List of Supporting Information (Theory part):

Table S1. The TPSS-D3/def2-TZVP + COSMO(toluene) predicted zero-point energies (ZPE), enthalpy (Hc) and Gibbs free energy (Gc) corrections at 298.15 K; COSMO-RS solvation enthalpy (Hsol) and free energy (Gsol) corrections in toluene; the PW6B95-D3/def2-QZVP computed total (TE, in hartrees) and relative electronic energies (RE) as well as final relative free energies (Grel) and relative enthalpies (Hrel) including thermal and solvation corrections; the differences of the relative electronic energies with respect to the TPSS-D3/def2-QZVP (Dif_T) calculations. All energy quantities are given in unit of kcal/mol unless specified otherwise. For each transition structure the imaginary frequency (in cm^{-1}) is also listed.

Table S2. The TPSS-D3/def2-TZVP + COSMO(toluene) optimized Cartesian coordinates (in Å). Each structure is labeled by the name as used in the manuscript, followed by the number of atoms, total energies in hartree, and atomic Cartesian coordinates in angstrom. Transition structures are indicated by the prefix **TS** together with the name of two structures. Some high-lying structures are further indicated by the suffix **'**.

Table S1. The TPSS-D3/def2-TZVP + COSMO(toluene) predicted zero-point energies (ZPE), enthalpy (Hc) and Gibbs free energy (Gc) corrections at 298.15 K; COSMO-RS solvation enthalpy (Hsol) and free energy (Gsol) corrections in toluene; the PW6B95-D3/def2-QZVP computed total (TE, in hartrees) and relative electronic energies (RE) as well as final relative free energies (Grel) and relative enthalpies (Hrel) including thermal and solvation corrections; the differences of the relative electronic energies with respect to the TPSS-D3/def2-QZVP (Dif_T) calculations. All energy quantities are given in unit of kcal/mol unless specified otherwise. For each transition structure the imaginary frequency (in cm^{-1}) is also listed.

Name	Frq1	ZPE	Hc	Gc	Hsol	Gsol	TE(PW6B95-D3)	RE	Grel	Hrel	Dif_T
2b	0	376.37	401.91	335.64	-26.21	-14.43	-3799.20001	0.0	0.0	0.0	0.0
2b'	-6	376.47	401.7	336.16	-23.23	-10.88	-3799.19236	4.8	8.9	7.6	1.3
a	-6	375.64	400.9	335.19	-25.96	-14.18	-3799.16789	20.2	20.0	19.4	2.8
TSab	-75	376.89	400.86	338.16	-25.96	-14.18	-3799.15999	25.1	27.9	24.3	1.7
b	0	377.15	402.82	336.23	-25.83	-14.1	-3799.21635	-10.3	-9.3	-9.0	-0.5
5	0	377.34	403.01	336.55	-26.48	-14.73	-3799.23077	-19.3	-18.7	-18.5	-0.6
5 + 5	0	754.68	806.01	673.1	-52.95	-29.46	-7598.46154	0.0	0.0	0.0	0.0
$(5)_2$	-6	756.13	807.1	692.58	-40.98	-25.59	-7598.49422	-20.5	2.9	-7.5	-0.6
E	0	560.43	597.04	510.14	-28.32	-15.31	-2572.90706	0.0	0.0	0.0	0.0
TSEF	-16	560.25	595.83	510.69	-27.17	-14.52	-2572.89859	5.3	6.7	5.3	0.9
F	0	560.57	597.21	509.93	-27.56	-14.78	-2572.89948	4.8	5.1	5.7	0.6
TSFG'	-139	560.16	596.29	510.59	-28.19	-15.41	-2572.84518	38.8	39.2	38.2	4.5
TSFG	-117	560.97	596.19	512.26	-28.08	-15.37	-2572.86355	27.3	29.4	26.7	3.3
G	-8	561.68	597.17	512.64	-26.21	-13.84	-2572.91902	-7.5	-3.5	-5.2	0.9
TSGH	-46	561.51	597.11	512.48	-26.87	-14.27	-2572.91972	-7.9	-4.5	-6.4	-0.1
H	0	561.49	597.74	511.75	-27.48	-14.74	-2572.93436	-17.1	-14.9	-15.6	-0.6
TSHD	0	561.55	597.83	512.21	-27.51	-14.82	-2572.93389	-16.8	-14.2	-15.2	0.2
D	0	561.64	597.77	512.57	-27.27	-14.63	-2572.93885	-19.9	-16.8	-18.2	-0.4

Table S2. The TPSS-D3/def2-TZVP + COSMO(toluene) optimized Cartesian coordinates (in Å). Each structure is labeled by the name as used in the manuscript, followed by the number of atoms, total energies in hartree, and atomic Cartesian coordinates in angstrom. Transition structures are indicated by the prefix **TS** together with the name of two structures. Some high-lying structures are further indicated by the suffix **'**.

2b'.xyz
71
Energy = -3796.405562349

Ge	-1.3626718	-0.3255867	-0.8683456
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C	0.0482993	1.0802491	-0.8420474
Al	1.3839413	-0.4735142	0.0690075
C	-0.5335074	-2.8743866	0.4354865
C	-4.1700416	0.5344445	-0.8433725
C	-2.8716866	1.2336006	1.0752533
C	0.3599506	2.2673222	-0.9231648
Cl	-1.7491519	-0.6486477	-3.0084645
C	1.9065349	0.1600443	1.9027715
C	2.7306301	-0.9101906	-1.3562257
C	-1.7756313	-3.7359282	0.3113582
H	0.2723603	-3.4212463	0.9437378
C	-5.2974093	1.1544513	-0.3025103
H	-4.2355388	0.0297380	-1.8031173
C	-4.0001182	1.8521603	1.6133910
H	-1.9300686	1.2740194	1.6153710
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C	2.0267811	-1.4863392	-2.5981338
C	3.5686259	0.3027927	-1.7886558
C	3.6704845	-1.9900088	-0.7779524
C	-1.4240501	-4.9151344	-0.6255170
C	-2.9913551	-2.9870297	-0.2374361
C	-2.1048132	-4.2886213	1.7157407
C	-5.2139650	1.8126096	0.9250434
H	-6.2402018	1.1251678	-0.8419933
H	-3.9307390	2.3651949	2.5688410
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C	-0.3027632	4.3133684	-2.0316429
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H	3.9687716	0.7541293	1.4388042
H	3.3143601	1.5025610	2.9056947
H	0.3519829	1.6941191	2.1252718
H	0.9684976	1.0611724	3.6629047
H	-0.1396785	0.0825826	2.6841948
H	3.2292877	-1.5684724	2.2645591
H	2.6081273	-0.8081553	3.7386271
H	1.5465659	-1.8332029	2.7594290
H	1.4169755	-2.3635717	-2.3524820
H	1.3664041	-0.7488882	-3.0688008
H	2.7694403	-1.7960707	-3.3528568
H	2.9399433	1.0774433	-2.2422050
H	4.1104220	0.7564750	-0.9501029
H	4.3181575	0.0073216	-2.5422558
H	3.1193896	-2.8807830	-0.4476212
H	4.2502532	-1.6176308	0.0758342
H	4.3922109	-2.3217437	-1.5433033
H	-0.5488847	-5.4613486	-0.2563315
H	-2.2656280	-5.6154355	-0.6820522
H	-1.2024142	-4.5525899	-1.6342409
H	-3.2692033	-2.1484874	0.4095119
H	-2.8106113	-2.6107303	-1.2510504
H	-3.8520445	-3.6630351	-0.2933146
H	-1.2480792	-4.8292819	2.1334675
H	-2.3649863	-3.4759662	2.4023444
H	-2.9526913	-4.9810157	1.6616657
H	-6.0924887	2.2951906	1.3441894
H	2.8494421	3.4229895	-0.8123808
H	2.2776701	3.4375294	-2.4920797
H	2.3496558	4.9541237	-1.5653847
H	1.1882381	3.9220423	1.1052965
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H	0.6955394	5.4224090	0.2896151
H	-0.1883294	3.8519952	-3.0160646
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H	-0.0919391	5.3848303	-2.1147165

2b.xyz
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Ge	0.6983373	0.7259755	-0.6103051
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C	0.5346180	0.2458516	4.0387054
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C	-0.2257288	2.5789993	3.4767478
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C	2.1396082	-0.4829013	-0.7441696
C	1.9231240	5.0613711	-2.0690410
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C	-2.7141021	-2.7107342	1.1895255
C	2.4221213	2.7039637	-1.8795156
C	2.9900754	-1.3547651	-0.7454038
C	2.7810730	3.9847379	-2.3000046
C	3.2737488	-3.7787196	-0.9175838
C	-3.0961937	-3.1473331	-1.2518626
C	-3.3786320	2.1567927	-0.8819940
C	3.9939274	-2.4197017	-0.7476490
C	-3.7617447	0.6646388	-0.8704459
C	4.7585493	-2.3965057	0.5965528
C	-4.3838912	0.3100895	-2.2339360
C	-4.8162296	0.4361518	0.2323276
C	4.9803439	-2.1975638	-1.9170729
H	-0.0820711	-2.5491695	0.3793660

H	0.9393695	-0.6963193	3.6543459
H	0.0381008	5.6985435	-1.2363960
H	-0.3652034	3.3244516	2.6867410
H	-0.3378696	-2.8795650	-1.3392903
H	-1.1920103	2.4128756	3.9655876
H	-0.7764845	-4.1010668	-0.1291632
H	1.2334446	0.6482009	4.7811516
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H	-0.6011901	3.4275056	-0.4813075
H	0.4681372	2.9870694	4.2209086
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H	2.5676106	-3.9484062	-0.1002130
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H	-2.9485881	2.4720057	0.0771534
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H	-2.7648586	-2.9782217	-2.2841087
H	3.0900360	1.8643194	-2.0558670
H	-3.0924033	-4.2372480	-1.0803939
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H	4.0722720	-2.5515258	1.4341771
H	3.7286720	4.1431319	-2.8074559
H	4.0149925	-4.5855057	-0.9178781
H	-3.6768102	0.4728023	-3.0569408
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H	-4.7115523	-0.7350179	-2.2772342
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H	-5.1612387	-0.6047670	0.2588932
H	5.4966666	-1.2387307	-1.8121304
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H	-5.2672584	0.9405517	-2.4318074
H	-5.7023813	1.0701685	0.0602798
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Energy = -7592.914966099

