

A DFT Study on the Mechanism of Hydrosilylation of Unsaturated Compounds with Neutral Hydrido(hydrosilylene)tungsten Complex

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Reference 10 - Complete List

Gaussian 03, Revision B.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

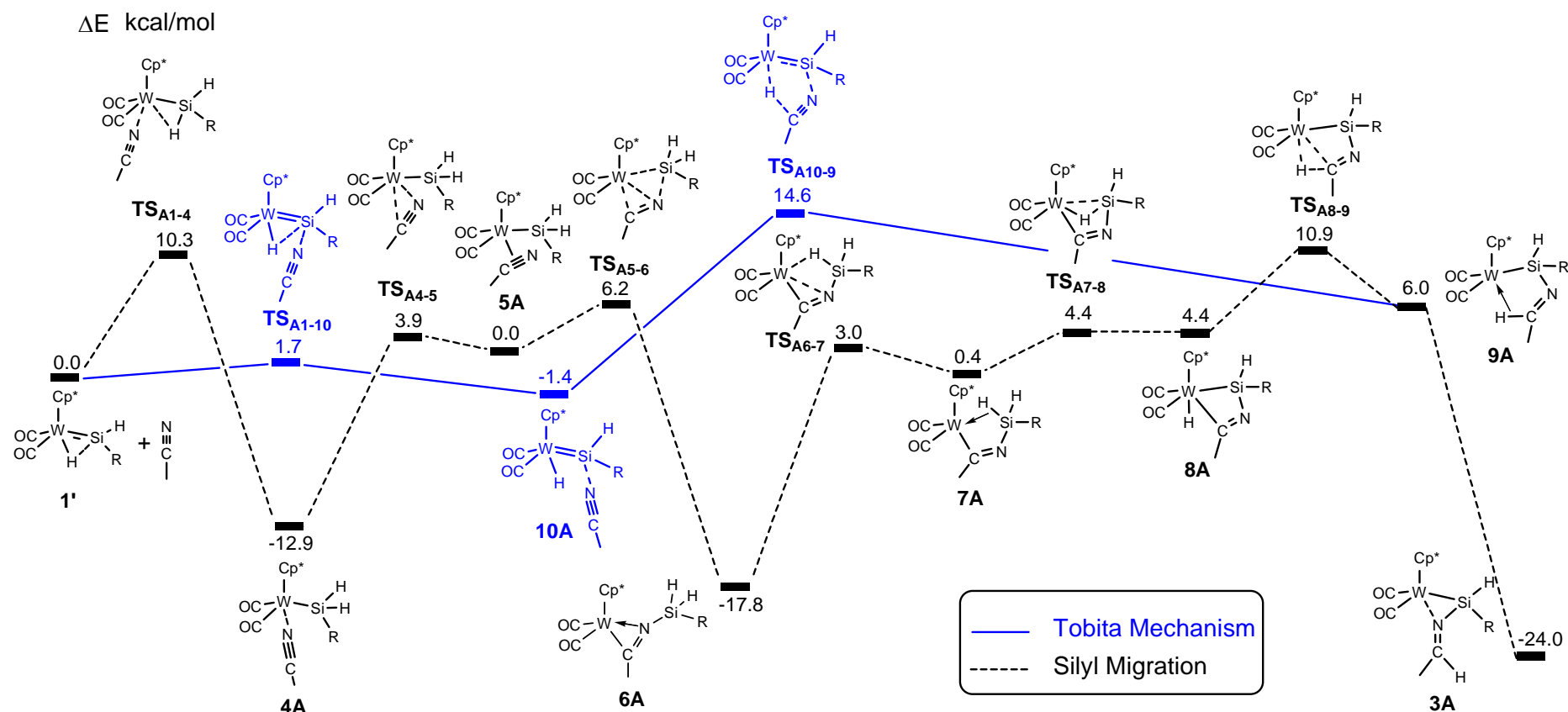


Figure S1. Potential energy profiles of the Tobita mechanism and the Silyl Migration mechanism for the reaction of acetonitrile with **1'**. The relative electronic energies with ZPE correction are given in kcal/mol.

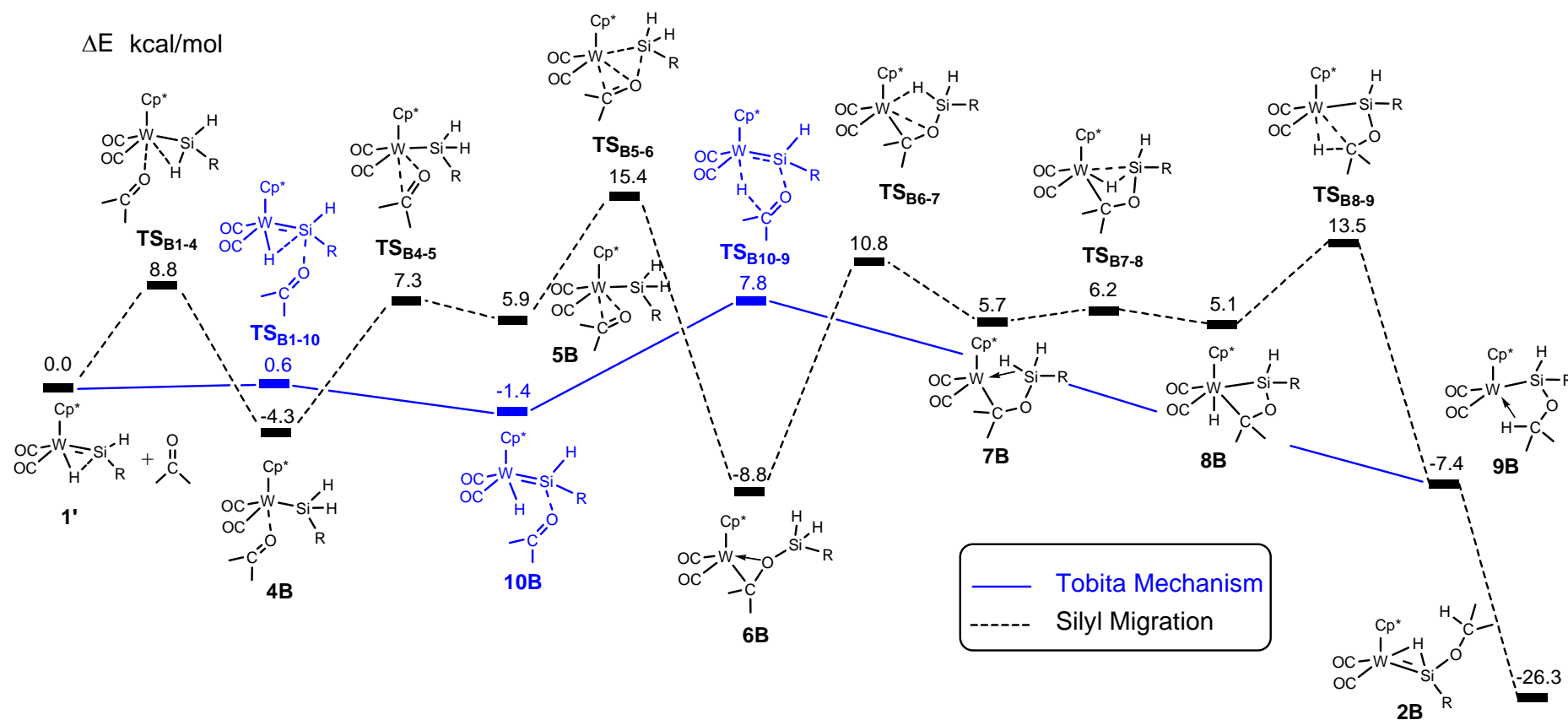


Figure S2. Potential energy profiles of the Tobita mechanism and the Silyl Migration mechanism for the reaction of acetone with **1'**. The relative electronic energies with ZPE correction are given in kcal/mol.

