Supplementary Material (ESI) for Dalton Transaction

SUPPLEMENTARY INFORMATION

Stable Lewis acid chelate of a bis(imido) tungsten compound and implications for α-olefin dimerisation catalysis: a DFT study

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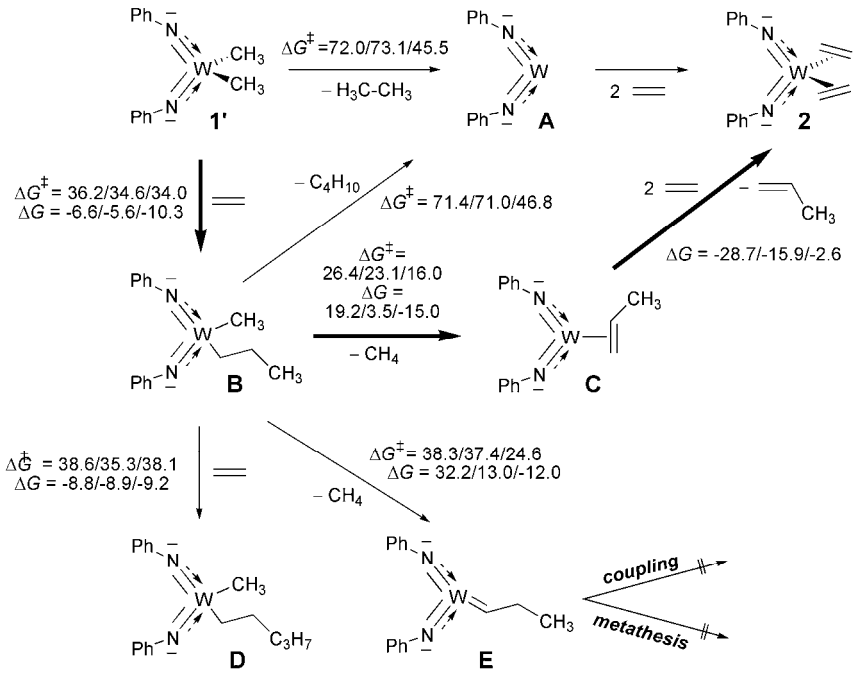

Scheme S1 Condensed Gibbs free-energy profile (kcal mol^{-1}) of alternative reaction routes for transformation of $[W^{VI}(NPh)_2Me_2]$ compound **1** into the $[W^{IV}(NPh)_2(C_2H_4)_2]$ active catalyst species **2**. The activation and reaction free energies for individual steps are given relative to the respective precursor for Lewis acid association modes **0**/**I**/**II**. The favorable route is indicated by bold reaction arrows.

Computational Details

All DFT calculations were performed with the program package TURBOMOLE[1] using the TPSS density functional[2] within the RI-*J* approximation[3] in conjunction with flexible basis sets of triple-ζ quality. For W we used the Stuttgart−Dresden quasirelativistic effective core potential (SDD) with the associate (8s7p6d)/[6s5p3d] valence basis set contracted according to a (311111/22111/411) scheme.[4] All other elements were represented by Ahlrich's valence triple-ζ TZVP basis set[5] with polarization functions on all atoms. The good to excellent performance of the TPSS functional for a wide range of applications has been demonstrated previously.[6] In view of the fact that all species investigated in this study show a large HOMO–LUMO gap, a spin-restricted formalism was used for all the calculations.

All stationary points were located by utilizing analytical/numerical gradients/Hessians according to standard algorithms without imposing any symmetry constraints and were identified exactly by the curvature of the potential-energy surface at these points corresponding to the eigenvalues of the Hessian. The reaction and activation free energies (ΔG, $\Delta G^{\ddagger}$ at 298 K and 1 atm) were evaluated according to standard textbook procedures[7] using computed harmonic frequencies. The influence of the solvent was taken into explicit consideration by making use of a continuum model. The experimentally used chlorobenzene solvent[8] was described as a homogeneous, isotropic dielectric medium (characterised by its relative static dielectric permittivity ε = 5.621 at 298 K)[9] within the conductor-like screening model (COSMO) due to Klamt and Schüürmann[10] as implemented in TURBOMOLE.[11] The optimised atomic COSMO radii (r_H = 1.3 Å, r_C = 2.0 Å, r_N = 1.83 Å, r_{Cl} = 2.06 Å)[12] have been used, in combination with the van der Waals radius[13] (multiplied by a standard scaling factor of 1.17) for aluminum; i.e. r_{Al} = 1.40 Å, and the radius of 2.22 Å for W. Nonelectrostatic contributions to solvation were not included. The solvation effects were included self-consistently in the calculations, and all stationary points were fully optimised including solvation at the TPSS/SDD+Ahlrichs-TZVP level.

The electronic structure and bonding of localised stationary points was studied by means of natural population analysis (NPA)[14] and related Wiberg bond indices (WBIs)[15] by using the NBO 5.0[16] program in conjunction with the MAG-ReSpect[17] module.

In order to account for real condensed-phase reaction condition, the entropy costs for Lewis acid and olefin substrate association/dissociation processes was approximated as being two-thirds of its gas-phase value. This approximation was successfully applied in former investigations on group 4 metal-assisted selective olefin oligomerisation[18] and is expected to reasonably estimate the true entropy contribution in condensed phase.

The relative stability of various adducts of **3** with the $AlClMe_2$ Lewis acid (Fig. 1) is calculated with respect to {**3** + n/2×$[AlClMe_2]_2$}, where n (1–3) is the number of associated $AlClMe_2$ moieties. The heat of 2 $AlClMe_2$ ⇄ $[AlClMe_2]_2$ dimer formation amounts to −2.6 kcal mol^{-1} at the TPSS-COSMO/TZVP level of approximation. DFT methods, however, are known tending to under-bind dimers of aluminium compounds. The MP2 method has been

demonstrated being superior in this case and reproduces experimental values satisfactory.[19] This is illustrated here for $[AlMe_3]_2 \rightleftarrows 2\ AlMe_3$, for which the following experimental binding values are reported:[20] ΔH = 20.4 kcal mol^{-1} and ΔS = 43.1 eu for gas phase; ΔH = 19.4 kcal mol^{-1} and ΔS = 29.3 eu for liquid phase. DFT(TPSS-COSMO/TZVP) gives ΔH = 10.5 kcal mol^{-1}, whilst 15.7 kcal mol^{-1} (TZVP basis)[5] and 17.2 kcal mol^{-1} (TZVPP basis)[21], respectively, result from SP-MP2(COSMO) calculations at DFT-optimised structures. Hence, to ensure a balanced description of Lewis acid association, the relative stabilities summarised in Fig. 1 are obtained by using the SP-MP2(COSMO) value of –7.9 kcal mol^{-1} for the heat of $AlClMe_2$ dimer formation.