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Ge	-4.4404721	-0.0812951	-0.4560204
Al	1.5515470	-0.2095508	-0.7360728
Al	-1.5515470	0.2095508	0.7360728
Cl	0.3945310	-1.2090083	0.9639537
Cl	-0.3945310	1.2090083	-0.9639537
C	0.1958278	-1.8865192	-2.7076328
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C	-1.4661100	-0.0968412	3.5693908
C	1.4866809	-1.0628083	-2.5455875
C	-1.4866809	1.0628083	2.5455875
C	1.5905752	-4.5887362	-0.1470731
C	-1.5905752	4.5887362	0.1470731
C	2.6978442	-1.9502338	-2.8813140
C	-2.6978442	1.9502338	2.8813140
C	2.6725319	2.4318897	-0.2605735
C	-2.6725319	-2.4318897	0.2605735
C	2.8908279	1.1080882	-0.1513003
C	-2.8908279	-1.1080882	0.1513003
C	2.8121614	-4.2083373	0.7183719
C	-2.8121614	4.2083373	-0.7183719
C	3.1559194	4.1556215	1.4397555
C	-3.1559194	-4.1556215	-1.4397555
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C	-2.4323946	4.3231152	-2.2143027
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C	-3.2435862	2.8308288	-0.4536237
C	3.5696564	0.1923953	3.1781584
C	-3.5696564	-0.1923953	-3.1781584
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C	4.9061477	0.1060387	2.4237152
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C	-5.7008867	-0.5695782	2.1164609
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C	-6.7200535	-0.6035837	3.0676312
C	7.2491382	-0.2707813	-0.4744943
C	-7.2491382	0.2707813	0.4744943
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C	-8.0115602	-0.2048462	2.7197930
C	8.2749912	-0.2298206	-1.4207783
C	-8.2749912	0.2298206	1.4207783
H	-0.1107383	2.2687344	3.7380880
H	0.1107383	-2.2687344	-3.7380880
H	0.1788633	-2.7493302	-2.0333279
H	-0.1788633	2.7493302	2.0333279
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H	-0.5804508	-0.7319865	3.4616218
H	0.6988700	1.2892167	2.5011614
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H	-0.7532358	3.9141085	-0.0464945
H	1.2822126	-5.6110413	0.0984892
H	-1.2822126	5.6110413	-0.0984892
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H	-1.8338042	4.5467643	1.2118149
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H	-2.0799392	-4.3477372	-1.5118733
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H	-2.7584873	2.8266369	2.2319326
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H	-1.6034831	3.6509983	-2.4522034
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H	-2.9115542	0.6445470	-2.9206998
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H	-3.0377993	-1.1215781	-2.9513327
H	2.1278869	-5.3519914	2.4369973
H	-2.1278869	5.3519914	-2.4369973
H	3.4153395	3.4119711	2.1989275
H	-3.4153395	-3.4119711	-2.1989275
H	3.3859123	4.4137854	-2.0195345
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H	-3.6471906	1.4123387	2.7816833
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H	-3.6905104	6.1939761	-0.6113087
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H	-3.6887002	-5.0873509	-1.6653634
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H	-3.2830286	4.0645794	-2.8518062
H	4.7007914	0.8976392	-2.3900596
H	-4.7007914	-0.8976392	2.3900596
H	4.8618323	-4.9159223	1.0122745
H	-4.8618323	4.9159223	-1.0122745
H	5.0128840	-2.0790862	2.5109955
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H	5.3025520	2.2477983	2.6821581
H	-5.3025520	-2.2477983	-2.6821581
H	5.3611028	2.5975179	0.6121988
H	-5.3611028	-2.5975179	-0.6121988
H	5.3238958	3.0986324	-1.0795360
H	-5.3238958	-3.0986324	1.0795360
H	5.7609905	-1.2385518	3.8859904
H	-5.7609905	1.2385518	-3.8859904
H	5.5941873	4.2949720	0.2047411
H	-5.5941873	-4.2949720	-0.2047411
H	6.0807178	1.1999665	3.8721651
H	-6.0807178	-1.1999665	-3.8721651
H	6.5942749	-1.3011443	2.3264381
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H	6.7356981	1.3064250	2.2286681
H	-6.7356981	-1.3064250	-2.2286681
H	6.5071348	0.9422363	-4.0782149
H	-6.5071348	-0.9422363	4.0782149
H	7.4745752	-0.6193167	0.5291622
H	-7.4745752	0.6193167	-0.5291622
H	8.8089643	0.2336536	-3.4572925
H	-8.8089643	-0.2336536	3.4572925
H	9.2793409	-0.5390739	-1.1432571
H	-9.2793409	0.5390739	1.1432571

5.xyz
71
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Ge	0.8531258	-0.3725320	-0.6990128
Al	-1.7238847	1.0423258	-0.5009025
Cl	-3.0690457	0.8306839	-2.1731865
C	2.4779522	4.3729881	-1.4868361
C	3.3937908	-1.1308716	0.6293544
C	3.1797978	1.9725663	-1.4997353
C	2.2732122	3.0006548	-0.8178461
C	4.2227331	-1.3816759	1.7237906
C	0.7954834	2.6380432	-0.8921092
C	1.2531978	-2.9714255	-1.8710523
C	0.1729644	1.4488957	-0.8785675
C	2.0409072	-0.8102142	0.8108490
C	2.6429744	3.1013020	0.6817659
C	-0.9228658	-1.0347559	-0.0763181
C	3.7092965	-1.3134299	3.0189092
C	1.1391610	-1.5115651	-2.3340885
C	-0.0831913	-1.3383488	-3.2483168
C	1.5371200	-0.7510949	2.1183542
C	-1.8706986	-1.7600240	0.2138174
C	2.3635435	-0.9988245	3.2140525
C	-4.2441885	-2.2215304	-0.2478459
C	2.4036649	-1.0972351	-3.0995477
C	-2.5382359	3.3831259	0.8817118
C	-2.9792714	-2.6611419	0.5254447
C	-2.5279871	1.8580409	1.1313795
C	-3.2474468	-2.6675732	2.0472987
C	-3.9691419	1.3972651	1.3959404
C	-1.6634684	1.5689997	2.3713409
C	-2.5568218	-4.0799552	0.0636225
H	0.3595588	-3.2862531	-1.3218502
H	1.8522157	5.1353718	-1.0088224
H	5.2685348	-1.6302657	1.5640146
H	3.0900430	0.9851959	-1.0363199
H	2.1230759	-3.1291336	-1.2245147
H	2.9400836	1.8843448	-2.5632195
H	1.3587658	-3.6275767	-2.7468260
H	3.5238599	4.6896826	-1.4044173
H	2.2140638	4.3334479	-2.5495900
H	3.8155550	-1.1866990	-0.3707285
H	4.2295583	2.2729970	-1.4049298
H	-1.0078981	-1.6480883	-2.7528981
H	0.1639604	3.5354354	-0.8888210
H	1.9918393	3.8158488	1.1970283
H	2.5366387	2.1269963	1.1681949
H	4.3542644	-1.5058180	3.8717243
H	0.0457547	-1.9565055	-4.1483857
H	-4.5644274	-1.2228353	0.0562079
H	3.6805678	3.4390121	0.7939435
H	-4.0561481	-2.2033646	-1.3239923
H	-1.5252195	3.7773908	0.7342946
H	-3.1385331	3.6501906	0.0029858
H	3.3116632	-1.1832356	-2.4934904
H	0.4901575	-0.5121857	2.2822208
H	2.5261905	-1.7554128	-3.9714529
H	-0.2087212	-0.2985056	-3.5665248
H	-3.5400315	-1.6741758	2.3965902
H	1.9566066	-0.9457421	4.2204260

H	-5.0507346	-2.9317952	-0.0367498
H	-4.6188125	1.5720818	0.5308676
H	-0.6220968	1.8806435	2.2223432
H	2.3326825	-0.0695379	-3.4662970
H	-2.3691346	-4.0966479	-1.0134270
H	-2.9705566	3.9104795	1.7481898
H	-4.0135097	0.3284739	1.6369690
H	-2.3550235	-2.9808903	2.5970379
H	-1.6623861	0.5003586	2.6201724
H	-1.6521277	-4.4078287	0.5837805
H	-4.0597817	-3.3680030	2.2681151
H	-4.3983190	1.9397945	2.2546566
H	-2.0485392	2.1117825	3.2505300
H	-3.3663167	-4.7817212	0.2906982

a.xyz
71
Energy = -3796.383097826

Ge	0.7884908	1.0099444	-0.2772404
Al	-2.3072900	-0.1146403	-0.7899568
Cl	-2.5768612	1.5946605	-2.1644244
C	-0.0935001	0.1160986	3.9917298
C	0.2486324	3.5723861	-1.5084675
C	-1.1666000	2.3698245	3.6445228
C	-0.3153383	1.2643768	2.9805024
C	0.5825769	4.7169155	-2.2288072
C	-1.1273900	0.7020054	1.8260947
C	-0.2279819	-0.8326833	-2.6260558
C	-0.8603403	0.5689980	0.5162396
C	1.2123017	2.5707395	-1.3121124
C	1.0348542	1.8448592	2.5611166
C	2.2542273	-0.1583688	-0.1756588
C	1.8707514	4.8681352	-2.7464514
C	-1.3072771	-1.5495994	-1.8272252
C	-0.6499295	-2.5567656	-0.8673581
C	2.5062812	2.7246420	-1.8347905
C	3.1227902	-1.0085797	-0.0742083
C	2.8327143	3.8741903	-2.5499092
C	3.5451256	-3.3837632	-0.4593656
C	-2.2100902	-2.3059096	-2.8225775
C	-4.6277740	0.7394687	0.8235028
C	4.1445762	-2.0475181	0.0431006
C	-4.0664590	-0.5070558	0.1123757
C	4.5571117	-2.1839664	1.5282093
C	-5.0749268	-0.8926006	-0.9927534
C	-3.9858496	-1.6723519	1.1159698
C	5.3737631	-1.6655232	-0.8131715
H	0.3166984	-0.0491358	-2.0246214
H	0.5189979	-0.6762240	3.5490030
H	-0.1651047	5.4872338	-2.3930313
H	-1.3353140	3.2000625	2.9509082
H	-0.6348719	-0.2721128	-3.4722392
H	-2.1426587	1.9771357	3.9481853
H	0.5838656	-1.4961422	-2.9658868
H	0.4126520	0.4906509	4.8889644
H	-1.0500895	-0.3211719	4.2964733
H	-0.7598556	3.4400055	-1.1292836
H	-0.6600615	2.7566474	4.5361375
H	0.0234622	-2.0646932	-0.1545980
H	-2.1115293	0.3659384	2.1666296
H	1.7040096	1.0722438	2.1591799
H	0.9158705	2.6514009	1.8233731
H	2.1256139	5.7619954	-3.3090191
H	-0.0514773	-3.3005136	-1.4220471
H	2.6699411	-3.6637891	0.1329052
H	1.5475189	2.2818687	3.4255352
H	3.2407443	-3.3023253	-1.5064321
H	-4.0072003	1.0583105	1.6699431
H	-4.7068647	1.5890025	0.1354112
H	-2.7323970	-1.6198907	-3.4994133
H	3.2471570	1.9436053	-1.6829191
H	-1.6225856	-3.0054858	-3.4411039
H	-1.3992439	-3.1053910	-0.2848069
H	3.6956424	-2.4532764	2.1459174
H	3.8323084	3.9944378	-2.9577333
H	4.2997044	-4.1728631	-0.3714760
H	-5.1709452	-0.1012963	-1.7455295
H	-3.3020960	-1.4622552	1.9485706
H	-2.9661277	-2.8975285	-2.2946887
H	5.0950411	-1.5621069	-1.8656956
H	-5.6371480	0.5339894	1.2199746
H	-4.7878420	-1.8149973	-1.5104903
H	4.9759644	-1.2455617	1.9031402
H	-3.6427137	-2.5982960	0.6374847
H	5.8060441	-0.7200955	-0.4722830
H	5.3155107	-2.9685137	1.6228519
H	-6.0744224	-1.0600027	-0.5556277
H	-4.9775118	-1.8801438	1.5534343
H	6.1347254	-2.4486346	-0.7279264