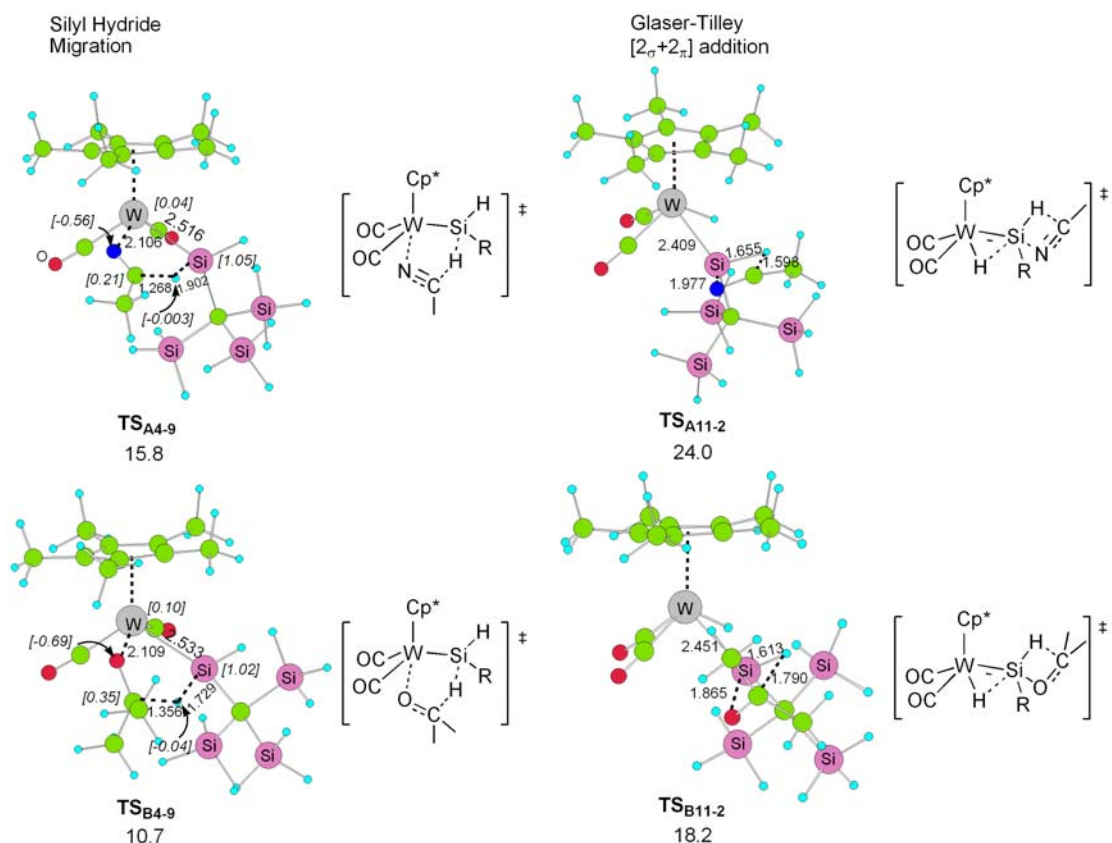


Figure S3. The rate-determining transition state structures calculated for the Silyl Hydride Migration mechanism and the Glaser-Tilley mechanism. Distances are in Å; NBO charges are shown in brackets; relative electronic energies (ΔE) are in kcal/mol.

Table S1. The relative electronic energies (kcal/mol) calculated for the transition states shown in Scheme 4 ^a

Acetonitrile	3A + SiH ₄	TS_{A3-12}	TS_{A3-1}	TS_{A2-1}	TS_{A6-1}
	-24.0	cannot be located	34.7	22.8	6.4
Acetone	2B + SiH ₄	TS_{B3-12}	TS_{B3-1}	TS_{B2-1}	TS_{B6-1}
	-26.3	cannot be located	39.9	11.6	12.1

^a The total energy of **1'**, SiH₄, and the substrate, acetonitrile or acetone, is set to be zero as the reference point.

Cartesian coordinates and electronic energies (hartree, without ZPE correction)

of all the calculated structures.

1'

E= -744.9664205

W	1.104635	0.044298	-0.070667
Si	-1.072649	-0.912609	-0.089727
H	-0.191061	-0.305715	-1.379041
H	-1.284778	-2.362324	-0.405570
O	0.148492	1.766608	2.363802
O	0.954526	2.824638	-1.531097
C	0.463491	1.136722	1.431871
C	0.970645	1.793014	-0.989643
C	-2.839012	-0.226291	-0.058729
C	2.266643	-2.014821	0.365691
C	2.581096	-1.652566	-0.984168
C	3.262126	-0.391843	-0.966891
C	3.390004	0.029583	0.406258
C	2.759881	-0.971419	1.228601
Si	-3.556693	-0.588896	1.662590
H	-5.038118	-0.590164	1.612145
H	-3.114313	-1.926368	2.131557
H	-3.110876	0.420854	2.648479
Si	-3.872715	-1.170539	-1.340090
H	-4.116072	-2.562916	-0.893553
H	-5.184706	-0.509055	-1.539824
H	-3.171862	-1.215906	-2.645863
Si	-2.931297	1.638398	-0.401062
H	-2.065680	2.408923	0.511993
H	-2.546503	1.914425	-1.804752
H	-4.331619	2.090819	-0.210698
C	2.329763	-2.500476	-2.201284
H	2.185259	-1.891278	-3.097864
H	3.185123	-3.164460	-2.388407
H	1.445007	-3.131892	-2.080579
C	3.888540	0.287059	-2.155556
H	4.921622	-0.059266	-2.297353
H	3.339697	0.075855	-3.077718
H	3.918567	1.373130	-2.032666
C	4.207859	1.193422	0.898600
H	5.255941	0.896841	1.046371
H	4.197029	2.024421	0.187479
H	3.834435	1.574145	1.853204
C	2.790054	-1.018100	2.733133
H	3.698871	-1.525440	3.085088
H	2.780545	-0.014746	3.167247
H	1.929599	-1.558462	3.137649
C	1.688065	-3.328854	0.813440
H	2.483241	-4.077874	0.933546
H	1.174180	-3.234665	1.773886
H	0.968755	-3.726071	0.091429