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Optimised structures and total electronic energies (hartree) of all species reported.

2-0

E = -797.576925

W	-0,9263	-0,0062	0,0062
C	-1,7877	-0,0105	-2,0826
C	-2,9480	-0,0061	-1,2766
C	-2,9224	-0,0552	1,3253
C	-1,7480	-0,0268	2,1106
H	-1,4650	0,9075	-2,5671
H	-1,4713	-0,9320	-2,5651
H	-3,5063	0,9134	-1,1333
H	-3,5180	-0,9191	-1,1396
H	-3,5145	0,8454	1,2006
H	-3,4633	-0,9865	1,1910
H	-1,4442	0,9000	2,5907
H	-1,3961	-0,9389	2,5862
N	0,0139	-1,5480	-0,0197
C	0,9849	-2,5257	-0,0572
N	-0,0152	1,5542	0,0201
C	0,9428	2,5446	0,0438
C	0,6872	3,7949	-0,5614
C	2,8845	4,5885	0,0893
C	2,1893	2,3405	0,6764
C	3,1428	3,3558	0,6998
H	4,0959	3,1836	1,1942
H	2,3878	1,3804	1,1448
C	1,6540	4,7988	-0,5419
H	-0,2723	3,9574	-1,0446
H	3,6333	5,3758	0,1063
H	1,4433	5,7536	-1,0174
C	2,2963	-2,2382	-0,4968
C	2,9504	-4,5448	-0,1338
C	0,6776	-3,8455	0,3404
C	1,6551	-4,8387	0,3051
H	1,4036	-5,8491	0,6183
H	-0,3312	-4,0705	0,6751
C	3,2623	-3,2409	-0,5362
H	2,5343	-1,2240	-0,8054
H	3,7084	-5,3228	-0,1634
H	4,2663	-3,0041	-0,8802

2-I

E = -1580.262399

W	-0,8472	-0,2027	-0,0004
C	-1,7183	-0,2924	-2,0734
C	-2,8953	-0,2500	-1,2919
C	-2,8990	-0,2470	1,2852
C	-1,7243	-0,2891	2,0702
H	-1,3869	0,5946	-2,6072
H	-1,4092	-1,2423	-2,5048
H	-3,4396	0,6830	-1,1877
H	-3,4724	-1,1525	-1,1333
H	-3,4423	0,6862	1,1776
H	-3,4758	-1,1494	1,1257
H	-1,3940	0,5985	2,6038
H	-1,4175	-1,2384	2,5043
N	0,8925	-1,0639	0,0014
C	2,1754	-0,4469	-0,0034
Al	0,8681	-3,0029	0,0042
Cl	-1,4531	-2,8913	0,0017
C	1,4734	-3,7878	-1,7154
C	1,4690	-3,7863	1,7262
N	-0,5113	1,5317	0,0006
C	-0,2932	2,8937	0,0035
H	2,5647	-3,7084	-1,8243
H	1,0216	-3,2975	-2,5881
H	1,2223	-4,8565	-1,7723
H	1,2138	-4,8540	1,7839
H	1,0178	-3,2935	2,5978
H	2,5604	-3,7111	1,8364
C	2,8152	-0,1378	-1,2172
C	4,7343	0,7344	-0,0142
C	2,8405	-0,1706	1,2046
C	4,1057	0,4193	1,1941
H	4,6010	0,6331	2,1382
H	2,3526	-0,4130	2,1444
C	4,0809	0,4509	-1,2174
H	2,3078	-0,3560	-2,1527
H	5,7191	1,1934	-0,0183
H	4,5570	0,6892	-2,1655
C	1,0239	3,3967	0,0258
C	0,1548	5,6591	0,0105
C	-1,3831	3,7876	-0,0151
C	-1,1522	5,1614	-0,0117
H	-1,9958	5,8461	-0,0261
H	-2,3945	3,3931	-0,0320
C	1,2374	4,7728	0,0292
H	1,8560	2,6998	0,0397
H	0,3291	6,7315	0,0132
H	2,2540	5,1562	0,0466

2-II

E = -2362.912531

W	-0,0204	-0,0000	-0,0000
C	-0,9530	-0,2442	2,0891
C	-2,0650	-0,2373	1,2505
C	-2,0648	0,2373	-1,2508
C	-0,9527	0,2441	-2,0893
H	-0,5564	-1,1838	2,4613
H	-0,6976	0,6370	2,6674
H	-2,5323	-1,1747	0,9667
H	-2,6881	0,6451	1,1743
H	-2,6880	-0,6451	-1,1747
H	-2,5322	1,1748	-0,9671
H	-0,6974	-0,6371	-2,6676
H	-0,5562	1,1837	-2,4616
N	-0,0762	-1,9368	-0,1271
N	-0,0762	1,9368	0,1269
C	-0,8011	-3,0738	0,2854
C	-0,8009	3,0738	-0,2855
Al	1,4137	-2,4870	-1,3224
Cl	2,0061	-0,2443	-1,6338
C	2,8655	-3,3712	-0,3104
C	0,7804	-3,2104	-3,0552
Al	1,4132	2,4869	1,3229
Cl	2,0058	0,2442	1,6338
C	2,8652	3,3715	0,3116
C	0,7794	3,2098	3,0557
H	-0,0424	2,6445	3,5123
H	0,4377	4,2478	2,9401
H	1,6080	3,2217	3,7780
H	2,5873	4,3953	0,0260
H	3,1305	2,8292	-0,6043
H	3,7712	3,4414	0,9297
H	2,5875	-4,3948	-0,0245
H	3,1307	-2,8286	0,6053
H	3,7716	-3,4414	-0,9285
H	-0,0400	-2,6440	-3,5129
H	0,4370	-4,2476	-2,9390
H	1,6096	-3,2242	-3,7768
C	-0,4358	3,7573	-1,4625
C	-2,2530	5,3308	-1,1384
C	-1,8908	3,5519	0,4692
C	-2,6121	4,6640	0,0362
H	-3,4546	5,0151	0,6268
H	-2,1619	3,0490	1,3931
C	-1,1604	4,8736	-1,8800
H	0,4190	3,4087	-2,0353
H	-2,8150	6,1997	-1,4692
H	-0,8656	5,3887	-2,7908
C	-1,8910	-3,5517	-0,4694
C	-2,2535	-5,3305	1,1381
C	-0,4362	-3,7572	1,4624
C	-1,1609	-4,8734	1,8799
H	-0,8664	-5,3884	2,7909
H	0,4186	-3,4087	2,0352
C	-2,6125	-4,6638	-0,0364
H	-2,1620	-3,0488	-1,3934
H	-2,8152	-6,1998	1,4686
H	-3,4550	-5,0147	-0,6270