b.xyz
71
Energy = -3796.426656028

Ge	0.2777321	0.2931357	-0.8318757
Al	-3.0159604	0.6258683	-0.3455153
Cl	-3.7357284	2.3702768	-1.3594664
C	0.4367793	-0.0795413	3.2013225
C	0.1069847	3.0482762	-1.8138806
C	-0.5434747	2.1572303	3.8041681
C	-0.0211591	1.2876828	2.6434920
C	0.5701227	4.2077073	-2.4379838
C	-1.1782173	1.0486916	1.6773537
C	0.4566348	-0.8798255	-3.4740573
C	-1.2051277	0.6852059	0.3762165
C	0.9456900	1.9348430	-1.6661058
C	1.1607128	2.0128020	1.9777877
C	1.7858345	-0.6474639	-0.1309128
C	1.8796895	4.2691735	-2.9157541
C	-0.4593621	-0.9397666	-2.2426279
C	-0.5104336	-2.3718048	-1.6922103
C	2.2599017	2.0085513	-2.1479222
C	2.7580049	-1.2576514	0.2777276
C	2.7255937	3.1684308	-2.7677397
C	3.5189655	-3.4217867	1.1577551
C	-1.8686496	-0.4842166	-2.6367808
C	-5.1208322	0.0565494	1.4720833
C	3.9242566	-1.9722668	0.8044915
C	-4.4309615	-0.6257412	0.2664850
C	4.4280341	-1.2476304	2.0746705
C	-5.4856271	-0.8782461	-0.8263657
C	-3.8336889	-1.9672615	0.7282351
C	5.0410593	-1.9879379	-0.2643149
H	1.4814934	-1.1644395	-3.2108423
H	0.8194803	-0.7119659	2.3962859

H -0.0912020 5.0633107 -2.5465466
H -0.8784792 3.1354414 3.4408302
H 0.4867641 0.1245308 -3.9087511
H -1.3875253 1.6723577 4.3089826
H 0.1014973 -1.5779749 -4.2458547
H 1.2324641 0.0672230 3.9421989
H -0.3947026 -0.5989266 3.6909330
H -0.9120677 3.0186578 -1.4360726
H 0.2475876 2.3207989 4.5440506
H 0.4896787 -2.7207956 -1.4182469
H -2.1422352 1.2017606 2.1867864
H 1.6563663 1.3908946 1.2289118
H 0.8315669 2.9397047 1.4979977
H 2.2419287 5.1731575 -3.3978617
H -0.9195809 -3.0581238 -2.4481222
H 2.7251561 -3.4279017 1.9104660
H 1.9099305 2.2629476 2.7383579
H 3.1577756 -3.9497050 0.2701266
H -4.4259201 0.2217578 2.3056764
H -5.5618788 1.0227990 1.1992866
H -1.9372579 0.5879689 -2.8553769
H 2.9263334 1.1576543 -2.0250637
H -2.2358089 -1.0217767 -3.5225408
H -1.1435401 -2.4385076 -0.7995931
H 3.6497671 -1.2296997 2.8430256
H 3.7485054 3.2153907 -3.1325577
H 4.3854483 -3.9605526 1.5574754
H -5.9226140 0.0566043 -1.1943015
H -3.0419734 -1.8300705 1.4745106
H -2.6101053 -0.7655767 -1.8535845
H 4.6994720 -2.4923876 -1.1731137
H -5.9342928 -0.5829478 1.8510542
H -5.0613516 -1.4113415 -1.6866081
H 4.7092059 -0.2158513 1.8444385
H -3.4074612 -2.5316159 -0.1101711
H 5.3395957 -0.9683059 -0.5254448
H 5.3042016 -1.7703953 2.4744784
H -6.3050025 -1.4984003 -0.4289857
H -4.6144376 -2.5984485 1.1814127
H 5.9164446 -2.5205337 0.1240782

TSab.xyz
71
Energy = -3796.373771716
Ge 0.4764117 0.7602520 0.2911690
C -1.1298234 0.1141715 1.0368328
C 0.9408012 2.6184293 0.1176524
C 1.9255315 -0.3294610 -0.1889813
C -0.9053176 0.1324268 -2.3421471
Al -2.2160541 0.2226589 -0.6744430
C -1.3701013 -0.1299071 2.3327119
C 0.0571010 3.6051496 0.5785868
C 2.1960640 2.9820642 -0.3929292
C 2.8769532 -1.0611922 -0.4055802
C 0.1251130 1.1977407 -2.7616380
C -0.3133296 -1.2695182 -2.5632018
C -2.0809498 0.2977947 -3.3491399
Cl -2.9280927 2.3051113 -0.6250087
C -3.7949185 -1.0576795 -0.7024102
C -0.4799324 -0.0288933 3.5584266
H -2.3812625 -0.4511891 2.6002720
C 0.4287891 4.9469389 0.5199350
H -0.9227743 3.3248471 0.9520972
C 2.5629087 4.3241535 -0.4442745
H 2.8779882 2.2139630 -0.7492341
C 3.9981277 -1.9524694 -0.6996198
H 1.1031611 1.0608929 -2.2843417
H -0.2227401 2.2128898 -2.5445373
H 0.3002008 1.1260372 -3.8487373
H 0.5671257 -1.4523207 -1.9414285
H -0.0024320 -1.3812440 -3.6161404
H -1.0421646 -2.0589125 -2.3549219
H -2.5873738 1.2632442 -3.2463851
H -1.6688526 0.2398562 -4.3705606
H -2.8258681 -0.4973776 -3.2520770
C -4.2476955 -1.2150954 0.7650462
C -4.9809094 -0.4589291 -1.4840666
C -3.4937535 -2.4615173 -1.2518531
C -0.4678141 -1.4151736 4.2412147
C -1.1284959 0.9999453 4.5126691
C 0.9549372 0.3971610 3.2467619
C 1.6779432 5.3055766 0.0101221
H -0.2597636 5.7125907 0.8652885
H 3.5337385 4.6071016 -0.8412916
C 3.6032842 -2.8608583 -1.8894744
C 4.2987960 -2.8193367 0.5457769
C 5.2412396 -1.1107706 -1.0695439
H -3.5046538 -1.7591023 1.3588126
H -4.4327648 -0.2459416 1.2455418
H -5.1882632 -1.7892044 0.8100712
H -5.2460712 0.5377848 -1.1162227
H -4.7765259 -0.3720642 -2.5564551
H -5.8652844 -1.1083577 -1.3701494
H -2.6632336 -2.9430607 -0.7201186
H -3.2453073 -2.4443687 -2.3196281
H -4.3772392 -3.1121699 -1.1371474
H -0.0053074 -2.1642727 3.5899677
H 0.0963462 -1.3728403 5.1801029
H -1.4874292 -1.7436713 4.4695969
H -1.1413126 1.9958221 4.0578228
H -2.1609824 0.7178862 4.7445688
H -0.5678999 1.0523071 5.4531732
H 1.4559390 -0.3210856 2.5858704
H 0.9905227 1.3968575 2.7916536
H 1.5431575 0.4529711 4.1698511
H 1.9628072 6.3530239 -0.0367866
H 2.7224404 -3.4606339 -1.6444369
H 3.3785129 -2.2627524 -2.7768685
H 4.4355880 -3.5346001 -2.1200739
H 3.4250495 -3.4162303 0.8222276
H 4.5762369 -2.1918675 1.3978645
H 5.1307170 -3.4965077 0.3242443
H 5.0424843 -0.4942006 -1.9508500
H 5.5258991 -0.4545867 -0.2417997
H 6.0807780 -1.7782860 -1.2914285

D.xyz
103
Energy = -2570.398316667
Si -0.1013355 -0.8798950 -0.6867470
Al 0.6680756 -2.4918542 1.6226155
Al -0.8987834 2.4073189 -1.2253904
Cl -0.1940158 -4.4178718 2.0893738
C -0.2791715 -1.4920682 -3.4079038