2A

E= -877.751092

C	-2.44132100	0.97546500	1.13568500
C	-1.90297600	1.84390600	0.12491300
C	-2.25558100	1.30225500	-1.15566100
C	-3.01869300	0.10999300	-0.94528400
C	-3.14310300	-0.09689400	0.47622600
W	-0.87067400	-0.33574000	-0.02107500
C	-0.91253000	-2.17129600	-0.73785100
O	-1.02948800	-3.24868700	-1.16998300
Si	1.42246800	0.31366700	-0.04195900
C	3.03669800	-0.68959900	-0.11894200
C	-0.32308700	-1.27514300	1.61604500
O	-0.06741900	-1.81168800	2.62322700
H	0.35293100	-0.29393000	-1.35909100
H	2.20806500	3.42440500	-1.49989400
Si	2.70845700	-2.56049500	-0.27111300
H	4.01826300	-3.25552400	-0.28707600
H	1.92749400	-3.07484700	0.87115400
H	2.01458300	-2.87069000	-1.53935100
Si	4.02609300	-0.37463700	1.47195700
H	5.14344200	-1.34358400	1.58196100
H	4.60381000	0.98930700	1.49190200
H	3.15848200	-0.53066200	2.66299200
Si	4.05839600	-0.15497800	-1.62550600
H	5.14257200	-1.13199000	-1.88830200
H	3.20239100	-0.08737500	-2.83505100
H	4.68710900	1.17190100	-1.42959100
N	1.98625200	1.90144100	-0.14349600
C	2.27992100	3.08512900	-0.45176200
C	-1.27542500	3.18804800	0.36856200
H	-0.58374000	3.46645300	-0.43132700
H	-2.04972000	3.96682400	0.41873900
H	-0.72104700	3.21261000	1.31060600
C	-1.97497000	1.94449200	-2.48731700
H	-2.78391500	2.63632600	-2.76106000
H	-1.04380200	2.51799600	-2.47165900
H	-1.89273800	1.20177600	-3.28561200
C	-2.43797600	1.24563900	2.61683600
H	-1.54844300	1.80537000	2.92013200
H	-3.31898400	1.83529000	2.90665700
H	-2.45414400	0.31871800	3.19657100
C	-4.01620500	-1.12463500	1.14517600
H	-3.64199800	-1.38559400	2.13908900
H	-5.04167700	-0.74683900	1.26469800
H	-4.07032000	-2.04910100	0.56310900
C	-3.70464800	-0.69884400	-2.01353000
H	-4.71741300	-0.31437100	-2.19796300
H	-3.15933800	-0.66250100	-2.96096400
H	-3.79712800	-1.75057500	-1.72908800
C	2.75756300	4.13101300	0.52045700
H	2.79391100	3.73228000	1.53687700
H	3.75647400	4.48317800	0.23046900

H 2.09443400 5.00584900 0.49050600

3A

E= -877.763029

C	-3.00350800	0.51396100	0.17174700
C	-2.91273700	-0.85700500	-0.27796200
C	-2.20423100	-1.60180600	0.73255500
C	-1.86094300	-0.69578700	1.79629000
C	-2.35792400	0.60173000	1.44548200
W	-0.73553200	-0.06613300	-0.24735800
Si	1.50661700	0.01101600	0.81608800
H	1.64700800	0.05495100	2.30224500
C	0.09114900	-1.52918800	-1.25546900
O	0.51869500	-2.45075200	-1.83675700
C	-0.73016800	0.80476000	-2.01646200
O	-0.78830400	1.31836200	-3.06414400
C	3.27970800	-0.18300200	0.14605700
Si	4.44571800	0.79796600	1.27011000
H	5.79942400	0.90590100	0.67261600
H	3.93726100	2.17555100	1.48813700
H	4.57791100	0.14772100	2.59597600
Si	3.76727600	-2.01574800	0.24953400
H	3.31600500	-2.76855500	-0.93976600
H	5.24140300	-2.14279300	0.36003300
H	3.16995800	-2.63690300	1.45838300
Si	3.48341200	0.41138600	-1.64078000
H	2.45706100	-0.15408000	-2.53744800
H	3.41708000	1.89241500	-1.70223200
H	4.82062900	0.00507000	-2.13913400
N	0.66495000	1.50243900	0.31653700
C	0.82190200	2.77344400	0.36390500
C	-3.80296900	1.59859400	-0.49941000
H	-4.85661000	1.54983700	-0.19092400
H	-3.43362300	2.59592700	-0.24307500
H	-3.77501500	1.50642600	-1.58866700
C	-3.63066900	-1.43964100	-1.46685000
H	-4.65908500	-1.72456700	-1.20284600
H	-3.68681800	-0.72567900	-2.29379200
H	-3.12505200	-2.33378500	-1.84207300
C	-2.02927500	-3.09660800	0.76742100
H	-2.89198900	-3.57524000	1.25115300
H	-1.93577700	-3.51694300	-0.23738600
H	-1.13373100	-3.38373200	1.32607900
C	-1.26633900	-1.07317100	3.12488300
H	-2.06080700	-1.26697700	3.85965300
H	-0.65686300	-1.97755000	3.05039900
H	-0.63008000	-0.28079800	3.53085300
C	-2.28713700	1.81801300	2.32725300
H	-3.07864400	1.78685900	3.08854100
H	-1.33059700	1.88373500	2.85498600
H	-2.41990700	2.74169000	1.75757100
C	-0.14321200	3.77929100	-0.18556000
H	0.35416000	4.39687100	-0.94553600
H	-1.01103600	3.29467700	-0.63774600
H	-0.47726800	4.46435300	0.60541400
H	1.73242000	3.17530500	0.82189000

2B

E= -938.1688042

C	-2.67730900	0.82881000	1.1893010
C	-1.86989500	1.84503200	0.5755910
C	-1.99548300	1.70988900	-0.8450610
C	-2.88737600	0.61864100	-1.1185040
C	-3.31859100	0.07318900	0.1471070
W	-1.02267400	-0.33889300	-0.0378550
C	-1.20773000	-2.04360300	-1.0096160
O	-1.40435000	-3.03357400	-1.5954060
Si	1.31033700	0.10848900	0.0888270
C	2.82174600	-1.04385500	-0.0472610
C	-0.69257100	-1.54258900	1.4823840
O	-0.56974300	-2.22687200	2.4223950
H	0.30136200	-0.24414200	-1.2948840
O	1.80586900	1.69662900	0.0250610
C	3.02060200	2.46311400	0.0112870
H	3.88177500	1.78644900	0.0254520
Si	3.88864600	-0.65697000	-1.5752270
H	4.98863000	0.29032000	-1.2755400
H	4.50671600	-1.90157100	-2.0898770
H	3.06333700	-0.07233700	-2.6586180
Si	2.27550600	-2.86509300	-0.2749490
H	1.34010800	-3.31135800	0.7711630
H	1.69032100	-3.06325400	-1.6182450
H	3.49907000	-3.70076900	-0.1843780
Si	3.89900600	-1.01066800	1.5159330
H	5.19405800	-1.68221400	1.2544750
H	4.19000300	0.37228500	1.9611820
H	3.22209900	-1.71452700	2.6297200
C	-2.94577600	0.69081000	2.6640290
H	-2.08794400	1.00992700	3.2625100
H	-3.80558500	1.30845100	2.9580160
H	-3.17095700	-0.34312700	2.9393250
C	-1.15971600	2.96178600	1.2885800
H	-1.80635800	3.84909200	1.3454000
H	-0.89441600	2.68289600	2.3121510
H	-0.23929300	3.24602400	0.7741360
C	-1.38437700	2.63567200	-1.8616200
H	-1.99631300	3.54120900	-1.9765350
H	-0.37910400	2.94665000	-1.5640400
H	-1.31009300	2.16186700	-2.8443470
C	-3.43032100	0.23279000	-2.4689780
H	-4.34672100	0.79623900	-2.6940340
H	-2.71198300	0.43729400	-3.2679850
H	-3.67743400	-0.83143400	-2.5157640
C	-4.39310000	-0.96372400	0.3382950
H	-5.38711900	-0.49472300	0.3585420
H	-4.39258300	-1.70051800	-0.4699850
H	-4.26481700	-1.50807500	1.2780920
C	3.05818100	3.33075500	1.2675670
H	3.98163900	3.92013500	1.2975680
H	2.20700800	4.02043600	1.2832940
H	3.01604600	2.71052700	2.1686310
C	3.05832100	3.28931700	-1.2729370
H	2.20457100	3.97546700	-1.3103720
H	3.97921700	3.88159300	-1.3197940
H	3.01988700	2.64297100	-2.1555630