TS_{OXC}-**0**

E = -797.566528

W	-0,9643	0,0580	0,0017
C	-2,1002	0,1557	-1,8381
C	-3,2392	0,4421	-0,9458
C	-3,2472	0,0021	1,0062
C	-2,0554	0,1037	1,8692
H	-1,7676	0,9808	-2,4672
H	-2,1451	-0,7930	-2,3721
H	-3,5010	1,4947	-0,8680
H	-4,1137	-0,1910	-1,0582
H	-4,0096	0,7625	1,1431
H	-3,6704	-0,9969	0,9333
H	-1,9429	1,0421	2,4120
H	-1,8348	-0,7696	2,4821
N	-0,0854	-1,5120	0,0001
C	0,8974	-2,4814	0,0197
N	0,0953	1,5099	-0,0159
C	1,1953	2,3452	-0,0489
C	1,0399	3,7244	0,2068
C	3,4176	4,0767	-0,1191
C	2,4841	1,8496	-0,3437
C	3,5791	2,7103	-0,3767
H	4,5650	2,3128	-0,6048
H	2,6053	0,7886	-0,5441
C	2,1438	4,5759	0,1720
H	0,0489	4,1086	0,4319
H	4,2748	4,7438	-0,1456
H	2,0081	5,6359	0,3723
C	1,9936	-2,3889	0,9043
C	2,8779	-4,4860	0,0660
C	0,8087	-3,5995	-0,8370
C	1,7944	-4,5847	-0,8131
H	1,7140	-5,4373	-1,4832
H	-0,0349	-3,6755	-1,5175
C	2,9690	-3,3837	0,9230
H	2,0620	-1,5312	1,5680
H	3,6423	-5,2580	0,0829
H	3,8065	-3,2979	1,6112

TS_{OXC}-**I**

E = -1580.253416

W	-0,8029	-0,2703	-0,0004
C	-1,9052	-0,3905	-1,8499
C	-3,1174	-0,3136	-0,9950
C	-3,1277	-0,4780	0,9624
C	-1,9266	-0,4189	1,8333
H	-1,7237	0,4695	-2,4927
H	-1,7639	-1,3401	-2,3641
H	-3,6275	0,6439	-1,0442
H	-3,7992	-1,1503	-1,1013
H	-3,8180	0,3506	1,0873
H	-3,6260	-1,4410	0,9735
H	-1,8322	0,4673	2,4586
H	-1,7076	-1,3409	2,3709
N	0,9922	-0,9533	0,0033
C	2,2395	-0,2675	-0,0001
Al	1,0818	-2,8997	-0,0035
Cl	-1,2474	-2,9695	-0,0174
C	1,7370	-3,6313	-1,7267
C	1,7165	-3,6452	1,7215
N	-0,5814	1,4814	0,0071
C	-0,4275	2,8518	0,0153
H	2,8153	-3,4555	-1,8492
H	1,2315	-3,1820	-2,5918
H	1,5801	-4,7180	-1,7803
H	1,5554	-4,7316	1,7658
H	1,2035	-3,2003	2,5846
H	2,7941	-3,4740	1,8565
C	0,8620	3,4194	-0,0426
C	-0,1159	5,6366	0,0316
C	-1,5586	3,6907	0,0821
C	-1,3952	5,0743	0,0894
H	-2,2707	5,7157	0,1406
H	-2,5487	3,2474	0,1276
C	1,0069	4,8044	-0,0337
H	1,7266	2,7657	-0,0932
H	0,0056	6,7161	0,0378
H	2,0027	5,2376	-0,0784
C	2,8562	0,0838	-1,2135
C	4,7141	1,0742	-0,0078
C	2,8851	0,0441	1,2088
C	4,1095	0,7149	1,2003
H	4,5919	0,9564	2,1442
H	2,4137	-0,2335	2,1474
C	4,0806	0,7546	-1,2124
H	2,3625	-0,1641	-2,1489
H	5,6672	1,5960	-0,0107
H	4,5406	1,0266	-2,1593

TS_{OXC}-**II**

E = -2362.892430

W	-0,6919	-0,4721	-0,1539
C	-1,9822	-0,6821	1,5474
C	-3,1001	-0,5672	0,5881
C	-2,8933	-0,4780	-1,4013
C	-1,6040	-0,4680	-2,1136
H	-1,8770	-1,6497	2,0340
H	-1,8458	0,1535	2,2354
H	-3,7311	-1,4454	0,5219
H	-3,6611	0,3595	0,6545
H	-3,4872	-1,3721	-1,5467
H	-3,4685	0,4384	-1,4889
H	-1,3614	-1,3668	-2,6773
H	-1,3563	0,4423	-2,6560
N	-0,5181	1,3121	0,1712
N	0,9775	-1,3329	0,1862
C	-0,8875	2,4050	0,9862
C	2,2190	-0,8816	0,7195
Al	0,7377	2,3139	-1,4246
Cl	1,5243	0,6782	-2,6906
C	-0,6069	3,3755	-2,4188
C	2,1912	3,1200	-0,3544
Al	0,9316	-3,2781	-0,0927
Cl	-1,3671	-3,0986	-0,4098
C	1,2501	-4,2335	1,6127
C	1,7357	-3,8748	-1,8015
H	-0,9096	4,2787	-1,8743
H	-1,5179	2,8258	-2,6867
H	-0,1426	3,7011	-3,3613
H	2,6887	2,3938	0,2996
H	1,8547	3,9621	0,2624
H	2,9503	3,5015	-1,0524
H	2,8291	-3,9551	-1,7292
H	1,5082	-3,1889	-2,6274
H	1,3585	-4,8687	-2,0799
H	0,6762	-3,8063	2,4451
H	2,3116	-4,2037	1,8959
H	0,9690	-5,2921	1,5240
C	-2,0332	3,1565	0,6708
C	-1,6925	4,4965	2,6596
C	-0,1386	2,7126	2,1353
C	-0,5489	3,7530	2,9662
H	0,0301	3,9840	3,8560
H	0,7507	2,1349	2,3620
C	-2,4321	4,1925	1,5135
H	-2,6019	2,9200	-0,2223
H	-2,0063	5,3070	3,3113
H	-3,3233	4,7645	1,2703
C	3,3984	-0,9860	-0,0375
C	4,6834	-0,0836	1,8124
C	2,2888	-0,3866	2,0331
C	3,5131	0,0090	2,5718
H	3,5518	0,3861	3,5907
H	1,3814	-0,3385	2,6288
C	4,6178	-0,5816	0,5084
H	3,3472	-1,3547	-1,0566
H	5,6360	0,2259	2,2335
H	5,5202	-0,6558	-0,0928