C	-0.4400730	2.4653829	-4.1546135
C	0.3653365	0.9257029	-0.8350287
C	0.8673657	-0.0682507	3.2571096
C	1.2450270	-2.0644751	-0.2078673
C	1.4437540	3.6467643	-0.7787313
C	1.4176406	-2.1937998	4.4778905
C	1.5126708	-1.4615235	3.1278891
C	1.6580357	1.1585798	-0.5055315
C	2.2924020	-2.3822076	-0.9913796
C	2.3762930	2.4908586	-0.4244833
C	2.9100143	2.6675847	1.0136104
C	3.0048293	-1.2414739	2.7972410
C	3.4437906	-4.3309673	-1.9809682
C	3.1116448	-4.2543773	0.5044878
C	3.3784066	-3.4100939	-0.7423714
C	3.5649136	2.4634250	-1.4099806
C	4.7226802	-2.6595619	-0.6049925
C	-4.0299869	-0.6403033	2.7562565
C	-3.7773508	-3.0794868	2.1103028
C	-3.3784615	2.1174327	0.2028620
C	-3.0421993	-1.8260909	2.6430766
C	-2.3637771	-0.5709924	-2.3274951
C	-2.4386408	-2.1296677	4.0320045
C	-2.7639311	3.0445967	-3.4132034
C	-2.0829367	2.9542818	0.2996766
C	-2.4621243	4.4459384	0.2686256
C	-1.9934512	-1.4608118	1.6858016
C	-1.4166815	2.6371338	1.6505992
C	-1.6527937	-2.9392500	-1.8778015
C	-0.9307725	4.6828580	-3.1155205
C	-1.1605728	-1.5056046	-2.1435153
C	-1.1746668	-1.1467957	0.8269130
C	-1.2638007	3.1730575	-3.0634879
H	-0.8124272	-3.6235937	-1.7219437
H	0.1414603	4.8838219	-3.0111500
H	0.1576682	-0.5042402	-3.5919742
H	-0.1875200	-0.1241077	3.5434325
H	-0.6114884	2.9373201	-5.1357987
H	0.5384898	-2.2153411	-3.3219981
H	-0.7105134	1.4082659	-4.2488160
H	0.3796091	-2.3421490	4.7924112
H	0.5941467	3.7025991	-0.0739349
H	0.6381655	2.5120279	-3.9523041
H	1.0846298	3.5468685	-1.8127209
H	0.9181967	0.4919620	2.3164660
H	1.3928183	0.5224074	4.0257804
H	1.9433522	4.6189367	-0.7180450
H	1.8918990	-3.1813010	4.4397040
H	1.9224204	-1.6103018	5.2654297
H	2.3197311	0.3245829	-0.2400204
H	2.4405072	-1.8726713	-1.9537454
H	2.0864731	2.7094834	1.7331899
H	2.5042973	-4.8796235	-2.1060933
H	2.1766213	-4.8141702	0.4126378
H	3.2125015	2.3567098	-2.4415024
H	3.1421557	-0.7806545	1.8117568
H	3.6250802	-3.7476820	-2.8911955
H	3.0507474	-3.6272655	1.4030448
H	3.4925571	3.5928779	1.0934050
H	3.4613188	-0.5732397	3.5454945
H	3.5575465	1.8297722	1.2910562
H	3.5750398	-2.1775934	2.8117117
H	4.1510344	3.3867818	-1.3345445
H	4.2572460	-5.0577481	-1.8735988
H	4.2265809	1.6196449	-1.1869488
H	3.9271945	-4.9679678	0.6674847
H	4.9091442	-2.0303117	-1.4830287
H	4.7195393	-2.0188818	0.2823536
H	5.5501480	-3.3732488	-0.5153835
H	-4.5717405	-3.3546060	2.8125594
H	-4.8161739	-0.9034103	3.4719428
H	-4.0580582	2.3709405	1.0336904
H	-4.4952101	-0.4229556	1.7912245
H	-4.2278769	-2.8776921	1.1339482
H	-3.9231859	2.2978391	-0.7313880
H	-3.1700104	1.0437555	0.2721720
H	-3.5207562	0.2612108	3.1072956
H	-3.0820415	-3.9165534	2.0123052
H	-2.9652837	-0.8715984	-3.1969449
H	-3.2498663	-2.4016068	4.7155367
H	-3.0155244	-0.5734955	-1.4476981
H	-3.3963588	3.5801722	-2.6957723
H	-3.1235766	4.6902703	1.1163398
H	-2.1019844	2.8741893	2.4817458
H	-2.0416475	0.4638504	-2.5148539
H	-2.9966708	4.7166524	-0.6491674
H	-2.9544926	3.4829894	-4.4063158
H	-1.4554992	5.2541567	-2.3417402
H	-2.2349945	-3.3023235	-2.7366144
H	-3.1050035	2.0042719	-3.4479252
H	-1.1460750	1.5797994	1.7315030
H	-2.2911944	-2.9852418	-0.9895682
H	-1.7347127	-2.9627989	3.9732513
H	-1.9240204	-1.2537020	4.4356135
H	-1.2378330	5.0926333	-4.0913563
H	-1.5820889	5.0975973	0.3464611
H	-0.8776568	-1.7657541	-4.2881441
H	-0.5041878	3.2259475	1.8119643

E.xyz

103

Energy = -2570.367122091

C	-1.1474170	-1.1832540	-0.0418197
Al	-3.0329568	-0.7486259	-0.4215843
C	-4.2224740	-0.1749505	1.0877045
C	-5.5007310	-1.0268394	1.2172376
Si	0.0917438	0.1749627	-0.0371772
Cl	0.8336266	0.4125190	-2.0815141
C	1.7412639	-0.0493330	0.7409633
Al	3.0350408	0.2218944	-0.7549354
C	3.7675122	-1.4212095	-1.6699099
C	5.1420779	-1.8682226	-1.1317127
C	-0.7160320	1.7720448	0.2596311
C	-1.1431850	2.8970062	0.4626608
C	-1.6051067	4.2664845	0.6928606
C	-2.2392058	4.3685806	2.0998164
C	-0.6808752	-2.4174557	0.2470637
C	-1.4814009	-3.7025046	0.2698737
C	-1.3168803	-4.3595656	1.6571399
C	-0.9043081	-4.6393665	-0.8151463
C	-2.9643282	-3.4399019	-0.0040825
C	-3.5329337	-0.4889494	-2.3385782
C	-3.4439794	-0.2320407	2.4161960
C	-4.6489171	1.2863071	0.8310896

C	1.8412847	-0.4190474	2.0317916
C	3.1149616	-0.6648396	2.8183242
C	2.9830790	0.0366723	4.1860979
C	4.3467269	-0.1287693	2.0873962
C	3.2480892	-2.1890202	3.0391964
C	3.8084763	2.0578522	-1.0394238
C	3.5535898	2.5713237	-2.4713800
C	5.3342638	2.0507341	-0.8085681
C	3.1545841	3.0479565	-0.0560765
C	3.9270796	-1.1300565	-3.1766749
C	2.7845924	-2.5953582	-1.4975602
C	-2.6452266	4.6499163	-0.3856875
C	-0.3855778	5.2152955	0.5999575
H	0.3777218	-2.5782223	0.4830039
H	-1.0220049	-4.1981120	-1.8100289
H	-1.4184633	-5.6073576	-0.7967546
H	0.1631186	-4.8138269	-0.6457055
H	-3.3952914	-2.7887086	0.7714942
H	-3.5526097	-4.3632312	0.0051425
H	-3.1090541	-2.9983400	-1.0056049
H	-0.2574112	-4.5281659	1.8776865
H	-1.8309639	-5.3269887	1.6890495
H	-1.7309881	-3.7188374	2.4430391
H	-2.5543537	0.4083267	2.3911484
H	-3.1093570	-1.2506869	2.6516164
H	-4.0779302	0.1077202	3.2517024
H	-5.2567937	1.6612853	1.6712643
H	-5.2544491	1.3827258	-0.0781192
H	-3.7808624	1.9469001	0.7303221
H	-5.2826390	-2.0710483	1.4740251
H	-6.0924212	-1.0271968	0.2943670
H	-6.1421901	-0.6272255	2.0197434
H	0.9447940	-0.5932694	2.6427937
H	4.4795913	-0.6212276	1.1151162
H	5.2587142	-0.3214797	2.6631284
H	4.2629966	0.9501969	1.9267515
H	2.3568500	-2.5902389	3.5350812
H	4.1181499	-2.4103204	3.6686465
H	3.3694807	-2.7069775	2.0822194
H	2.8851011	1.1202304	4.0595091
H	3.8659146	-0.1605478	4.8049426
H	2.1001935	-0.3256686	4.7250260
H	5.8493467	1.3940628	-1.5203108
H	5.6053804	1.7232094	0.2022894
H	5.7458835	3.0650120	-0.9433949
H	3.5615518	4.0632447	-0.1998386
H	3.3279560	2.7677843	0.9901921
H	2.0688615	3.1016370	-0.2006629
H	2.4838989	2.6655569	-2.6880215
H	3.9919487	1.9144408	-3.2315802
H	4.0059776	3.5690983	-2.5994890
H	4.6713129	-0.3466405	-3.3622924
H	2.9847916	-0.8146574	-3.6404133
H	4.2663098	-2.0360619	-3.7063566
H	1.7942904	-2.3653090	-1.9075462
H	2.6544532	-2.8572425	-0.4399106
H	3.1574964	-3.4934112	-2.0185566
H	5.5232982	-2.7149435	-1.7268373
H	5.0872923	-2.2107275	-0.0912655
H	5.8916497	-1.0695474	-1.1828780
H	-2.2136542	4.5636068	-1.3868882
H	-2.9652208	5.6857057	-0.2285077
H	-3.5236596	4.0014466	-0.3296155
H	0.3680717	4.9527308	1.3475285
H	-0.7139676	6.2455942	0.7760022
H	0.0759570	5.1574209	-0.3896406
H	-3.1015528	3.7025131	2.1893994
H	-2.5720402	5.3976910	2.2735363
H	-1.5114574	4.1005975	2.8711452
C	-3.1738190	0.9798896	-2.6722513
C	-2.7077639	-1.4048976	-3.2621459
C	-5.0304979	-0.7069106	-2.6187018
H	-2.8991387	-1.1574406	-4.3189624
H	-1.6309243	-1.3015649	-3.0868911
H	-2.9676287	-2.4636647	-3.1300350
H	-3.3908705	1.1900248	-3.7325461
H	-3.7525317	1.6925784	-2.0726380
H	-2.1106828	1.1946169	-2.5103247
H	-5.2599854	-0.4988346	-3.6767144
H	-5.3396285	-1.7403548	-2.4157761
H	-5.6620045	-0.0462003	-2.0128756

F.xyz
103
Energy = -2570.360412909

C	-1.2126520	-1.1696871	0.6901281
Al	-0.4962832	-2.8518395	-0.0787022
C	-1.1677745	-3.4376987	-1.8818618
C	-2.0186627	-4.7233757	-1.8025972
Si	-0.5230369	0.3726253	-0.0458030
Cl	1.1059357	-0.4196851	-1.2846786
C	0.4886430	1.6054487	0.8722426
Al	2.2540861	1.6817724	-0.0577763
C	3.9010238	0.7765839	0.6660478
C	3.5655812	-0.0377646	1.9290458
C	-1.6849920	1.0981393	-1.2225234
C	-2.4843392	1.5779793	-2.0073761
C	-3.4147365	2.1441386	-2.9826013
C	-2.9907931	1.6724613	-4.3946623
C	-2.1942999	-1.0530830	1.6071528
C	-2.9816707	-2.1819680	2.2442438
C	-4.4813676	-1.9212790	1.9838812
C	-2.7172314	-2.1740408	3.7653933
C	-2.5908533	-3.5355227	1.6493151
C	0.9657740	-3.8561611	0.8661445
C	-2.0277740	-2.3265729	-2.5138681
C	0.0283578	-3.7264274	-2.8146446
C	-0.0487733	2.2926644	1.8982444
C	0.6119979	3.3733220	2.7304073
C	2.0919584	3.5301692	2.3862689
C	0.4637289	2.9960193	4.2199381
C	-0.1366282	4.6984812	2.4633043
C	2.3740359	2.9386019	-1.6298983
C	3.3469650	2.3841729	-2.6896005
C	2.8845645	4.3296077	-1.1965982
C	0.9943800	3.1272188	-2.2871436
C	4.9900562	1.8160026	1.0098754
C	4.5072876	-0.1861545	-0.3776440
C	-3.3597565	3.6877065	-2.9080199
C	-4.8467627	1.6491792	-2.6743233
H	-2.5334326	-0.0719385	1.9657614
H	-1.6605701	-2.3657164	3.9765217
H	-3.3196279	-2.9420994	4.2644000
H	-2.9799896	-1.2019244	4.1967862

