.864725	0.527300	-0.171094
C	5.956289	1.815724	-0.700096
H	4.919428	3.527298	-1.522009
H	2.657229	2.526993	-1.335351
H	6.751239	-0.023483	0.149383
H	6.937514	2.285877	-0.796985
N	4.145856	-1.252374	0.396784
H	4.728213	-1.992734	0.772064
N	2.313559	-0.142215	-0.251291
C	2.790252	-1.292641	0.279137
C	-0.462531	-2.846383	0.590970
C	-0.224345	-4.113267	1.111744
C	1.100352	-4.498811	1.398998
C	2.158516	-3.606572	1.144108
C	1.874440	-2.347018	0.626558
N	0.574418	-1.967992	0.374482
H	1.305757	-5.489626	1.806169
H	-1.051595	-4.803513	1.291257
H	3.190829	-3.899449	1.347090
C	-1.717447	-2.263018	0.189204
C	-3.679073	0.344234	-1.278612
C	-5.061591	0.310229	-1.463150
C	-5.831902	-0.799369	-1.061054
C	-5.240794	-1.914404	-0.465751
C	-3.856319	-1.875730	-0.283934
C	-3.066412	-0.761818	-0.672731
H	-3.094313	1.203408	-1.603748
H	-5.558469	1.161473	-1.934125
H	-6.912062	-0.789080	-1.223384
H	-5.831597	-2.779902	-0.159474
N	-2.969206	-2.793285	0.250429
H	-3.204172	-3.708241	0.619159
N	-1.737865	-1.026067	-0.359019
Cr	0.205107	-0.166784	-0.398428
C	-0.158916	1.940998	-1.581875
C	-2.677374	6.002147	2.042387
C	-0.098170	2.305950	-0.274658
H	0.742510	1.862975	-2.198270
H	-1.115577	1.840464	-2.104119
C	-2.563937	4.502600	1.773439
H	-2.801160	6.569498	1.104459
H	-1.775274	6.388720	2.546127
C	-1.274362	2.631330	0.602128
H	0.889157	2.492659	0.169871
C	-1.375704	4.144032	0.876931
H	-3.494704	4.137048	1.303042
H	-2.473280	3.957345	2.730352
H	-2.208618	2.277791	0.140639
H	-1.173255	2.104805	1.567785
H	-1.460665	4.678939	-0.085657
H	-0.438750	4.497928	1.343704
H	-3.541766	6.231243	2.686187

^{6}12B
Geometry with 62 atoms:
Total energy: -2363.574253320

C	-3.510357	-4.383334	-1.110577
C	-2.687313	-3.258035	-1.046290
C	-3.188520	-2.111950	-0.411531
C	-4.502216	-2.124565	0.128092
C	-5.328353	-3.248963	0.066036
C	-4.808276	-4.381737	-0.562015
H	-3.140180	-5.287251	-1.599827
H	-1.689050	-3.278330	-1.482370
H	-6.334677	-3.240573	0.489292
H	-5.420570	-5.283701	-0.631460
N	-4.698609	-0.863622	0.664719
H	-5.535201	-0.538393	1.136467
N	-2.627941	-0.859936	-0.184472
C	-3.567622	-0.133183	0.464556
C	-1.513904	2.833723	0.707483
C	-2.315662	3.799909	1.304546
C	-3.630949	3.461440	1.680058
C	-4.115846	2.162475	1.435543
C	-3.279833	1.228647	0.832587
N	-1.987943	1.561552	0.490937
H	-4.275945	4.206938	2.146925
H	-1.933815	4.809973	1.470640
H	-5.138840	1.893621	1.707940
C	-0.165187	2.968418	0.219749
C	2.751087	1.765281	-1.475347
C	3.910427	2.505910	-1.709500
C	4.035886	3.839892	-1.274038
C	2.999417	4.477274	-0.591521
C	1.841376	3.731573	-0.359166
C	1.697801	2.383828	-0.783930
H	2.678902	0.737113	-1.826145
H	4.739785	2.039790	-2.246388
H	4.959402	4.386470	-1.477951
H	3.085887	5.512392	-0.255330
N	0.650487	4.055562	0.264922
H	0.422461	4.949279	0.685249
N	0.438267	1.928280	-0.402372
Cr	-0.837857	0.224868	-0.444163
C	7.798900	-3.687297	1.383141
C	6.639286	-2.707449	1.555800
H	7.513617	-4.705577	1.698078
H	8.675369	-3.387933	1.980578
C	0.410929	-1.268808	-1.844866
C	5.398474	-3.085287	0.741716
H	6.365289	-2.641869	2.624687
H	6.966564	-1.691931	1.266056
C	0.671129	-1.758997	-0.602671
H	-0.406759	-1.666333	-2.454616

```
H   1.086685  -0.565550  -2.341112
C   4.237597  -2.102525   0.907696
H   5.670796  -3.151796  -0.328221
H   5.065226  -4.099326   1.031155
C   1.871019  -1.428601   0.241746
H   8.119775  -3.746801   0.329043
H   0.013491  -2.544190  -0.207274
C   3.003522  -2.462596   0.077264
H   4.575714  -1.087325   0.628195
H   3.955441  -2.043178   1.974946
H   2.263558  -0.434029  -0.013938
H   1.574113  -1.392752   1.303777
H   3.277325  -2.522842  -0.991029
H   2.637509  -3.465841   0.359046
```