3-0

E = -797.582169

W	-0,9485	-0,0092	0,0059
C	-2,3681	-0,0822	-1,5923
C	-3,5479	-0,4526	-0,6355
C	-3,5436	0,3671	0,7049
C	-2,3330	0,0282	1,6344
H	-2,5375	0,8984	-2,0510
H	-2,2253	-0,8274	-2,3780
H	-4,5020	-0,2783	-1,1480
H	-3,5108	-1,5232	-0,3930
H	-3,5401	1,4382	0,4620
H	-4,4808	0,1679	1,2390
H	-2,1916	0,7773	2,4166
H	-2,4658	-0,9564	2,0967
N	0,0350	-1,5115	0,0197
C	1,1240	-2,3619	0,0276
N	0,0018	1,5143	-0,0246
C	1,0726	2,3870	-0,0473
C	1,6324	2,8040	-1,2739
C	3,2285	4,1981	-0,0941
C	1,6060	2,8982	1,1550
C	2,6746	3,7924	1,1248
H	3,0772	4,1753	2,0593
H	1,1732	2,5812	2,0996
C	2,7016	3,6977	-1,2896
H	1,2197	2,4142	-2,2001
H	4,0614	4,8955	-0,1121
H	3,1254	4,0067	-2,2420
C	1,5101	-3,0379	-1,1493
C	3,3157	-4,1300	0,0463
C	1,8500	-2,5914	1,2159
C	2,9355	-3,4653	1,2174
H	3,4875	-3,6297	2,1395
H	1,5509	-2,0749	2,1235
C	2,5970	-3,9102	-1,1335
H	0,9498	-2,8647	-2,0638
H	4,1620	-4,8113	0,0536
H	2,8843	-4,4222	-2,0486

3-I

E = -1580.263881

W	-0,7885	-0,3420	0,0005
C	-2,1268	-0,5577	-1,6522
C	-3,3676	-0,7789	-0,7234
C	-3,3547	-0,0799	0,7034
C	-2,1600	-0,4504	1,6375
H	-2,2295	0,3429	-2,2622
H	-1,9546	-1,4228	-2,2955
H	-4,2616	-0,4060	-1,2357
H	-3,5003	-1,8521	-0,5633
H	-3,3880	1,0065	0,5687
H	-4,2937	-0,3735	1,1869
H	-2,0410	0,2712	2,4478
H	-2,2661	-1,4583	2,0480
N	1,0453	-0,9160	0,0141
C	2,2284	-0,1276	0,0448
Al	1,2683	-2,8510	0,0243
Cl	-1,0471	-3,0600	0,0202
C	1,9503	-3,6010	-1,6820
C	1,9656	-3,5110	1,7595
N	-0,6107	1,4140	-0,0229
C	-0,4756	2,7832	-0,0604
H	3,0352	-3,4559	-1,7834
H	1,4731	-3,1500	-2,5623
H	1,7669	-4,6842	-1,7275
H	1,9122	-4,6070	1,8203
H	1,4086	-3,1041	2,6139
H	3,0206	-3,2321	1,8939
C	3,0890	-0,0942	-1,0668
C	4,5840	1,4115	0,1076
C	2,5699	0,6091	1,1925
C	3,7352	1,3751	1,2181
H	3,9828	1,9426	2,1118
H	1,9152	0,5703	2,0589
C	4,2549	0,6726	-1,0320
H	2,8284	-0,6600	-1,9566
H	5,4929	2,0066	0,1314
H	4,9057	0,6940	-1,9026
C	-0,5605	3,5378	1,1277
C	-0,2237	5,5712	-0,1462
C	-0,2608	3,4364	-1,2916
C	-0,1365	4,8229	-1,3253
H	0,0310	5,3222	-2,2758
H	-0,1900	2,8463	-2,2002
C	-0,4353	4,9238	1,0759
H	-0,7205	3,0266	2,0720
H	-0,1252	6,6525	-0,1794
H	-0,5014	5,5019	1,9937

3-II

E = -2362.914368

W	-0,1171	-0,3481	-0,6586
C	-2,2811	-0,4215	-0,6759
C	-2,8801	0,0499	-2,0030
C	-2,0962	-0,6768	-3,1003
C	-0,6072	-0,4263	-2,8321
H	-2,5400	-1,4745	-0,5000
H	-2,6342	0,1469	0,1981
H	-3,9578	-0,1614	-2,0545
H	-2,7555	1,1355	-2,1142
H	-2,3035	-1,7529	-3,0383
H	-2,3882	-0,3460	-4,1073
H	0,0484	-1,1052	-3,3833
H	-0,3435	0,5999	-3,1348
N	-0,0642	1,4549	-0,3036
N	-0,0067	-1,3931	0,9637
C	-0,5244	2,6335	0,3184
C	0,1434	-0,8163	2,2604
Al	1,7633	2,0382	-1,2326
Cl	2,2646	-0,1924	-1,6746
C	1,4280	3,0058	-2,9157
C	2,9504	2,6518	0,2138
Al	-0,0721	-3,3446	0,8588
Cl	0,0068	-3,0507	-1,4129
C	-1,8240	-4,1029	1,4012
C	1,6247	-4,1217	1,5261
H	1,2255	4,0670	-2,7205
H	0,5967	2,6078	-3,5086
H	2,3301	2,9545	-3,5400
H	2,9275	1,9976	1,0924
H	2,6819	3,6648	0,5399
H	3,9850	2,6849	-0,1528
H	1,6714	-4,0945	2,6239
H	2,5082	-3,5935	1,1446
H	1,7158	-5,1751	1,2251
H	-2,6826	-3,5653	0,9781
H	-1,9380	-4,0990	2,4945
H	-1,9022	-5,1496	1,0747
C	-1,1276	3,6364	-0,4645
C	-1,5015	4,9594	1,5288
C	-0,4007	2,8075	1,7091
C	-0,8948	3,9656	2,3042
H	-0,8033	4,0945	3,3792
H	0,0718	2,0334	2,3044
C	-1,6196	4,7887	0,1466
H	-1,2245	3,4937	-1,5360
H	-1,8824	5,8609	2,0004
H	-2,0947	5,5543	-0,4603
C	1,4070	-0,3986	2,7124
C	0,4521	0,2213	4,8541
C	-0,9624	-0,7253	3,1247
C	-0,8039	-0,2000	4,4079
H	-1,6689	-0,1239	5,0617
H	-1,9384	-1,0561	2,7818
C	1,5552	0,1141	4,0021
H	2,2643	-0,4918	2,0520
H	0,5706	0,6244	5,8560
H	2,5385	0,4311	4,3396