H	-2.7728245	-3.5502024	0.5649314
H	-3.1804500	-4.3523797	2.0782899
H	-1.5373838	-3.7722869	1.8598667
H	-4.7797240	-0.9466284	2.3852518
H	-5.0940788	-2.6912934	2.4667446
H	-4.6958397	-1.9275585	0.9098838
H	-1.4570214	-1.4050446	-2.6717859
H	-2.8902743	-2.0687373	-1.8868924
H	-2.4116604	-2.6510551	-3.4956468
H	-0.3346717	-4.0084796	-3.8166763
H	0.6428607	-4.5562456	-2.4462631
H	0.6794902	-2.8531826	-2.9362683
H	-1.4791493	-5.5553694	-1.3352660
H	-2.9507659	-4.5726542	-1.2440722
H	-2.3040787	-5.0450522	-2.8177249
H	-1.0855589	2.1201794	2.2176867
H	-0.5918628	2.8640602	4.4834584
H	0.8785436	3.7844260	4.8585178
H	0.9896949	2.0604354	4.4375989
H	-0.0333689	4.9957259	1.4144887
H	0.2672265	5.4984572	3.0948231
H	-1.2046905	4.5944811	2.6848747
H	2.6361367	2.6026724	2.5879395
H	2.5528187	4.3267766	2.9803179
H	2.2282791	3.8048643	1.3311750
H	3.8547645	4.2833187	-0.6867102
H	2.1760850	4.8366816	-0.5295970
H	3.0095390	4.9765863	-2.0809498
H	1.0653989	3.8442022	-3.1230401
H	0.2525074	3.5128247	-1.5782548
H	0.6011272	2.1886896	-2.6925259
H	3.0491634	1.3890895	-3.0420948
H	4.3718769	2.3123523	-2.3073519
H	3.3721674	3.0504537	-3.5681539
H	4.6695950	2.5275911	1.7792839
H	5.2933494	2.3929828	0.1277360
H	5.8904653	1.3071435	1.3918030
H	4.8176682	0.3370316	-1.2881544
H	3.8102883	-0.9777807	-0.6700777
H	5.4011274	-0.6766911	0.0418152
H	4.4641650	-0.5495541	2.3112035
H	2.8129998	-0.8072800	1.7246176
H	3.1754919	0.5893304	2.7400135
H	-3.6513991	4.0375490	-1.9133431
H	-4.0478570	4.1151626	-3.6458393
H	-2.3489539	4.0477833	-3.1193029
H	-4.8959718	0.5574377	-2.7232010
H	-5.5449173	2.0658665	-3.4088309
H	-5.1594436	1.9666333	-1.6751877
H	-1.9766379	2.0105804	-4.6254632
H	-3.6787804	2.0881834	-5.1392209
H	-3.0169685	0.5811060	-4.4612963
C	2.3152929	-3.6050471	0.1595641
C	1.1089237	-3.4149532	2.3351950
C	0.6856962	-5.3733961	0.8287261
H	1.9644926	-3.9257606	2.8056994
H	1.2742475	-2.3359223	2.4273409
H	0.2217963	-3.6623755	2.9318294
H	3.1121159	-4.1847464	0.6534801
H	2.2957465	-3.9044368	-0.8942567
H	2.6077903	-2.5517565	0.2013586
H	0.6345419	-5.7540350	-0.1980337
H	1.4929710	-5.9216565	1.3412664
H	-0.2544800	-5.6384522	1.3299204

G.xyz

103

Energy = -2570.381081803

C	0.4987904	-1.3449780	-0.2661929
Al	2.2709218	-0.8166316	0.5483778
C	4.0438683	-1.2307419	-0.4144199
C	4.9474764	-2.1877935	0.4002723
Si	-0.8226717	-0.1598441	-0.8925362
Cl	2.4649168	1.7373714	-0.0971526
C	-0.8218053	1.4930140	-0.0009186
Al	0.5685814	2.7347107	-0.5060743
C	0.8870779	4.4924662	-1.4008508
C	1.5905748	5.4338634	-0.3954500
C	-2.4873762	-0.8911696	-0.6398082
C	-3.5900041	-1.3627894	-0.4209539
C	-4.9024307	-1.9513544	-0.1428319
C	-5.0018054	-3.3264872	-0.8432793
C	-0.0113990	-2.6028229	-0.3100473
C	0.5508916	-3.9390082	0.1324798
C	0.6540685	-4.8483515	-1.1121557
C	-0.4598777	-4.5613523	1.1213358
C	1.9145219	-3.8075598	0.7934229
C	2.1394949	-0.5288136	2.5696369
C	3.7451701	-1.8744970	-1.7859668
C	4.9313657	0.0028409	-0.6955212
C	-1.6799922	1.6572101	1.0266215
C	-1.7850323	2.8299149	1.9803636
C	-3.1696674	3.4885674	1.7881464
C	-0.6882183	3.8615641	1.7276895
C	-1.6747588	2.2912544	3.4232818
C	-0.6649526	0.1718667	-2.7699402
C	0.6355984	0.9324494	-3.0470900
C	-1.8583402	1.0228480	-3.2405456
C	-0.6395446	-1.1641311	-3.5338856
C	-0.4224082	5.1429926	-1.8856533
C	1.8327432	4.3232442	-2.6102551
C	-6.0125817	-1.0146319	-0.6716722
C	-5.0583105	-2.1351541	1.3849812
H	-1.0289206	-2.7557027	-0.6948127
H	-0.5564480	-3.9436551	2.0201148
H	-0.1328488	-5.5641392	1.4208963
H	-1.4501721	-4.6461541	0.6597909
H	2.6393592	-3.4043668	0.0834123
H	2.2951246	-4.7767013	1.1347675
H	1.8655044	-3.1507792	1.6703024
H	-0.3165378	-4.9271811	-1.6147081
H	0.9745726	-5.8569641	-0.8250695
H	1.3766072	-4.4448281	-1.8290437
H	3.1737934	-1.1966203	-2.4319098
H	3.1700170	-2.8043468	-1.7096990
H	4.6859901	-2.1141134	-2.3088297
H	5.8937330	-0.3318899	-1.1163199
H	5.1536995	0.5747065	0.2134546
H	4.4807906	0.6862397	-1.4212450
H	5.3076124	-1.7089923	1.3166562
H	4.4645416	-3.1253492	0.6895912
H	5.8338600	-2.4513725	-0.2002540
H	-2.4073046	0.8682775	1.2556395
H	0.3147182	3.4048735	1.8148171

H -0.7159407 4.6760022 2.4591015
H -0.8084925 4.3254646 0.7390926
H -2.4369851 1.5263897 3.6059335
H -1.8231846 3.1028160 4.1451028
H -0.6940071 1.8408743 3.6009342
H -3.2707684 3.8930044 0.7754560
H -3.3125710 4.3030697 2.5077896
H -3.9666811 2.7533180 1.9415162
H -1.9077973 1.9763935 -2.6990845
H -2.8046594 0.4986726 -3.0735557
H -1.7720145 1.2474770 -4.3136586
H -0.5696389 -0.9849190 -4.6164998
H -1.5533666 -1.7383873 -3.3443800
H 0.2145160 -1.7791192 -3.2319811
H 1.5221289 0.4129894 -2.6728616
H 0.6174055 1.9441197 -2.5930225
H 0.7700841 1.1187043 -4.1221967
H -1.1249454 5.3357841 -1.0652095
H -0.9381747 4.5184980 -2.6246902
H -0.2091783 6.1121026 -2.3623464
H 1.3645799 3.7647337 -3.4271786
H 2.7626275 3.8113193 -2.3383018
H 2.1019002 5.3152834 -3.0041412
H 1.8337233 6.3857602 -0.8923138
H 2.5312838 5.0068216 -0.0279373
H 0.9638263 5.6702717 0.4711133
H -5.9522957 -0.0345076 -0.1891631
H -6.9962516 -1.4495440 -0.4610205
H -5.9164427 -0.8734674 -1.7522972
H -4.2732872 -2.7886744 1.7765361
H -6.0334753 -2.5835867 1.6066270
H -4.9920471 -1.1710009 1.8982070
H -4.8869393 -3.2175706 -1.9257270
H -5.9793654 -3.7771039 -0.6375426
H -4.2217401 -4.0015681 -0.4789536
C 2.2906342 0.9415393 3.0053440
C 0.7450185 -0.9912323 3.0427503
C 3.2072150 -1.3295976 3.3445196
H 0.6380052 -0.8273113 4.1286140
H -0.0569032 -0.4424927 2.5367306
H 0.5696871 -2.0566371 2.8560638
H 2.2041820 1.0161815 4.1026987
H 3.2589971 1.3672026 2.7191004
H 1.5091507 1.5753374 2.5712789
H 4.2185623 -0.9656198 3.1320863
H 3.0420710 -1.2251171 4.4301201
H 3.1889772 -2.4016814 3.1163874