3B

E= -938.1545698

C	-3.07601300	0.42930000	0.2447150
C	-2.93572400	-0.98327900	-0.0209060
C	-2.10387400	-1.53888100	1.0172590
C	-1.74958000	-0.47417600	1.9239850
C	-2.35800800	0.72942100	1.4448120
W	-0.81676300	-0.12145300	-0.2774620
Si	1.45770800	0.12277300	0.6661650
H	1.62146300	0.58460900	2.0809390
C	-0.10411200	-1.64808800	-1.2391160
O	0.22335700	-2.62933700	-1.7935130
C	-0.99277100	0.49860000	-2.1527370
O	-1.14353800	0.83822200	-3.2575610
O	0.90321500	1.53141900	-0.2111890
C	0.75038300	2.89967700	0.2533810
H	0.32094600	2.86706400	1.2640350
C	3.17932400	-0.48501500	0.1286100
Si	4.53450300	0.20535400	1.2569520
H	5.87942800	-0.12165400	0.7239430
H	4.45010100	1.67773600	1.3905170
H	4.42588700	-0.38067000	2.6153690
Si	3.23183300	-2.37793300	0.3296730
H	2.78432800	-3.08241200	-0.8873790
H	4.62076900	-2.79971700	0.6370110
H	2.37883100	-2.79905100	1.4699880
Si	3.56278400	-0.05218000	-1.6762380
H	2.41265500	-0.32058600	-2.5627380
H	3.94814500	1.37484600	-1.7971410
H	4.71477300	-0.86516700	-2.1389390
C	-1.06346700	-0.64077100	3.2520160
H	-0.48139500	0.24323900	3.5278800
H	-1.80429600	-0.81075900	4.0460960
H	-0.38083200	-1.49458600	3.2496010
C	-2.35715500	2.05151800	2.1613850
H	-3.21887800	2.11551800	2.8405720
H	-1.45768800	2.18500300	2.7694310
H	-2.42802300	2.89648400	1.4705950
C	-3.97635900	1.37446100	-0.5053260
H	-4.99652800	1.34087700	-0.0980330
H	-3.62992000	2.41003600	-0.4354830
H	-4.03723700	1.11808900	-1.5665060
C	-3.70412600	-1.76652400	-1.0518400
H	-4.68380500	-2.07272800	-0.6584680
H	-3.88021500	-1.17837700	-1.9573590
H	-3.16833900	-2.67203400	-1.3494070
C	-1.83959600	-3.00427500	1.2402300
H	-2.64995300	-3.45724200	1.8280890
H	-1.76737400	-3.54909800	0.2953310
H	-0.90398300	-3.16732900	1.7825930
C	-0.20854000	3.61640900	-0.6893940
H	0.21105000	3.66093400	-1.7001350
H	-1.16936200	3.09583600	-0.7441290
H	-0.38567500	4.63990200	-0.3400030
C	2.11628800	3.57485600	0.3026680
H	2.79022400	3.06210400	0.9941850
H	2.57631100	3.58064800	-0.6913070
H	2.00913400	4.61197400	0.6409260

TS_{A1-4}

E= -877.701831

C	-1.77559200	-1.58519800	1.35775600
C	-2.40618000	-0.32787300	1.58887500
C	-3.01740400	0.11594100	0.36585600
C	-2.79694200	-0.90108500	-0.63277200
C	-2.00184400	-1.94068800	-0.02540700
W	-0.72061000	-0.02227900	-0.16781300
C	-0.76254200	1.44240400	-1.48483100
O	-0.82556900	2.30368400	-2.27451700
Si	1.53915300	-0.33708500	0.93645800
C	0.19708800	-0.86183500	-1.66479900
O	0.65358500	-1.43699700	-2.57601300
H	1.62381300	-1.31594000	2.06217200
H	1.38742600	1.00982100	1.60790500
C	3.30965700	-0.32567300	0.18386700
Si	4.50983000	0.25644800	1.52616800
H	4.25251200	-0.43126600	2.81325900
H	5.91835200	-0.01247000	1.13864100
H	4.37819000	1.71874600	1.74625500
Si	3.80796100	-2.07198900	-0.34136800
H	4.96569600	-2.03920000	-1.26895700
H	4.20346300	-2.87310400	0.84455400
H	2.69497700	-2.77944200	-1.01500700
Si	3.43415600	0.87474500	-1.26910100
H	2.73005100	2.14477900	-0.95827000
H	4.85647300	1.21564700	-1.52909500
H	2.86749000	0.32019800	-2.51656300
N	-0.78617300	2.98754200	1.33057400
C	-0.20527300	3.78050200	0.71277500
C	-3.43550600	-0.95542700	-1.99408100
H	-2.83751600	-1.54189000	-2.69687000
H	-4.43104300	-1.41757200	-1.93640900
H	-3.55796600	0.04396000	-2.42134600
C	-1.66923700	-3.27117500	-0.64356400
H	-2.46526600	-3.99863300	-0.43418800
H	-1.56054800	-3.19751800	-1.72854700
H	-0.73384000	-3.67661900	-0.24764300
C	-1.15858300	-2.47799500	2.39732200
H	-1.92880700	-3.11178200	2.85892100
H	-0.40177400	-3.13720600	1.96502200
H	-0.67607300	-1.90717300	3.19498300
C	-2.46800200	0.40382000	2.89961800
H	-3.45366000	0.26071000	3.36389900
H	-1.71468200	0.03651800	3.60163700
H	-2.30865100	1.47663000	2.76761300
C	-3.90221500	1.32574400	0.22671000
H	-4.92168300	1.10315600	0.57149100
H	-3.52456200	2.16605800	0.81546200
H	-3.97051400	1.65390000	-0.81420000
C	0.52577700	4.74750100	-0.09960500
H	0.21216900	5.76715900	0.14427300
H	1.60087300	4.65102300	0.08039800
H	0.32470700	4.55044600	-1.15752000