$TS_{\beta Hab}$-**0**

E = -797.519106

W	-0,5701	-0,6487	0,1716
C	-1,9692	-2,4654	0,6435
C	-2,4670	-1,3123	1,3535
C	-3,1338	-0,3332	0,3461
C	-2,3728	-0,3874	-1,0259
H	-2,4916	-2,7595	-0,2598
H	-1,5298	-3,2788	1,2185
H	-1,3332	-0,6640	1,8464
H	-2,8637	-1,3374	2,3712
H	-4,1580	-0,7089	0,2105
H	-3,1934	0,6808	0,7455
H	-2,7043	-1,2153	-1,6527
H	-2,4448	0,5542	-1,5690
N	-0,2636	1,1428	0,2103
C	-0,2935	2,5091	0,3207
N	0,9091	-1,5506	-0,3695
C	2,2221	-1,7037	-0,7471
C	2,5871	-1,6575	-2,1130
C	4,9100	-2,0459	-1,5326
C	3,2316	-1,9363	0,2158
C	4,5581	-2,0953	-0,1786
H	5,3230	-2,2653	0,5753
H	2,9551	-1,9816	1,2656
C	3,9163	-1,8273	-2,4937
H	1,8129	-1,4848	-2,8555
H	5,9455	-2,1758	-1,8346
H	4,1793	-1,7876	-3,5480
C	-0,3714	3,1362	1,5862
C	-0,3388	5,3236	0,5338
C	-0,2313	3,3218	-0,8355
C	-0,2636	4,7102	-0,7216
H	-0,2192	5,3186	-1,6217
H	-0,1599	2,8454	-1,8092
C	-0,3899	4,5258	1,6827
H	-0,4093	2,5172	2,4785
H	-0,3550	6,4067	0,6162
H	-0,4452	4,9902	2,6646

$TS_{\beta Hab}$-**I**

E = -1580.205253

W	-0,0730	0,1127	0,4298
C	-1,4000	-1,8861	0,3078
C	-2,1731	-0,9461	1,0419
C	-2,8264	0,1320	0,1681
C	-1,7548	0,5093	-0,9025
H	-1,5712	-1,9725	-0,7595
H	-1,0218	-2,7693	0,8103
H	-1,2002	-0,1137	1,8387
H	-2,6171	-1,1988	2,0045
H	-3,7429	-0,2768	-0,2789
H	-3,1025	1,0005	0,7710
H	-1,8087	-0,1580	-1,7670
H	-1,8480	1,5425	-1,2389
N	1,5440	-0,5344	-0,4609
C	2,2049	0,2780	-1,4141
Al	2,3608	-2,0468	0,4512
Cl	1,0669	-1,4638	2,3207
C	1,8086	-3,8021	-0,2880
C	4,2507	-1,8462	1,0349
N	0,1103	1,8776	0,6911
H	2,4019	-4,0339	-1,1855
H	0,7518	-3,8504	-0,5769
H	1,9943	-4,6114	0,4322
H	4,4563	-0,9024	1,5560
H	4,9587	-1,9297	0,1986
H	4,4882	-2,6611	1,7351
C	-0,0330	3,2326	0,8867
C	3,5427	0,6892	-1,2392
C	3,4724	1,9018	-3,3406
C	1,5216	0,6861	-2,5779
C	2,1512	1,4889	-3,5295
H	1,6074	1,7878	-4,4222
H	0,5020	0,3445	-2,7326
C	4,1610	1,4981	-2,1903
H	4,0789	0,3914	-0,3443
H	3,9635	2,5265	-4,0816
H	5,1889	1,8153	-2,0326
C	0,6142	4,1383	0,0188
C	-0,2997	5,9991	1,2732
C	-0,8108	3,7307	1,9539
C	-0,9374	5,1046	2,1408
H	-1,5354	5,4809	2,9666
H	-1,2995	3,0283	2,6230
C	0,4709	5,5102	0,2127
H	1,2147	3,7478	-0,7972
H	-0,4033	7,0700	1,4231
H	0,9684	6,2013	-0,4623

$TS_{\beta Hab}$-**II**

E = -2362.872919

W	-0,1184	-0,0093	0,2133
C	-1,5194	-1,5140	1,3873
C	-2,0267	-0,2294	1,6275
C	-2,7695	0,3981	0,4434
C	-2,0465	-0,0552	-0,8532
H	-1,9090	-2,0988	0,5645
H	-1,0300	-2,0617	2,1857
H	-0,5512	0,5611	1,7907
H	-2,1611	0,1768	2,6276
H	-3,8083	0,0335	0,4911
H	-2,7953	1,4851	0,5401
H	-2,3899	-1,0223	-1,2190
H	-2,1123	0,6871	-1,6507
N	1,4121	-0,9925	0,8919
N	-0,0385	1,9327	0,2570
C	2,3564	-0,4081	1,7783
C	-0,4709	2,8985	1,1998
Al	1,7953	-2,7899	0,1900
Cl	0,0129	-2,5806	-1,2172
C	3,4605	-2,8642	-0,8884
C	1,4722	-4,1501	1,6000
Al	0,8519	2,6725	-1,3212
Cl	1,1214	0,4676	-2,0133
C	-0,3486	3,5469	-2,6372
C	2,6154	3,4548	-0,8774
H	3,1949	2,8189	-0,1964
H	2,5040	4,4370	-0,3960
H	3,2172	3,6077	-1,7842
H	-0,5220	4,6053	-2,3986
H	-1,3286	3,0593	-2,7220
H	0,1161	3,5163	-3,6335
H	4,3646	-2,8788	-0,2648
H	3,5508	-2,0289	-1,5941
H	3,4613	-3,7921	-1,4791
H	0,4744	-4,0875	2,0527
H	2,2075	-4,0539	2,4119
H	1,5803	-5,1635	1,1879
C	-1,3607	3,9174	0,8053
C	-1,3219	4,8540	3,0423
C	-0,0015	2,8861	2,5262
C	-0,4278	3,8540	3,4363
H	-0,0500	3,8320	4,4555
H	0,7182	2,1283	2,8222
C	-1,7831	4,8803	1,7233
H	-1,7294	3,9392	-0,2161
H	-1,6493	5,6077	3,7529
H	-2,4789	5,6518	1,4037
C	3,6553	-0,0889	1,3361
C	4,2475	0,6516	3,5698
C	2,0226	-0,2018	3,1301
C	2,9675	0,3153	4,0173
H	2,6982	0,4576	5,0607
H	1,0321	-0,4799	3,4782
C	4,5818	0,4508	2,2261
H	3,9180	-0,2458	0,2950
H	4,9796	1,0604	4,2605
H	5,5739	0,7118	1,8671