H.xyz
103
Energy = -2570.393447556
Si 0.3760604 -0.4431152 1.0543275
C 0.8428784 -1.9918195 0.0985712
C 1.8611692 -1.8657310 -0.7803055
H 2.3491595 -0.8942537 -0.9143225
C 2.4733132 -2.9282354 -1.6724943
C 3.9648049 -3.0710090 -1.2971333
H 4.0732721 -3.4277591 -0.2676547
H 4.4647785 -3.7794690 -1.9678565
H 4.4736099 -2.1048590 -1.3794783
C 1.7756636 -4.2810127 -1.5222785
H 0.7088933 -4.2108894 -1.7998007
H 2.1997040 -5.0375800 -2.1906641
H 1.8941811 -4.6860397 -0.5037165
C 2.3581064 -2.4486350 -3.1360738
H 2.8434969 -1.4751925 -3.2603063
H 2.8433204 -3.1620850 -3.8122053
H 1.3091628 -2.3422835 -3.4310322
Al -0.0473727 -3.7167222 0.3015036
Cl 0.5781260 -5.0862383 1.8356443
C -1.7594377 -4.1766582 -0.5842606
C -2.8833202 -3.8759304 0.4308105
H -2.7968418 -4.4972188 1.3302043
H -2.8719708 -2.8256748 0.7448570
H -3.8700785 -4.0766444 -0.0177903
C -1.8330364 -5.6604419 -0.9852356
H -2.8179554 -5.8906318 -1.4224203
H -1.0762102 -5.9190799 -1.7371093
H -1.6870017 -6.3212469 -0.1236090
C -1.9559607 -3.2905551 -1.8287208
H -1.8758433 -2.2241898 -1.5903066
H -1.2150881 -3.5095929 -2.6089231
H -2.9492474 -3.4634549 -2.2729757
C 1.4405729 1.0092741 0.6105411
C 2.7727069 1.0041092 0.8095401
H 3.2680211 0.1523740 1.2965311
C 3.7771536 2.0697342 0.4127591
C 3.1226080 3.2018545 -0.3776874
H 2.3518743 3.7062613 0.2183399
H 3.8569334 3.9621515 -0.6652874
H 2.6675719 2.8168825 -1.2974270
C 4.4319123 2.6244480 1.6968010
H 4.8874270 1.8157927 2.2794074
H 5.2163304 3.3485634 1.4466892
H 3.6874568 3.1206707 2.3275514
C 4.8622950 1.3969668 -0.4566095
H 4.4296041 1.0129638 -1.3871889
H 5.6508047 2.1141652 -0.7128291
H 5.3235512 0.5588640 0.0780599
Al 0.2098198 2.3128167 -0.2123106
C -0.2538893 2.1478910 -2.1701631
C 0.5288873 3.1526987 -3.0428582
H 0.3745290 4.1919300 -2.7308864
H 1.6074220 2.9570116 -3.0343255
H 0.1977689 3.0716526 -4.0916517
C 0.0734197 0.7283673 -2.6687300
H -0.1828532 0.6237816 -3.7368269
H 1.1406103 0.5028091 -2.5616524
H -0.4816687 -0.0378218 -2.1163594
C -1.7548601 2.4089937 -2.3910460
H -2.3674541 1.6905878 -1.8365812
H -2.0496156 3.4189356 -2.0806763
H -2.0092593 2.3065925 -3.4593727
C -0.3870801 3.9175680 0.8592373
C -1.8799988 3.8215574 1.2204772
H -2.5107035 3.7677487 0.3274045
H -2.0926110 2.9404062 1.8360980
H -2.1930184 4.7119328 1.7919050
C 0.4033136 4.0624916 2.1725613
H 0.2516247 3.2036030 2.8333764
H 1.4826123 4.1615517 2.0073716
H 0.0742106 4.9642541 2.7152291
C -0.1889548 5.2002358 0.0225373
H -0.5083362 6.0827728 0.6014968

H 0.8593901 5.3604016 -0.2591994
H -0.7821043 5.1828888 -0.8993230
C -1.3288074 0.1362894 0.5648809
C -2.5411647 0.2720156 0.4362847
C -4.0069210 0.3163777 0.3228999
C -4.4465974 -0.4449406 -0.9495992
H -4.1256611 -1.4877691 -0.9130773
H -5.5391328 -0.4168199 -1.0252323
H -4.0229116 0.0181134 -1.8452139
C -4.6034938 -0.3716726 1.5762735
H -4.3000372 0.1544774 2.4859374
H -5.6967877 -0.3540756 1.5089973
H -4.2771690 -1.4120749 1.6487659
C -4.5405188 1.7635911 0.2558850
H -4.1345332 2.2963969 -0.6068550
H -5.6310509 1.7272639 0.1604772
H -4.2877202 2.3195891 1.1608821
C 0.2273115 -0.8468543 2.9166615
C -0.0362194 0.4444287 3.7097508
H -0.1505054 0.2156770 4.7788598
H 0.7940564 1.1494543 3.6010564
H -0.9534310 0.9409871 3.3719131
C 1.5458325 -1.4873910 3.3933763
H 1.7648928 -2.4136745 2.8519505
H 2.3907697 -0.8018349 3.2621744
H 1.4782399 -1.7319309 4.4627676
C -0.9379517 -1.8232316 3.1469835
H -1.8908763 -1.3924335 2.8260341
H -0.7924545 -2.7765722 2.6196024
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TSEF.xyz
103
Energy = -2570.359965789
C -1.6679026 0.1410470 0.6263451
Al -2.6899600 -1.3190140 -0.2270824
C -3.8688174 -0.8114030 -1.7713451
C -5.3058050 -1.3499762 -1.6144689
Si -0.0443946 0.7091761 -0.0381244
Cl 0.1939319 -0.1876314 -2.0062638
C 1.5397185 0.0695771 0.6533575
Al 2.6177351 -0.5537346 -0.9073668
C 2.9217949 -2.5165770 -1.2786210
C 4.4348750 -2.7963061 -1.4127261
C -0.0718825 2.4955484 -0.3175740
C -0.1166184 3.7037782 -0.4710710
C -0.1477878 5.1505345 -0.6833362
C -1.0821193 5.8011236 0.3630858
C -2.1063901 0.8440642 1.6936850
C -3.3761429 0.5984664 2.4866659
C -4.2246045 1.8879026 2.4597276
C -2.9855802 0.2705385 3.9442462
C -4.1802924 -0.5607403 1.8958594
C -2.2460539 -3.2052862 0.2705179
C -3.9248054 0.7250692 -1.8848385
C -3.2954236 -1.3785868 -3.0888459
C 1.7125496 0.0498561 1.9886841
C 2.9435697 -0.3854985 2.7576704
C 3.3305979 0.7587795 3.7198315
C 4.1185190 -0.6892997 1.8273473
C 2.5753233 -1.6372766 3.5851824
C 3.6632047 0.8073586 -1.9609484
C 3.6697077 0.4342330 -3.4573375
C 5.1277710 0.8774855 -1.4776169
C 3.0519425 2.2122627 -1.8171236
C 2.2583981 -2.9177424 -2.6142929
C 2.3583867 -3.4291833 -0.1751609
C -0.6797017 5.4341613 -2.1082952
C 1.2836055 5.7180370 -0.5372602
H -1.5471363 1.7080462 2.0787272
H -2.3887674 -0.6464298 3.9882740
H -3.8808183 0.1360350 4.5624501
H -2.3928590 1.0844647 4.3754374
H -4.4900648 -0.3341751 0.8618020
H -5.1046997 -0.7452096 2.4524258
H -3.6058424 -1.4998659 1.9328877
H -3.6520493 2.7328586 2.8571066
H -5.1269877 1.7687574 3.0704712
H -4.5257221 2.1336834 1.4359964
H -2.9316902 1.1607048 -2.0449947
H -4.3400977 1.1896085 -0.9810182
H -4.5628448 1.0249986 -2.7321482
H -3.9206841 -1.0584311 -3.9383759
H -3.2807133 -2.4743144 -3.0903417
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H -5.3303525 -2.4437336 -1.5445508
H -5.9146899 -1.0627498 -2.4871987
H 0.9064899 0.3708029 2.6638622
H 3.8726546 -1.5025176 1.1331594
H 4.9979353 -1.0096235 2.3965904
H 4.3970257 0.1984761 1.2494028
H 1.7216085 -1.4305747 4.2404755
H 3.4211263 -1.9429837 4.2121944
H 2.3063124 -2.4711059 2.9297691
H 3.6009186 1.6613612 3.1613832
H 4.1860824 0.4640718 4.3385408
H 2.4961998 1.0052828 4.3862657
H 5.6382534 -0.0909019 -1.5342131
H 5.2010281 1.2359322 -0.4435790
H 5.6960524 1.5860855 -2.1032348
H 3.6618243 2.9511087 -2.3653151
H 3.0015179 2.5328697 -0.7700264
H 2.0354980 2.2595263 -2.2220501
H 2.6549536 0.3774389 -3.8699031
H 4.1610196 -0.5285045 -3.6404508
H 4.2180979 1.1957573 -4.0369110
H 2.6231645 -2.3166106 -3.4549735
H 1.1687216 -2.8164455 -2.5813939
H 2.4827478 -3.9730777 -2.8413851
H 1.2892202 -3.2666155 -0.0115189
H 2.8636641 -3.2772912 0.7857798
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H 4.6037580 -3.8657279 -1.6213198
H 4.9899586 -2.5534423 -0.4979450
H 4.8850712 -2.2294217 -2.2355861
H -0.0334806 4.9721563 -2.8599227
H -0.7022890 6.5159256 -2.2808993
H -1.6917195 5.0372023 -2.2295275
H 1.6785323 5.5179205 0.4630779
H 1.2660740 6.8018192 -0.6976845
H 1.9555619 5.2639699 -1.2706044
H -2.0973071 5.4028431 0.2755465
H -1.1144656 6.8844471 0.2025677

H	-0.7197085	5.6088859	1.3773639
C	-1.4852827	-3.8452164	-0.9121106
C	-1.3272689	-3.1997557	1.5085902
C	-3.4827539	-4.0728653	0.5726024
H	-1.0013148	-4.2238451	1.7526365
H	-0.4289509	-2.5910959	1.3564054
H	-1.8391265	-2.8017066	2.3950403
H	-1.1156744	-4.8456665	-0.6349634
H	-2.1291809	-3.9644475	-1.7905712
H	-0.6144870	-3.2544703	-1.2184905
H	-3.1761851	-5.1016301	0.8230396
H	-4.0599579	-3.6926456	1.4254970
H	-4.1606007	-4.1342774	-0.2866912