4A

E= -877.741348

C	-1.82000600	-0.24980500	1.90237800
C	-2.38965800	0.90755800	1.28275400
C	-3.05087400	0.50487000	0.07712400
C	-2.90029800	-0.92507200	-0.05362100
C	-2.13018000	-1.38809300	1.07380400
W	-0.77536300	-0.04584200	-0.27176700
C	-0.87842100	0.31311800	-2.21244800
O	-1.00662100	0.50575100	-3.35630700
Si	1.48177500	-0.37281300	0.99877800
C	0.06603200	-1.66518100	-0.99636200
O	0.48584800	-2.67820900	-1.40434900
H	1.50965700	-1.65092600	1.77671300
H	1.56916400	0.67366000	2.06994200
C	3.23406400	-0.29763900	0.15486900
Si	4.27005800	0.96262900	1.10112300
H	4.32248900	0.65850200	2.55026100
H	5.66826700	1.01385500	0.60015200
H	3.70851200	2.33218900	0.94990300
Si	4.05519200	-1.99619600	0.32930800
H	5.34727900	-2.03241300	-0.40391000
H	4.34127000	-2.29589800	1.75360800
H	3.19153500	-3.06769900	-0.21321900
Si	3.21570500	0.17328800	-1.67414400
H	2.52583700	1.46536800	-1.90642900
H	4.61004000	0.34759800	-2.15720400
H	2.57792900	-0.86313700	-2.51353600
N	0.15226900	1.84478500	-0.26737300
C	0.61515700	2.91128600	-0.22393500
C	-3.90822800	1.37832900	-0.79976200
H	-4.95124900	1.36990000	-0.45394000
H	-3.56888200	2.41849000	-0.79411700
H	-3.90237000	1.03655900	-1.83842600
C	-3.60721000	-1.79326000	-1.06070500
H	-4.61775300	-2.04924700	-0.71242100
H	-3.70691700	-1.29093600	-2.02732900
H	-3.06914600	-2.72957300	-1.23249600
C	-2.36574200	2.29945800	1.84930700
H	-2.45062300	3.05683100	1.06434000
H	-3.20661400	2.44825800	2.54014400
H	-1.44476900	2.49382800	2.40724900
C	-1.19906900	-0.29875000	3.27041500
H	-0.66919000	0.62723300	3.51052700
H	-1.97474100	-0.44668800	4.03494400
H	-0.48345500	-1.11984300	3.36311100
C	-1.87635200	-2.82599900	1.43937500
H	-0.94274700	-2.94074400	1.99709800
H	-2.69145700	-3.21318400	2.06613200
H	-1.80776600	-3.46119100	0.55235400
C	1.22743400	4.23256700	-0.19105900
H	0.48326400	5.00866200	-0.40066400
H	1.67520600	4.42238100	0.79027600
H	2.01626700	4.28960900	-0.94912600

TS_{A4-5}

E= -877.714152

C	1.72313200	-1.65195000	1.15629500
C	2.02251600	-1.78919600	-0.24991800
C	2.85370100	-0.67735300	-0.63727500

C	3.04864300	0.15320000	0.52983600
C	2.36579200	-0.46637700	1.62556800
W	0.77852800	0.16321000	-0.15675000
C	1.07654700	1.78336600	-1.22498200
O	1.34049700	2.71970900	-1.88247100
Si	-1.53357000	-0.97511300	0.41466900
C	-0.01973200	-0.39765500	-1.85030900
O	-0.39034800	-0.80790200	-2.88109800
H	-1.58448200	-1.25573000	1.88331300
H	-1.57982100	-2.34011400	-0.19706100
C	-3.31877800	-0.27162700	0.07568200
Si	-3.49581800	0.78524200	-1.47551200
H	-4.92758700	1.09078800	-1.72588500
H	-2.80563400	2.09181100	-1.32448600
H	-2.95617000	0.11683700	-2.67662700
Si	-4.43728900	-1.79089900	-0.12332100
H	-4.21715100	-2.75892100	0.97674400
H	-5.87073900	-1.39827900	-0.09516200
H	-4.17997200	-2.47176500	-1.41412000
Si	-3.95641400	0.69529900	1.56451400
H	-4.10310600	-0.17592000	2.75459100
H	-3.05038300	1.81056900	1.93496100
H	-5.28074300	1.30235300	1.27629000
N	-0.03056400	1.45130200	1.65544800
C	-0.36531000	2.40258400	1.05380700
C	2.37142800	0.00975600	3.04910600
H	1.43285200	-0.22508400	3.55728900
H	3.18566400	-0.47379300	3.60605600
H	2.52140800	1.09058400	3.11449700
C	3.97154600	1.33943700	0.61976800
H	3.66091600	2.03379600	1.40614300
H	4.99647400	1.01780900	0.85114200
H	4.00497400	1.89750400	-0.32004800
C	3.56859400	-0.52476800	-1.95344100
H	3.72967300	0.52701700	-2.20600500
H	4.55144000	-1.01503400	-1.91799000
H	3.00237600	-0.97583200	-2.77283700
C	1.72118200	-3.00334100	-1.08643900
H	1.67140300	-2.76031300	-2.15080900
H	2.50421900	-3.76182700	-0.95143000
H	0.76536900	-3.45544300	-0.80870000
C	1.06456100	-2.69065400	2.01950300
H	0.32450600	-3.27420300	1.46595400
H	1.81769500	-3.39238500	2.40493000
H	0.55606800	-2.24473900	2.87831600
C	-0.82200200	3.68945200	0.54141700
H	-0.89486900	4.40355000	1.36878400
H	-0.11702100	4.06218300	-0.20758900
H	-1.80331300	3.57083200	0.07306000

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E= -877.721305

C	1.99995300	-1.74010700	0.64286000
C	2.74699100	-1.06337400	-0.39222700
C	3.10665000	0.24123200	0.09825900
C	2.55474100	0.38225900	1.40462600
C	1.86636900	-0.83546200	1.74335300
W	0.71497000	0.07190100	-0.21267100

C	0.78825300	1.28230500	-1.75552000
O	0.89751000	2.01487100	-2.65915600
Si	-1.60699400	-1.06422800	0.40168000
C	-0.01577700	-1.07371100	-1.63734700
O	-0.33901100	-1.76629400	-2.52150300
H	-1.49971800	-1.34148400	1.85924900
H	-1.80760000	-2.41319800	-0.20217400
C	-3.28354200	-0.15606800	0.13842500
Si	-3.36795500	0.71133000	-1.53859100
H	-4.75227700	1.18119200	-1.80218500
H	-2.48748600	1.90132300	-1.57970500
H	-2.97864100	-0.19915100	-2.63891200
Si	-4.59756300	-1.52912300	0.15387600
H	-4.48831500	-2.34412700	1.38865800
H	-5.96304900	-0.95152700	0.11031700
H	-4.44319600	-2.42812300	-1.01326100
Si	-3.71888600	1.07727600	1.51300700
H	-3.29958200	0.58535600	2.84441400
H	-3.12598000	2.41511800	1.28313500
H	-5.19129300	1.27490000	1.55143700
N	-0.42492100	1.24870000	1.31777600
C	-0.12685600	2.02976300	0.43192000
C	1.23169400	-1.10579600	3.07725900
H	0.51236000	-0.32299900	3.34033800
H	0.70111800	-2.06029500	3.08629200
H	1.99666400	-1.14030500	3.86438000
C	1.58641100	-3.18697400	0.61785600
H	2.41152200	-3.82455500	0.96334800
H	0.72689600	-3.37472000	1.26685400
H	1.31541100	-3.51268900	-0.39010400
C	3.26882000	-1.69820900	-1.65519200
H	4.23522600	-2.18727700	-1.47168600
H	2.58179900	-2.45568900	-2.04180800
H	3.41776400	-0.95754400	-2.44639500
C	4.01758600	1.21460000	-0.59966500
H	5.06703100	0.98432500	-0.37152400
H	3.89997700	1.17310200	-1.68583800
H	3.83174100	2.24590200	-0.28638900
C	2.70831600	1.55310400	2.33159500
H	3.42247700	1.31773700	3.13197500
H	3.08083900	2.43910300	1.80948600
H	1.75670500	1.81281300	2.80651100
C	-0.21031700	3.47236700	0.08584600
H	-0.73088700	3.59835200	-0.86771300
H	-0.74311800	4.01807100	0.87035100
H	0.79607700	3.88708000	-0.03247600