4-0

E = -797.556845

W	-0,6559	-0,7008	-0,2095
C	-4,7612	-3,0705	-1,9168
C	-3,6327	-2,6931	-2,5240
C	-2,3125	-2,4623	-1,8356
C	-1,8229	-0,9957	-1,9712
H	-4,7975	-3,2555	-0,8442
H	-5,6869	-3,2069	-2,4705
H	-1,3715	-1,0870	1,3351
H	-3,6338	-2,5105	-3,6000
H	-1,5434	-3,1230	-2,2540
H	-2,4282	-2,7498	-0,7734
H	-1,3539	-0,8078	-2,9412
H	-2,6649	-0,2911	-1,8593
N	-0,2037	1,0261	-0,0944
N	0,7650	-1,7805	-0,3366
C	0,5556	2,1787	-0,0252
C	2,0829	-2,1930	-0,4037
C	2,6653	-2,5085	-1,6488
C	4,7465	-3,0779	-0,5429
C	2,8496	-2,3349	0,7717
C	4,1705	-2,7713	0,6945
H	4,7532	-2,8744	1,6064
H	2,3956	-2,0982	1,7298
C	3,9882	-2,9416	-1,7107
H	2,0713	-2,4024	-2,5521
H	5,7767	-3,4189	-0,5968
H	4,4289	-3,1780	-2,6760
C	1,1518	2,7175	-1,1848
C	2,0614	4,5489	0,1184
C	0,7171	2,8479	1,2057
C	1,4670	4,0209	1,2695
H	1,5862	4,5272	2,2241
H	0,2522	2,4343	2,0959
C	1,9003	3,8900	-1,1052
H	1,0217	2,2036	-2,1329
H	2,6443	5,4641	0,1742
H	2,3583	4,2930	-2,0049

4-I

E = -1580.248622

W	0,0136	-0,0041	0,5212
C	-2,4756	-0,8307	1,4851
C	-2,7340	0,0942	0,5322
C	-2,6569	-0,1623	-0,9549
C	-1,2432	0,3393	-1,2862
H	-2,3779	-1,8856	1,2427
H	-2,4715	-0,5660	2,5380
H	-0,0845	-0,9484	1,9725
H	-2,9000	1,1287	0,8346
H	-2,7412	-1,2353	-1,1541
H	-3,4506	0,3572	-1,5044
H	-0,7885	-0,1926	-2,1276
H	-1,2316	1,4148	-1,4925
N	1,8044	-0,1780	-0,1066
C	2,9249	0,6907	-0,0328
Al	2,1144	-1,9556	-0,9009
Cl	-0,0883	-2,5335	-0,4089
C	2,2845	-1,9440	-2,8779
C	3,3260	-3,0348	0,2338
N	-0,0152	1,5939	1,2786
H	3,3005	-1,6765	-3,2005
H	1,5883	-1,2469	-3,3624
H	2,0760	-2,9463	-3,2786
H	3,0386	-2,9987	1,2925
H	4,3630	-2,6774	0,1611
H	3,3248	-4,0888	-0,0764
C	-0,0702	2,8208	1,9023
C	3,3779	1,1747	1,2067
C	5,1543	2,4005	0,1011
C	3,6097	1,0623	-1,2039
C	4,7111	1,9165	-1,1326
H	5,2229	2,2043	-2,0475
H	3,2604	0,6976	-2,1658
C	4,4825	2,0235	1,2682
H	2,8606	0,8717	2,1126
H	6,0153	3,0612	0,1536
H	4,8212	2,3891	2,2344
C	0,0833	4,0027	1,1488
C	-0,1896	5,3181	3,1657
C	-0,2833	2,9002	3,2940
C	-0,3421	4,1457	3,9142
H	-0,5066	4,2022	4,9868
H	-0,3966	1,9838	3,8654
C	0,0235	5,2401	1,7851
H	0,2523	3,9321	0,0787
H	-0,2350	6,2866	3,6557
H	0,1448	6,1483	1,2008

4-II

E = -2362.885112

W	-0,3567	-0,1843	-0,4401
C	-5,7294	-1,5091	-1,1985
C	-4,5916	-1,1940	-1,8242
C	-3,2093	-1,4533	-1,2825
C	-2,4302	-0,1416	-1,0532
H	-5,7274	-1,9985	-0,2255
H	-6,7009	-1,2935	-1,6370
H	-1,3432	-0,6238	0,8434
H	-4,6359	-0,7021	-2,7980
H	-3,2809	-2,0029	-0,3371
H	-2,6563	-2,0820	-1,9916
H	-2,3517	0,4195	-2,0052
H	-2,9774	0,4902	-0,3454
N	-0,3748	1,3124	0,7670
N	0,2790	-1,8961	0,0026
C	-1,1179	1,6033	1,9369
C	0,4819	-2,6731	1,1707
Al	1,0172	2,6429	0,3513
Cl	1,8337	1,0600	-1,1745
C	0,3934	4,1994	-0,7004
C	2,2963	2,7970	1,8514
Al	0,8444	-2,8131	-1,7099
Cl	-0,1019	-1,0437	-2,9139
C	-0,2539	-4,4238	-2,0308
C	2,8083	-2,7835	-1,8943
H	-0,0426	4,9791	-0,0604
H	-0,3599	3,9289	-1,4519
H	1,2372	4,6600	-1,2335
H	2,5729	1,8183	2,2634
H	1,8749	3,3944	2,6718
H	3,2193	3,2962	1,5264
H	3,2709	-3,4860	-1,1873
H	3,2403	-1,7926	-1,7113
H	3,1047	-3,0966	-2,9045
H	-1,3256	-4,2606	-1,8685
H	0,0628	-5,2493	-1,3793
H	-0,1216	-4,7591	-3,0686
C	-1,8422	2,8082	2,0143
C	-2,5933	2,2330	4,2460
C	-1,1266	0,7275	3,0370
C	-1,8598	1,0437	4,1799
H	-1,8534	0,3602	5,0250
H	-0,5432	-0,1872	2,9883
C	-2,5823	3,1102	3,1584
H	-1,8457	3,4859	1,1650
H	-3,1643	2,4744	5,1382
H	-3,1521	4,0349	3,1963
C	1,6138	-2,4511	1,9732
C	0,8888	-4,2075	3,4772
C	-0,4385	-3,6751	1,5201
C	-0,2338	-4,4301	2,6750
H	-0,9553	-5,1959	2,9465
H	-1,3100	-3,8427	0,8953
C	1,8098	-3,2172	3,1216
H	2,3249	-1,6798	1,6922
H	1,0448	-4,8005	4,3740
H	2,6844	-3,0369	3,7407