TSFG'.xyz
103
Energy = -2570.312629753

C	-1.3514334	-1.3489414	-0.2446292
Al	-2.8365595	-0.0378951	0.0989367
C	-3.3289818	0.2488026	2.0348020
C	-4.6429312	-0.4605418	2.4265234
Si	0.0141983	-0.1754541	-0.0646822
Cl	2.4383089	2.5727524	-0.0302503
C	1.6030501	-0.5353005	0.7542514
Al	2.8159360	0.4537308	-0.5264340
C	1.8028107	0.0467285	-2.3365627
C	1.8346792	-1.4766939	-2.5616135
C	-0.8725468	1.4174470	0.0195262
C	-0.9889992	2.6432274	0.0634240
C	-1.0423267	4.0986912	0.1202806
C	-0.2914612	4.5564310	1.3975122
C	-1.1728202	-2.6782117	-0.3928238
C	-2.2115933	-3.7684818	-0.3045374
C	-1.7376629	-4.7788983	0.7654585
C	-2.2694685	-4.4766143	-1.6781758
C	-3.5878641	-3.2204293	0.0686108
C	-4.0025121	0.4229443	-1.4787299
C	-2.1903979	-0.3082129	2.9126265
C	-3.5027613	1.7439140	2.3580071
C	1.4174626	-1.4788544	1.7122601
C	2.4816741	-2.1777632	2.5491119
C	3.1424146	-1.1389728	3.4807815
C	3.5250849	-2.8246478	1.6229405
C	1.8069130	-3.2690043	3.3993163
C	4.8454106	0.2872409	-0.6085561
C	5.4551023	1.4997070	-1.3482938
C	5.3994412	-0.9924406	-1.2609468
C	5.3751035	0.3724618	0.8402432
C	2.7907820	0.7072181	-3.3247726
C	0.4207282	0.5814382	-2.7581361
C	-2.4962540	4.6245743	0.1570354
C	-0.3326782	4.6465826	-1.1468223
H	-0.1746313	-3.0789993	-0.6103502
H	-2.6121546	-3.7879822	-2.4568163
H	-2.9623237	-5.3244565	-1.6325494
H	-1.2824336	-4.8551358	-1.9651202
H	-3.5533643	-2.7287782	1.0458538
H	-4.3285299	-4.0252320	0.1221656
H	-3.9378942	-2.4966534	-0.6765384
H	-0.7422740	-5.1667689	0.5226067
H	-2.4316908	-5.6251104	0.8174670
H	-1.6909024	-4.3074065	1.7526700
H	-1.2366431	0.1990233	2.7126440
H	-2.0363827	-1.3821627	2.7480690
H	-2.4154252	-0.1650963	3.9822460
H	-3.7832853	1.8759313	3.4158088
H	-4.2912601	2.2069512	1.7517078
H	-2.5738854	2.3002019	2.1948367
H	-4.5970630	-1.5459875	2.2868489
H	-5.4992019	-0.0882894	1.8537177
H	-4.8582028	-0.2820651	3.4926855
H	0.4041604	-1.8039343	1.9763256
H	3.0655878	-3.6167104	1.0211873
H	4.3410627	-3.2627460	2.2089198
H	3.9463659	-2.0848086	0.9412311
H	1.0501023	-2.8353912	4.0633729
H	2.5469560	-3.7865863	4.0192756
H	1.3165146	-4.0142202	2.7618576
H	3.5648700	-0.3131380	2.9052174
H	3.9421077	-1.6094975	4.0648590
H	2.4041779	-0.7260818	4.1769469
H	5.1421772	-1.0550703	-2.3252429
H	5.0350068	-1.9078089	-0.7805400
H	6.5003024	-1.0074053	-1.1949627
H	6.4750805	0.4510094	0.8313813
H	5.1214626	-0.5089619	1.4350622
H	4.9880181	1.2574654	1.3604803
H	5.1171352	2.4474419	-0.9172791
H	5.2164095	1.5124683	-2.4157081
H	6.5538338	1.4623645	-1.2601345
H	3.7922533	0.2760718	-3.2556700
H	2.8712590	1.7883780	-3.1649244
H	2.4311819	0.5473982	-4.3564781
H	0.3062547	1.6490168	-2.5507062
H	-0.4280883	0.0586726	-2.2776159
H	0.2687274	0.4158103	-3.8397702
H	1.6096675	-1.7231316	-3.6128961
H	1.0950112	-1.9983165	-1.9408599
H	2.8161924	-1.9038756	-2.3252091
H	-3.0318490	4.3671696	-0.7582115
H	-2.4564555	5.7148824	0.2449075
H	-3.0432908	4.2253666	1.0136196
H	0.6983210	4.2909995	-1.1949806
H	-0.3369331	5.7405512	-1.0980314
H	-0.8648819	4.3338273	-2.0500259
H	-0.8038980	4.1949320	2.2938790
H	-0.2765313	5.6511863	1.4189274
H	0.7334832	4.1810782	1.3964050
C	-3.9679288	1.9261105	-1.8022756
C	-3.5485348	-0.3519145	-2.7297451
C	-5.4662615	0.0428947	-1.1643066
H	-4.2194327	-0.1358607	-3.5771341
H	-2.5333435	-0.0751370	-3.0343708
H	-3.5578549	-1.4371444	-2.5732278
H	-4.6214887	2.1475775	-2.6620284
H	-4.3239809	2.5283079	-0.9586383
H	-2.9576791	2.2641153	-2.0597383
H	-6.1048976	0.2490106	-2.0387006
H	-5.5846440	-1.0199894	-0.9208331
H	-5.8660084	0.6223814	-0.3242011

TSFG.xyz
103
Energy = -2570.329447310

C	-1.2756463	-1.0752868	-0.0776809
Al	-0.0316360	-2.6180698	0.3569189
C	-0.0024532	-4.2711363	-0.8295986
C	-1.0752656	-5.3415168	-0.5443549
Si	-0.6004912	0.6158519	-0.1364678
Cl	1.9176500	-1.6401294	-0.6325306
C	0.9538088	1.2372239	0.5946077
Al	2.1115052	0.6327682	-0.9040712
C	4.1236120	0.8080510	-1.0922530
C	4.7222304	0.5790332	0.3144822
C	-1.8189745	1.9326750	-0.3327021
C	-2.5575852	2.9024446	-0.3957668
C	-3.4313712	4.0701363	-0.4802125
C	-3.2553896	4.7171015	-1.8757634
C	-2.6328199	-1.0042648	-0.1709634
C	-3.6654127	-2.0718521	0.1254583
C	-4.0344874	-2.7433934	-1.2191744
C	-4.9182139	-1.3788832	0.7005483
C	-3.1548262	-3.1046236	1.1317622
C	0.4460895	-2.7558902	2.3195319
C	-0.1210155	-3.8712542	-2.3141975
C	1.3675398	-4.9591873	-0.6229430
C	0.7666282	2.0409418	1.6660551
C	1.8141135	2.8247102	2.4438603
C	2.7363451	3.5806998	1.4759633
C	2.6232025	1.8314680	3.3082052
C	1.1006682	3.8333668	3.3619824
C	0.9008556	1.0207645	-2.5798689
C	1.9103787	0.5434403	-3.6550354
C	0.7928621	2.5562973	-2.6668297
C	-0.4387950	0.3812446	-3.0067013
C	4.6007178	2.1754936	-1.6194280
C	4.7340065	-0.2866506	-1.9957175
C	-3.0297084	5.0807335	0.6205066
C	-4.9008977	3.6301474	-0.2842840
H	-3.1096925	-0.0718993	-0.5014583
H	-4.6856372	-0.8712800	1.6431288
H	-5.7047267	-2.1165614	0.8931347
H	-5.3103227	-0.6345982	-0.0020486
H	-2.2427031	-3.5969757	0.7797747
H	-3.8978288	-3.8942108	1.2877106
H	-2.9426327	-2.6319298	2.0944741
H	-4.3946661	-2.0006716	-1.9394069
H	-4.8286843	-3.4821030	-1.0603133
H	-3.1675733	-3.2482783	-1.6524896
H	0.6738887	-3.1803730	-2.6161311
H	-1.0818707	-3.3876871	-2.5317606
H	-0.0472890	-4.7619512	-2.9604644
H	1.4480914	-5.8392246	-1.2824888
H	1.4938242	-5.3131408	0.4074347
H	2.2092105	-4.2986325	-0.8561203
H	-1.0823802	-5.6585166	0.5053357
H	-2.0848436	-5.0024693	-0.7995003
H	-0.8756109	-6.2374405	-1.1553874
H	-0.2402782	2.1681019	2.0839499
H	1.9676454	1.3112874	4.0147498
H	3.3913560	2.3662633	3.8792292
H	3.1079359	1.0788795	2.6824213
H	0.4990751	4.5380457	2.7757575
H	1.8300365	4.4091256	3.9421167
H	0.4361602	3.3187539	4.0657920
H	3.1797413	2.8961030	0.7512069
H	3.5469004	4.0767063	2.0217196
H	2.1729768	4.3397234	0.9221571
H	1.7499075	3.0458066	-2.4416379
H	0.0460682	2.9545586	-1.9718560
H	0.5032701	2.8642834	-3.6851503
H	-0.6207307	0.6126039	-4.0703215
H	-1.3142077	0.7671855	-2.4670989
H	-0.4279383	-0.7073607	-2.8961194
H	2.0872990	-0.5369168	-3.6057957
H	2.8736612	1.0542636	-3.5771584
H	1.4971151	0.7666860	-4.6528809
H	4.2446909	3.0136515	-1.0099560
H	4.2728288	2.3543050	-2.6507542
H	5.7020831	2.2168485	-1.6189491
H	4.4428569	-0.1864955	-3.0449169
H	4.4599416	-1.2936175	-1.6641976
H	5.8328350	-0.2144743	-1.9533936
H	5.8221391	0.5596280	0.2513109
H	4.4030788	-0.3803628	0.7404271
H	4.4531450	1.3677341	1.0217487
H	-3.1395679	4.6361303	1.6138202
H	-3.6757034	5.9630622	0.5577871
H	-1.9902095	5.3965824	0.4944003
H	-5.1972737	2.9152973	-1.0573492
H	-5.5558288	4.5058375	-0.3471622
H	-5.0377008	3.1605561	0.6941369
H	-2.2187102	5.0288098	-2.0308745
H	-3.9025460	5.5976690	-1.9493852
H	-3.5286049	4.0133332	-2.6670258
C	1.9740142	-2.7267390	2.5316360
C	-0.1558922	-1.5809111	3.1140540
C	-0.0824761	-4.0751242	2.9206925
H	0.0999483	-1.6654077	4.1840093
H	0.2305541	-0.6179576	2.7597637
H	-1.2497134	-1.5457301	3.0402078
H	2.2087948	-2.8580354	3.6014598
H	2.4850407	-3.5262126	1.9820795
H	2.4102714	-1.7746281	2.2113049
H	0.3512207	-4.9517809	2.4253386
H	0.1822895	-4.1399893	3.9896405
H	-1.1732769	-4.1605904	2.8523042