TS_{A5-6}

E= -877.711761

C	2.58737800	-1.43087100	-0.2050770
C	3.15740300	-0.12662900	-0.0300240
C	2.69514800	0.39897700	1.2237030
C	1.83372000	-0.57594900	1.8227390
C	1.76415100	-1.71338700	0.9442980
W	0.81034100	0.10885100	-0.2637740
Si	-1.61641100	-0.72789000	0.6735650
C	-0.16254600	-0.82628200	-1.6865170
O	-0.67352700	-1.42996700	-2.5498600

C	1.03279200	1.24681000	-1.8537820
O	1.22346700	1.92222900	-2.7869250
C	-0.05097100	1.93752600	0.4638670
H	-1.56546500	-0.88603600	2.1492610
H	-1.58957500	-2.15873700	0.2091200
C	-3.34793500	-0.13840600	0.1158280
Si	-4.32305600	0.39761300	1.6498300
H	-3.57449600	1.39453500	2.4479740
H	-5.61860700	1.00565300	1.2540520
H	-4.62269900	-0.76825000	2.5174000
Si	-3.36562600	1.31614900	-1.0977830
H	-3.34617800	2.62010500	-0.3896410
H	-2.22715400	1.28300900	-2.0404390
H	-4.61712500	1.27759500	-1.8941690
Si	-4.24296400	-1.61211000	-0.6812630
H	-4.21863700	-2.79984800	0.2039450
H	-5.66626000	-1.26122500	-0.9151280
H	-3.63130300	-1.96928900	-1.9803410
N	-0.92328600	1.18023500	0.9065920
C	1.22544900	-0.45313800	3.1932020
H	0.55250400	-1.28470700	3.4109640
H	2.01027000	-0.44761200	3.9608130
H	0.64706800	0.47125800	3.3034090
C	1.13658800	-3.04526900	1.2512540
H	1.87263700	-3.71240000	1.7206900
H	0.28816300	-2.95286700	1.9337580
H	0.77242200	-3.53708500	0.3451510
C	3.16076500	1.67135100	1.8766440
H	2.40175000	2.08384200	2.5481730
H	4.06068300	1.48676500	2.4798010
H	3.41583700	2.43895600	1.1397980
C	4.18669100	0.51363400	-0.9221550
H	4.13396500	1.60554800	-0.8836570
H	5.19810400	0.21844500	-0.6116610
H	4.05934300	0.21487400	-1.9658830
C	2.92967800	-2.40838000	-1.2974460
H	3.21848400	-1.89703800	-2.2197320
H	3.77029200	-3.04754200	-0.9935410
H	2.08561900	-3.06166100	-1.5349510
C	0.10275300	3.41981100	0.5210980
H	0.00816900	3.81757500	-0.4957910
H	-0.65624200	3.87704900	1.1634370
H	1.10314600	3.68292200	0.8779640

6A

E= -877.749801

C	-3.29329300	0.29384400	-0.64087400
C	-3.21330100	0.24518300	0.79834200
C	-2.34536900	1.30736300	1.23454800
C	-1.89195600	2.00594900	0.07142900
C	-2.45818500	1.38143200	-1.08667200
W	-1.11738500	-0.31329600	-0.06810300
C	0.38028300	-0.50941700	1.35003000
Si	2.44840700	1.18530500	0.25515800
C	-1.46764400	-2.22132800	0.19716700
O	-1.71058000	-3.35297000	0.37606600
C	-0.48079700	-1.04733100	-1.77917500
O	-0.17204300	-1.46003700	-2.83043800

H	2.73683800	2.06854700	1.41562100
H	2.17178100	2.03367900	-0.92477700
C	3.97884700	0.11980100	-0.08868700
Si	5.07421100	1.08538900	-1.30426600
H	5.15304100	2.51206500	-0.90775700
H	6.44848500	0.53023900	-1.30561600
H	4.52738900	1.00836400	-2.67868000
Si	4.97817200	-0.15957200	1.49534800
H	5.68257500	1.08272600	1.89361600
H	4.10084300	-0.56530600	2.61900200
H	5.98769400	-1.22556000	1.29431400
Si	3.53577300	-1.55209400	-0.87309100
H	2.94050000	-2.45587500	0.13921900
H	2.58808700	-1.37868500	-1.99194400
H	4.77243700	-2.18820300	-1.38769500
N	0.94686300	0.33890600	0.57010800
C	-1.01743900	3.22820900	0.07489400
H	-0.45122900	3.32652800	-0.85556700
H	-1.62589300	4.13621500	0.18760700
H	-0.30118300	3.21387700	0.90218700
C	-2.34810200	1.87791200	-2.50353000
H	-3.15025000	2.59512000	-2.72721500
H	-1.39447900	2.38243600	-2.68365500
H	-2.42696600	1.05917600	-3.22386000
C	-2.07957000	1.70840800	2.66025000
H	-1.06986800	2.11177900	2.78928900
H	-2.78433200	2.48565700	2.98742400
H	-2.18943400	0.86146500	3.34384500
C	-4.04671500	-0.63112100	1.69528100
H	-3.54320900	-0.83086600	2.64576000
H	-5.00772100	-0.14888900	1.92217500
H	-4.26142600	-1.59695400	1.23034400
C	-4.24094000	-0.49754100	-1.50306800
H	-5.20709300	0.01838000	-1.59917600
H	-3.84135000	-0.64288600	-2.51086800
H	-4.43516400	-1.48862100	-1.08356200
C	0.88868200	-1.15597400	2.59427300
H	1.08343600	-2.21394700	2.37691100
H	1.80517100	-0.69714400	2.98146700
H	0.11188800	-1.13644000	3.36610800

TS_{A6-7}

E= -877.715801

C	-3.06783100	0.77976400	-0.19758800
C	-3.04191200	-0.44739100	0.57008800
C	-2.23325300	-0.21945600	1.74194800
C	-1.77880300	1.13922700	1.70287500
C	-2.27966100	1.75497700	0.51532100
W	-0.93639400	-0.06369200	-0.27662900
C	0.19355200	-1.79234400	0.39142800
N	1.37385100	-1.51845600	0.83788900
Si	2.06487400	0.07314200	0.94889400
C	-1.28207400	-1.26211800	-1.76923200
O	-1.59275900	-1.98071100	-2.63978200
C	-0.29010400	1.00861200	-1.82020500
O	0.02560200	1.65671000	-2.73633100
H	2.22057800	0.43182600	2.37976000
H	1.15331000	1.13435100	0.37896400