TS_{RECH}-**0**

E = -797.459835

W	-0,3240	-0,5022	0,7881
C	-5,7769	-0,7710	-1,4480
C	-4,6080	-1,4177	-1,4169
C	-3,7219	-1,5300	-0,2053
C	-2,3635	-0,8202	-0,4633
H	-6,1774	-0,2743	-0,5654
H	-6,3765	-0,7210	-2,3536
H	-1,9531	-1,2345	0,8147
H	-4,2407	-1,9020	-2,3235
H	-3,5360	-2,5892	0,0193
H	-4,2172	-1,0859	0,6654
H	-1,8641	-1,2672	-1,3239
H	-2,5285	0,2457	-0,6231
N	-0,2294	1,2974	0,8423
N	0,8971	-1,3116	-0,2632
C	0,0122	2,6340	0,6213
C	1,9023	-1,5966	-1,1608
C	1,6011	-2,0155	-2,4761
C	3,9659	-2,2243	-2,9767
C	3,2574	-1,4992	-0,7732
C	4,2722	-1,8149	-1,6743
H	5,3098	-1,7359	-1,3590
H	3,4900	-1,1728	0,2364
C	2,6259	-2,3177	-3,3702
H	0,5611	-2,0926	-2,7807
H	4,7608	-2,4646	-3,6774
H	2,3771	-2,6336	-4,3804
C	-0,5563	3,3021	-0,4868
C	0,4749	5,3863	0,2081
C	0,8214	3,3711	1,5151
C	1,0426	4,7310	1,3065
H	1,6675	5,2824	2,0049
H	1,2671	2,8588	2,3632
C	-0,3216	4,6610	-0,6855
H	-1,1709	2,7390	-1,1834
H	0,6548	6,4457	0,0475
H	-0,7645	5,1581	-1,5453

TS_{RECH}-**I**

E = -1580.165173

W	-0,5499	-0,2373	0,7326
C	-5,1387	-0,4463	2,0440
C	-4,7341	-0,3321	0,7755
C	-3,9725	-1,3834	0,0210
C	-2,5501	-0,9047	-0,4083
H	-4,9548	-1,3507	2,6215
H	-5,6726	0,3568	2,5460
H	-2,2137	-0,8352	0,9016
H	-4,9388	0,5921	0,2314
H	-3,8979	-2,2997	0,6175
H	-4,5023	-1,6333	-0,9092
H	-2,0585	-1,6942	-0,9819
H	-2,6372	-0,0017	-1,0125
N	0,8310	-1,2535	-0,1097
C	1,7973	-1,0725	-1,1278
Al	1,1697	-2,7713	1,1241
Cl	-0,3771	-1,8733	2,7072
C	0,3813	-4,5044	0,5790
C	2,9699	-2,5934	1,9214
N	-0,5368	1,5093	0,3671
H	0,9940	-5,0065	-0,1829
H	-0,6305	-4,3951	0,1671
H	0,3153	-5,1867	1,4377
H	3,1593	-1,5742	2,2804
H	3,7535	-2,8391	1,1918
H	3,0881	-3,2778	2,7723
C	-0,6887	2,8786	0,2842
C	2,4338	0,1674	-1,3201
C	3,7207	-0,7546	-3,1576
C	2,1403	-2,1508	-1,9650
C	3,0941	-1,9889	-2,9714
H	3,3443	-2,8310	-3,6114
H	1,6417	-3,1081	-1,8345
C	3,3835	0,3210	-2,3276
H	2,1714	0,9987	-0,6716
H	4,4639	-0,6298	-3,9402
H	3,8666	1,2853	-2,4639
C	-1,1044	3,4705	-0,9275
C	-0,9842	5,6688	0,0899
C	-0,4155	3,7053	1,3949
C	-0,5647	5,0865	1,2914
H	-0,3505	5,7131	2,1535
H	-0,0851	3,2485	2,3236
C	-1,2531	4,8535	-1,0148
H	-1,3025	2,8338	-1,7848
H	-1,0966	6,7468	0,0144
H	-1,5752	5,2977	-1,9533

TS_{RECH}-**II**

E = -2362.848766

W	-0,4685	-0,2371	-0,0856
C	-6,1938	-0,5882	-1,7399
C	-4,9500	-1,0331	-1,9389
C	-3,9037	-1,1595	-0,8642
C	-2,6924	-0,2429	-1,1630
H	-6,5397	-0,2829	-0,7536
H	-6,9101	-0,5189	-2,5549
H	-2,1711	-0,4674	0,0864
H	-4,6390	-1,3291	-2,9421
H	-4,3403	-0,9118	0,1108
H	-3,5543	-2,1998	-0,8149
H	-2,2549	-0,4996	-2,1299
H	-2,9750	0,8116	-1,1569
N	0,0951	-1,8181	0,7370
N	-0,2713	1,1260	1,1649
C	0,0769	-2,4906	1,9896
C	-0,3722	1,4005	2,5561
Al	0,9502	-3,0063	-0,6709
Cl	0,1672	-1,5919	-2,3185
C	2,9257	-2,9213	-0,6596
C	-0,0836	-4,6896	-0,7464
Al	0,2198	2,8257	0,1410
Cl	-0,2621	1,7612	-1,8508
C	-1,1851	4,1635	0,5166
C	2,1583	3,2092	0,1950
H	2,7669	2,3089	0,0425
H	2,4651	3,6650	1,1457
H	2,4159	3,9208	-0,6015
H	-1,0846	4,5701	1,5320
H	-2,1962	3,7473	0,4241
H	-1,1069	5,0068	-0,1827
H	3,3644	-3,5607	0,1179
H	3,2988	-1,9009	-0,5049
H	3,3169	-3,2727	-1,6245
H	-1,1660	-4,5113	-0,7691
H	0,1299	-5,3305	0,1193
H	0,1779	-5,2595	-1,6483
C	-1,6196	1,3182	3,1958
C	-0,5835	1,9457	5,2960
C	0,7674	1,7628	3,2914
C	0,6558	2,0250	4,6581
H	1,5452	2,2915	5,2229
H	1,7332	1,8116	2,7974
C	-1,7182	1,5927	4,5579
H	-2,4960	1,0400	2,6183
H	-0,6660	2,1534	6,3592
H	-2,6872	1,5262	5,0462
C	1,2815	-2,7960	2,6437
C	0,0421	-3,8392	4,4475
C	-1,1454	-2,8653	2,5710
C	-1,1560	-3,5383	3,7906
H	-2,1068	-3,8257	4,2321
H	-2,0725	-2,6255	2,0593
C	1,2563	-3,4610	3,8711
H	2,2252	-2,4903	2,2020
H	0,0271	-4,3601	5,4007
H	2,1933	-3,6818	4,3755