TSGH.xyz

103

Energy = -2570.380050374

C	0.6174220	-1.3128440	-0.4087711
Al	2.4268448	-0.7910768	0.2709366
C	4.0463944	-0.7856776	-0.9776751
C	5.2064374	-1.5996814	-0.3560603
Si	-0.8051721	-0.1485559	-0.7990510
Cl	2.3309280	2.4436289	-0.0031195
C	-0.8355505	1.3662170	0.3060405
Al	0.2343609	2.9097253	-0.1805057
C	-0.1041881	4.7144982	-0.9721066
C	0.6656182	5.7540599	-0.1250144
C	-2.3977204	-1.0276628	-0.5557248
C	-3.4559985	-1.5942132	-0.3432034
C	-4.7191793	-2.2851221	-0.0731316
C	-4.4387252	-3.7912480	0.1381969
C	0.2150969	-2.6024121	-0.5332854
C	0.9635427	-3.8982871	-0.2887689
C	1.0503260	-4.6630936	-1.6280162

C	0.1387741	-4.7361318	0.7129419
C	2.3617878	-3.6585566	0.2675182
C	2.5399961	-0.6506989	2.3004810
C	3.6827730	-1.4236506	-2.3360433
C	4.6271335	0.6098902	-1.2854175
C	-1.5458413	1.2828466	1.4506997
C	-1.6592968	2.3139600	2.5573131
C	-3.1175735	2.8243275	2.5918829
C	-0.7065024	3.4885617	2.3328630
C	-1.3298579	1.6304796	3.9014600
C	-0.7623701	0.4026039	-2.6280014
C	0.5133871	1.2119068	-2.8892700
C	-1.9935917	1.2747094	-2.9310162
C	-0.7658729	-0.8389616	-3.5382166
C	-1.5986777	5.0856377	-0.9953580
C	0.4418388	4.7916460	-2.4143538
C	-5.6772166	-2.0956445	-1.2714622
C	-5.3581742	-1.6907587	1.2037433
H	-0.8185112	-2.8194822	-0.8339027
H	0.0600864	-4.2235645	1.6772809
H	0.6093224	-5.7131678	0.8748649
H	-0.8753264	-4.9017837	0.3330392
H	2.9674425	-3.0867295	-0.4440260
H	2.8964576	-4.5969421	0.4504997
H	2.3145874	-3.1268963	1.2259612
H	0.0505804	-4.8157946	-2.0492194
H	1.5136964	-5.6458803	-1.4801430
H	1.6442935	-4.1038207	-2.3579727
H	2.8933578	-0.8667490	-2.8525823
H	3.3395170	-2.4608347	-2.2469755
H	4.5670454	-1.4327905	-2.9939912
H	5.5378227	0.4965475	-1.8966699
H	4.9062911	1.1552025	-0.3770859
H	3.9286416	1.2356093	-1.8484805
H	5.5944154	-1.1205615	0.5486437
H	4.9310030	-2.6271187	-0.0935639
H	6.0381189	-1.6605966	-1.0769652
H	-2.1359194	0.3821013	1.6630706
H	0.3386368	3.1455300	2.2514248
H	-0.7340883	4.2018251	3.1632165
H	-0.9940840	4.0618545	1.4383965
H	-1.9783236	0.7620617	4.0587693
H	-1.4853048	2.3288334	4.7320390
H	-0.2917855	1.2873780	3.9246991
H	-3.3751708	3.3274938	1.6539952
H	-3.2605088	3.5285254	3.4199719
H	-3.8115393	1.9884030	2.7302727
H	-2.0264359	2.1599965	-2.2824790
H	-2.9212390	0.7152901	-2.7721776
H	-1.9739696	1.6233218	-3.9736669
H	-0.7604283	-0.5368693	-4.5953790
H	-1.6590456	-1.4493280	-3.3638495
H	0.1130615	-1.4669206	-3.3577431
H	1.4207904	0.6713210	-2.6050914
H	0.5167411	2.1699510	-2.3394299
H	0.5958429	1.4937329	-3.9484354
H	-2.0423798	5.1083685	0.0079786
H	-2.1855602	4.3858361	-1.6011817
H	-1.7312714	6.0897470	-1.4273881
H	-0.1352446	4.1678409	-3.1054572
H	1.4927310	4.4845798	-2.4739748
H	0.3786087	5.8293701	-2.7775755
H	0.5426384	6.7555469	-0.5661656
H	1.7391850	5.5362098	-0.0915576
H	0.3002800	5.8074581	0.9076169
H	-5.8844004	-1.0340338	-1.4355597
H	-6.6237549	-2.6115619	-1.0740720
H	-5.2382435	-2.5071630	-2.1851251
H	-4.6923441	-1.8183298	2.0625642
H	-6.3053096	-2.1997671	1.4159094
H	-5.5557027	-0.6224308	1.0741686
H	-3.9861023	-4.2281008	-0.7569975
H	-5.3768152	-4.3172875	0.3486836
H	-3.7554468	-3.9417408	0.9792357
C	2.6360778	0.7924455	2.8317123
C	1.2539694	-1.2611506	2.8982302
C	3.7546305	-1.4145788	2.8707053
H	1.2722715	-1.1753581	3.9976031
H	0.3562876	-0.7511092	2.5329203
H	1.1383350	-2.3247427	2.6595288
H	2.6893555	0.7763344	3.9335357
H	3.5232083	1.3179840	2.4628656
H	1.7609378	1.3859739	2.5500189
H	4.7008584	-0.9496710	2.5744254
H	3.7155470	-1.4053265	3.9725734
H	3.7904290	-2.4649121	2.5579595

TSHD.xyz

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Energy = -2570.394399166

Si	-0.3531715	-0.5008704	1.0203928
C	-1.9868946	-1.1332089	0.4040481
C	-2.3906656	-2.4159711	0.4221072
H	-1.7011610	-3.2176513	0.7196755
C	-3.7606443	-2.9723878	0.0859676
C	-4.2307996	-3.8169256	1.2909767
H	-4.3450931	-3.1909433	2.1823102
H	-5.1956052	-4.2896141	1.0735573
H	-3.5067919	-4.6079952	1.5177426
C	-4.7828943	-1.8689151	-0.1890660
H	-4.4760610	-1.2499476	-1.0427471
H	-5.7582243	-2.2974082	-0.4452667
H	-4.9156561	-1.2222198	0.6845786
C	-3.6191350	-3.8914657	-1.1477031
H	-2.8757479	-4.6758558	-0.9642892
H	-4.5759504	-4.3754786	-1.3761298
H	-3.2997086	-3.3184408	-2.0238822
Al	-2.8552880	0.5421171	-0.1624987
Cl	-4.1960340	1.5643729	1.1937002
C	-3.0964135	1.0254090	-2.0963555
C	-2.2494145	2.2379862	-2.5234635
H	-2.5644301	3.1449866	-1.9995211
H	-1.1812066	2.0946137	-2.3362186
H	-2.3761755	2.4219948	-3.6028625
C	-4.5780700	1.3750257	-2.3534382
H	-4.7251104	1.6244510	-3.4169293
H	-5.2504906	0.5410898	-2.1180618
H	-4.9012533	2.2355543	-1.7578450
C	-2.7161938	-0.1777647	-2.9839051
H	-1.6843007	-0.5060821	-2.8255007
H	-3.3648601	-1.0424004	-2.8022188
H	-2.8216286	0.0911099	-4.0472300
C	1.2245896	-1.0604620	0.1937446
C	1.3161618	-2.3964826	0.0098203

H	0.5083865	-3.0709747	0.3232046
C	2.4567951	-3.1694208	-0.6275895
C	3.5180351	-2.2286453	-1.2021150
H	3.9900108	-1.6277723	-0.4054717
H	4.3371669	-2.7769615	-1.6785591
H	3.0876486	-1.5802894	-1.9808817
C	3.0921017	-4.0782541	0.4471880
H	2.3379241	-4.7420303	0.8833056
H	3.8817054	-4.7006043	0.0097565
H	3.5256721	-3.4783601	1.2540367
C	1.8779670	-4.0417274	-1.7619052
H	1.4224790	-3.4183735	-2.5385034
H	2.6644149	-4.6525009	-2.2201545
H	1.1066522	-4.7145824	-1.3721573
Al	2.6173063	0.1685206	-0.4854156
C	2.3012683	0.9983143	-2.2840062
C	3.5070854	0.9322816	-3.2402184
H	4.3836715	1.4533723	-2.8409055
H	3.8065140	-0.1006090	-3.4608910
H	3.2526189	1.4047632	-4.2031580
C	1.1098263	0.2849882	-2.9466247
H	0.8427551	0.7664871	-3.9011017
H	1.3289579	-0.7691382	-3.1615176
H	0.2229623	0.3036704	-2.3057370
C	1.9291495	2.4830756	-2.0738533
H	1.0600136	2.5968151	-1.4150137
H	2.7598440	3.0539693	-1.6409185
H	1.6740272	2.9545615	-3.0371714
C	4.0586201	0.8666387	0.7251339
C	3.4780305	2.0997973	1.4558976
H	3.1992822	2.8940383	0.7533972
H	2.5921599	1.8521115	2.0502721
H	4.2273943	2.5218573	2.1460484
C	4.4964796	-0.1683449	1.7782932
H	3.6483780	-0.5863759	2.3319951
H	5.0386907	-1.0083176	1.3245237
H	5.1787569	0.2923166	2.5111349
C	5.3055349	1.3217748	-0.0568921
H	6.0704594	1.7122467	0.6344717
H	5.7650130	0.4992148	-0.6198914
H	5.0709051	2.1218400	-0.7680694
C	-0.6404509	1.3185936	0.6909114
C	-0.8280825	2.5182843	0.8726691
C	-1.0044224	3.9306205	1.2216740
C	-1.9630691	4.6409951	0.2426504
H	-2.9371167	4.1454592	0.2257968
H	-2.1005890	5.6750279	0.5759907
H	-1.5489378	4.6534009	-0.7683249
C	-1.5884063	3.9937736	2.6550682
H	-0.9155826	3.5101463	3.3691248
H	-1.7122368	5.0430927	2.9442657
H	-2.5599450	3.4954575	2.6934185
C	0.3810657	4.6194414	1.1870961
H	0.8119878	4.5801112	0.1831063
H	0.2621826	5.6688318	1.4771935
H	1.0738125	4.1402901	1.8838024
C	-0.2899591	-0.6493330	2.9345131
C	0.8248827	0.2216768	3.5302910
H	0.8404914	0.1167114	4.6245182
H	1.8102296	-0.0700071	3.1544920
H	0.6679739	1.2811339	3.2990817
C	-0.0288709	-2.1278416	3.2818913
H	-0.8160578	-2.7780552	2.8821173
H	0.9355285	-2.4709622	2.8918880
H	-0.0181675	-2.2558609	4.3734862
C	-1.6431955	-0.2169446	3.5282222
H	-1.8780979	0.8231486	3.2809771
H	-2.4624136	-0.8395968	3.1570862
H	-1.6108949	-0.3071882	4.6235673