C	3.72356300	0.15168500	0.06547100
Si	4.04610400	1.92433300	-0.51577800
H	3.70078400	2.89230000	0.55458600
H	5.47846900	2.10505300	-0.85281500
H	3.23288500	2.24253300	-1.71217000
Si	5.08972400	-0.36504900	1.27511600
H	5.37431200	0.73065900	2.23364500
H	4.69130400	-1.56684800	2.04304400
H	6.33856500	-0.67016000	0.53678600
Si	3.74738600	-1.02220700	-1.42944400
H	4.03292800	-2.41341400	-1.01376900
H	2.46378600	-0.97840600	-2.16289800
H	4.82597900	-0.59053900	-2.35275500
C	-0.22713500	-3.24546700	0.37054000
H	-0.26582200	-3.59376800	-0.66952000
H	0.47973200	-3.86691700	0.93053600
H	-1.23667000	-3.37489400	0.77698000
C	-2.05361900	-1.15931200	2.90319000
H	-1.04264000	-1.10893500	3.31865600
H	-2.75710100	-0.91127600	3.70996200
H	-2.23918100	-2.19724600	2.61675600
C	-0.97891500	1.81991100	2.77859200
H	-1.65004500	2.25274700	3.53357400
H	-0.31421700	1.12253300	3.29665900
H	-0.36772700	2.63459000	2.38031100
C	-2.13578200	3.20748500	0.14775200
H	-2.94123600	3.80121600	0.60167000
H	-1.18471600	3.62256800	0.49419200
H	-2.18597400	3.35735000	-0.93390200
C	-3.95495500	1.05699900	-1.38215700
H	-4.94145200	1.41463300	-1.05537900
H	-3.52521900	1.82030100	-2.03749800
H	-4.10976800	0.15869300	-1.98594100
C	-3.90518700	-1.65210600	0.30975300
H	-4.90073400	-1.50999900	0.75231700
H	-4.03854500	-1.83000700	-0.76044300
H	-3.47868300	-2.56042000	0.74321900

7A

E= -877.721482

C	-3.00974100	0.77202100	-0.1130280
C	-2.98729800	-0.57117000	0.4190210
C	-2.22153000	-0.54853900	1.6410810
C	-1.77231300	0.79248400	1.8560740
C	-2.24948700	1.60989400	0.7808340
W	-0.84707100	0.01115100	-0.2737180
Si	1.92481000	-0.28216000	0.9111570
C	-0.30113800	1.38596900	-1.5971470
O	-0.04640500	2.21201800	-2.3794610
C	-1.02731900	-0.93144500	-1.9802480
O	-1.22634100	-1.49353500	-2.9856800
C	0.24190700	-1.91508300	0.1472560
H	1.93513700	0.15296400	2.3291570
H	0.86771900	0.68321300	0.2956320
C	3.55648700	0.15443700	0.1001250
Si	4.95009700	-0.28618500	1.3140690
H	4.69821900	-1.59588700	1.9574000
H	6.24355600	-0.35081600	0.5942370

H	5.05601100	0.74459600	2.3751840
Si	3.80386100	-0.83421100	-1.5068610
H	4.24550900	-2.21517600	-1.2118690
H	2.56224800	-0.86896200	-2.3083180
H	4.86271500	-0.17156400	-2.3074450
Si	3.64479900	2.01075600	-0.2695360
H	3.06015800	2.78532300	0.8533570
H	5.05605100	2.43268000	-0.4348720
H	2.89942900	2.34063300	-1.5042490
N	1.42085600	-1.91997900	0.6985540
C	-0.33206800	-3.27949600	-0.1907250
H	0.21184100	-4.06605000	0.3433170
H	-1.40208900	-3.34891200	0.0264960
H	-0.22421500	-3.45040700	-1.2697870
C	-1.02763900	1.28369000	3.0667200
H	-1.73587400	1.59143000	3.8485150
H	-0.38520300	0.50934400	3.4950640
H	-0.39998600	2.14896300	2.8354620
C	-2.12941900	3.10821600	0.6925000
H	-2.96794900	3.59247800	1.2119350
H	-1.20437400	3.46966200	1.1511530
H	-2.13929000	3.45460000	-0.3444250
C	-2.06589000	-1.68101000	2.6180690
H	-1.09936300	-1.64806000	3.1288190
H	-2.85040300	-1.63109000	3.3859100
H	-2.14622100	-2.65491900	2.1302730
C	-3.83923000	-1.70901500	-0.0773960
H	-3.47129000	-2.67710100	0.2717260
H	-4.86973500	-1.59977500	0.2876880
H	-3.87520900	-1.74363700	-1.1698220
C	-3.87245300	1.25123200	-1.2505700
H	-4.02176000	0.46881600	-1.9999110
H	-4.86343600	1.55398300	-0.8839990
H	-3.43015300	2.11259200	-1.7592470

TS_{A7-8}

E= -877.713628

C	-2.87229900	0.91317900	0.13210500
C	-2.96162300	-0.51374600	0.29292600
C	-2.15659900	-0.88104000	1.42469500
C	-1.55666400	0.30626100	1.95834300
C	-1.99285500	1.41601200	1.16206600
W	-0.74281400	0.05954000	-0.32914100
C	-1.08817100	-0.61624400	-2.16554500
O	-1.38709700	-1.01511000	-3.21378400
C	-0.33236500	1.80562300	-1.22996900
O	-0.15490900	2.83009100	-1.74333700
Si	1.61796700	-0.27520400	0.74183200
C	0.23545900	-2.00410700	-0.04731800
H	0.89130700	0.06614100	-0.97725200
H	1.64872600	0.23470900	2.14299300
C	3.35545200	0.12668600	0.07326200
Si	3.47981500	1.93082200	-0.47290300
H	2.74819700	2.81833400	0.46513800
H	4.89641300	2.36941400	-0.50303200
H	2.91055800	2.11828700	-1.82784200
Si	3.83739100	-0.99826000	-1.37422300
H	4.25098300	-2.33980400	-0.90533100

H	2.72285200	-1.14513100	-2.33872900
H	4.98445700	-0.39672300	-2.10028600
Si	4.57644100	-0.15246300	1.49745700
H	5.96392000	-0.24173200	0.97880400
H	4.52115900	0.97719200	2.45789900
H	4.27210500	-1.40368600	2.22832400
N	1.32696200	-2.01729300	0.63791000
C	-0.29992300	-3.29294700	-0.63679500
H	-1.38637600	-3.38141600	-0.53756700
H	-0.08162600	-3.30068700	-1.71302700
H	0.19080600	-4.15675500	-0.17417500
C	-0.84177600	0.38813000	3.27623800
H	-1.57528800	0.44240600	4.09309800
H	-0.21184900	-0.48726600	3.45612300
H	-0.20504200	1.27331900	3.34294000
C	-1.74770300	2.86561200	1.48609700
H	-2.50501400	3.22904200	2.19413000
H	-0.76597100	3.01322200	1.94482300
H	-1.79692600	3.50058700	0.59772500
C	-3.71212300	1.74875800	-0.79774200
H	-4.66470000	2.01504400	-0.31953800
H	-3.21117900	2.68077100	-1.07383000
H	-3.94486100	1.21468000	-1.72327000
C	-3.90164300	-1.41986500	-0.45625200
H	-4.87869800	-1.45545700	0.04414900
H	-4.06804800	-1.07513000	-1.48041700
H	-3.52387000	-2.44428300	-0.51231600
C	-2.12098500	-2.22312100	2.09998800
H	-2.77860000	-2.20780400	2.98016600
H	-2.47219300	-3.02239400	1.44432700
H	-1.11540700	-2.48334300	2.44111500