TS_{INS}-**0**

E = -876.194767

W	-0,1254	-0,4956	0,5883
C	-2,3866	-0,7914	1,6948
C	-3,2273	0,4378	1,3748
C	-3,0110	0,7904	-0,0910
C	-1,5142	0,9762	-0,3025
N	1,2820	0,4773	0,0248
C	2,3433	1,2309	-0,4092
H	-2,4643	-1,5470	0,8995
H	-2,7281	-1,2664	2,6117
H	-4,2858	0,2261	1,5940
H	-2,9417	1,2883	2,0118
H	-3,3856	-0,0337	-0,7147
H	-3,5736	1,6920	-0,3758
C	-0,5899	-0,9429	3,0775
H	-1,1882	1,9113	0,1850
N	-0,2072	-2,0455	-0,3323
H	-1,2459	1,0670	-1,3632
C	0,7489	-0,8612	2,6271
H	1,3216	0,0358	2,8546
H	1,3281	-1,7801	2,5583
H	-1,0323	-0,1159	3,6227
H	-0,9914	-1,9210	3,3130
C	3,2742	0,7039	-1,3342
C	4,5115	2,7882	-1,3113
C	2,5238	2,5541	0,0546
C	3,5962	3,3205	-0,3968
C	4,3449	1,4777	-1,7747
C	0,2181	-2,9305	-1,3023
C	0,3003	-4,3098	-1,0101
C	1,0267	-4,7745	-3,2784
C	0,5413	-2,4939	-2,6063
C	0,9416	-3,4097	-3,5773
H	1,1868	-3,0558	-4,5758
H	0,4737	-1,4342	-2,8362
C	0,7063	-5,2151	-1,9896
H	0,0473	-4,6504	-0,0099
H	1,3388	-5,4845	-4,0394
H	0,7677	-6,2730	-1,7460
H	3,1375	-0,3126	-1,6916
H	5,3473	3,3886	-1,6603
H	1,8100	2,9615	0,7653
H	3,7205	4,3376	-0,0333
H	5,0533	1,0588	-2,4851

TS_{INS}-**I**

E = -1658.876729

W	-0,9018	-0,2066	0,0495
C	-3,1099	-0,3516	1,4824
C	-3,8411	0,8479	0,8864
C	-3,7748	0,8529	-0,6550
C	-2,7681	-0,1928	-1,1369
H	-3,3868	-1,3031	1,0238
H	-3,3530	-0,4151	2,5414
H	-4,8847	0,8110	1,2382
H	-3,4264	1,7797	1,2899
H	-4,7699	0,6485	-1,0753
H	-3,4769	1,8428	-1,0179
H	-3,1919	-1,2032	-1,1263
H	-2,4307	0,0186	-2,1605
C	-1,1943	-0,5466	2,6038
C	0,0974	-0,6118	2,0152
N	-0,6626	1,5427	0,0360
C	-0,4662	2,9080	0,0371
H	0,7767	0,2245	2,1675
H	0,5678	-1,5897	1,9417
H	-1,4718	0,3442	3,1568
H	-1,6462	-1,4686	2,9490
C	0,0690	3,5453	-1,1010
C	-0,0642	5,6817	0,0371
C	-0,7990	3,6720	1,1742
C	-0,5947	5,0502	1,1667
C	0,2649	4,9242	-1,0921
H	0,3250	2,9498	-1,9713
H	0,0922	6,7566	0,0368
H	-1,2110	3,1761	2,0476
H	-0,8526	5,6336	2,0465
H	0,6782	5,4102	-1,9719
N	0,3120	-0,8441	-1,2944
C	1,2233	-0,1292	-2,1199
Al	0,2953	-2,7881	-1,5145
Cl	-1,2859	-2,9267	0,1756
C	-0,5470	-3,3895	-3,2073
C	1,9922	-3,5935	-0,8774
H	0,1305	-3,2665	-4,0638
H	-1,4718	-2,8434	-3,4359
H	-0,8027	-4,4572	-3,1506
H	1,9015	-4,6845	-0,7802
H	2,3021	-3,2000	0,0995
H	2,8120	-3,3998	-1,5836
C	0,9686	0,0204	-3,4948
C	3,0366	1,2611	-3,7636
C	2,4030	0,4125	-1,5814
C	3,2993	1,1007	-2,3999
H	4,2070	1,5142	-1,9673
H	2,6060	0,2875	-0,5214
C	1,8667	0,7194	-4,3036
H	0,0600	-0,3980	-3,9178
H	3,7354	1,7997	-4,3978
H	1,6489	0,8373	-5,3623

TS_{INS}-**II**

E = -2441.510822

W	-0,7496	-0,5782	0,1203
C	-3,1008	-0,8548	1,0637
C	-3,8538	-1,7979	0,1482
C	-3,5085	-1,5268	-1,3288
C	-2,3098	-0,5804	-1,4362
H	-3,2297	0,1966	0,7875
H	-3,4321	-0,9583	2,0948
H	-4,9318	-1,6709	0,3367
H	-3,6239	-2,8374	0,4088
H	-4,3671	-1,0783	-1,8460
H	-3,2849	-2,4650	-1,8443
H	-2,6335	0,4685	-1,3669
H	-1,7841	-0,6811	-2,3901
C	-1,3065	-1,5670	2,4085
C	0,0465	-1,5239	2,0181
H	0,5520	-2,4439	1,7452
H	0,6773	-0,7396	2,4350
H	-1,8500	-2,5034	2,3857
H	-1,6737	-0,8109	3,0927
N	-0,6603	1,1136	0,8357
C	-0,5744	1,7837	2,0878
Al	-0,9560	2,8163	-0,5502
Cl	-0,5277	2,0771	-2,5877
C	0,4744	4,0746	-0,0086
C	-2,8834	3,2505	-0,3546
H	0,2965	4,5408	0,9681
H	1,4634	3,6002	0,0173
H	0,5201	4,8773	-0,7592
H	-3,1760	3,8743	-1,2117
H	-3,5570	2,3837	-0,3509
H	-3,0843	3,8315	0,5546
C	0,6734	2,0199	2,6890
C	-0,4326	3,0303	4,5941
C	-1,7505	2,1879	2,7431
C	-1,6730	2,8032	3,9924
H	-2,5882	3,1047	4,4947
H	-2,7133	2,0107	2,2763
C	0,7368	2,6363	3,9376
H	1,5822	1,7326	2,1718
H	-0,3772	3,5123	5,5661
H	1,7062	2,8124	4,3955
N	0,7840	-0,9341	-0,9783
C	1,9407	-0,1976	-1,3407
Al	0,8895	-2,8088	-1,5907
Cl	-1,0091	-3,2431	-0,3376
C	2,4328	-3,7114	-0,7362
C	0,4289	-3,1100	-3,4954
H	3,3767	-3,4201	-1,2178
H	2,5272	-3,4801	0,3327
H	2,3436	-4,8025	-0,8315
H	0,0355	-4,1291	-3,6179
H	-0,3366	-2,4188	-3,8704
H	1,3064	-3,0230	-4,1500
C	2,7331	0,4357	-0,3691
C	4,2808	1,1767	-2,0795
C	2,3423	-0,1441	-2,6888
C	3,4966	0,5480	-3,0502
H	3,7833	0,5944	-4,0976
H	1,7264	-0,6136	-3,4497
C	3,8948	1,1119	-0,7378
H	2,4448	0,3643	0,6746
H	5,1843	1,7086	-2,3643
H	4,5017	1,5883	0,0279