8A

E= -877.714367

C	-2.83732600	0.96010900	0.14802600
C	-2.95813600	-0.46296300	0.34517700
C	-2.13389100	-0.82958000	1.46068800
C	-1.49275800	0.35381000	1.95419900
C	-1.92075000	1.45938500	1.14318400
W	-0.73033300	0.04043500	-0.34160100
C	-1.28471500	-0.62568700	-2.14005200
O	-1.67630100	-1.00526200	-3.16227300
C	-0.22761200	1.77752000	-1.21402100
O	-0.00363400	2.80358400	-1.70188600
Si	1.59596700	-0.27963300	0.76624500
C	0.23360100	-2.01632600	-0.02170800
H	0.69344000	-0.15317700	-1.32071500
H	1.70769400	0.17625000	2.18367600
C	3.32172600	0.10690300	0.04393700
Si	3.46592400	1.90534200	-0.50856600
H	2.73711400	2.80729800	0.41838200
H	4.88687300	2.33268900	-0.52726100
H	2.91602500	2.09781100	-1.87049200
Si	3.77326000	-1.02918100	-1.40144900
H	4.18653900	-2.37111000	-0.93248100
H	2.64712100	-1.17939900	-2.35238300
H	4.91358200	-0.44166900	-2.15027100
Si	4.56637200	-0.18005600	1.44632500

H	5.94634700	-0.27503900	0.90705100
H	4.53468200	0.94973200	2.40793800
H	4.26993100	-1.43020300	2.18184200
N	1.31671100	-2.03579400	0.67139000
C	-0.77378900	0.45473600	3.26833200
H	-1.50942500	0.55573000	4.07900600
H	-0.17064900	-0.43250600	3.47686000
H	-0.11212000	1.32262700	3.30852400
C	-1.61560300	2.90551800	1.42940700
H	-2.29110500	3.28985100	2.20539600
H	-0.58933100	3.03346500	1.78552900
H	-1.73937000	3.53433100	0.54416200
C	-3.67650500	1.79641000	-0.78157100
H	-4.60949500	2.10038700	-0.28770300
H	-3.15604700	2.70675900	-1.09152400
H	-3.94627400	1.24832500	-1.68863000
C	-3.93766400	-1.36367700	-0.35896600
H	-4.89309800	-1.38105500	0.18206800
H	-4.14288600	-1.02647900	-1.37839300
H	-3.57487100	-2.39336700	-0.41930800
C	-2.10808600	-2.16184100	2.15531300
H	-2.48640600	-2.96349700	1.51756400
H	-1.09905500	-2.43453900	2.47574000
H	-2.74540500	-2.12382300	3.04951400
C	-0.31850100	-3.29782300	-0.61405200
H	-0.11729100	-3.29919600	-1.69374200
H	0.17357700	-4.16776700	-0.16433000
H	-1.40424600	-3.38023200	-0.49714000

TS_{A8-9}
E= -877.703037

C	-2.86134100	0.95207100	0.04091700
C	-2.92831000	-0.38929700	0.58353800
C	-2.03617000	-0.45920500	1.70369100
C	-1.41941700	0.82510200	1.86056600
C	-1.91404000	1.69129800	0.82296400
W	-0.78416900	-0.03815800	-0.34087800
C	-1.51882200	-0.80007900	-2.02729800
O	-2.00658400	-1.21501300	-2.99735500
C	0.04038300	1.30403800	-1.54258300
O	0.43620000	2.15848200	-2.22445500
Si	1.59275700	-0.20335100	0.79732800
C	0.27259800	-2.07165200	0.10677700
H	0.39169900	-1.15513000	-1.06705000
H	1.74297800	0.31320200	2.18614300
C	3.31737100	0.09869200	0.03125900
Si	3.58004000	1.93328700	-0.36006800
H	2.79589200	2.78378800	0.57105500
H	5.01125600	2.28995200	-0.19695200
H	3.18429100	2.26697100	-1.74480200
Si	3.65798400	-0.93587400	-1.51449900
H	3.96636000	-2.34164200	-1.16202900
H	2.50293100	-0.92728600	-2.44244200
H	4.82916100	-0.38587000	-2.24110700
Si	4.58519900	-0.37826200	1.36449300
H	5.93678500	-0.50351300	0.76368200
H	4.65166100	0.66972700	2.41249100
H	4.23720500	-1.66519000	2.00651000

N	1.28528700	-1.97316100	0.88492400
C	-1.88609100	-1.60691800	2.66380900
H	-0.84015800	-1.77494300	2.93621800
H	-2.44786700	-1.40854700	3.58673500
H	-2.27042900	-2.53892000	2.24197100
C	-0.65266100	1.27624100	3.07046800
H	-1.35783300	1.67762400	3.81234900
H	-0.10775700	0.45635400	3.54332700
H	0.06587400	2.06499200	2.83500200
C	-1.63501000	3.16644800	0.71285800
H	-2.33996700	3.73820300	1.33159500
H	-0.62406200	3.41191000	1.05000800
H	-1.73471200	3.52253700	-0.31609100
C	-3.77449200	1.52286900	-1.01174300
H	-4.70559000	1.88607300	-0.55548700
H	-3.31131800	2.36559800	-1.53233400
H	-4.04540200	0.77928400	-1.76649200
C	-3.92856900	-1.44045700	0.18103000
H	-4.86674800	-1.30511600	0.73621700
H	-4.16705000	-1.39151700	-0.88480800
H	-3.56667200	-2.45059700	0.39155700
C	-0.34857500	-3.39276700	-0.28607300
H	-1.39332600	-3.45180900	0.03876500
H	-0.34611200	-3.50444000	-1.37692400
H	0.21861900	-4.21312600	0.16525800

9A
E= -877.713467

C	-2.77524700	-1.12899400	0.24282500
C	-1.89484400	-1.18883100	1.38660200
C	-1.74655000	0.15088000	1.90766000
C	-2.52673400	1.02335000	1.08395300
C	-3.15306300	0.24975300	0.05659300
W	-0.81769900	-0.05454800	-0.30511700
C	0.07757900	-1.70062600	-0.84734700
O	0.50424700	-2.75429900	-1.12163700
C	-1.04990600	-0.00199900	-2.27396400
O	-1.24239500	-0.00238000	-3.42361100
Si	1.54001400	0.37558900	0.73187700
H	0.02356800	1.78179200	-0.89386000
H	1.62686500	0.20892600	2.21346000
C	3.24675300	-0.23549100	0.11767100
Si	4.58591600	0.97802400	0.70715300
H	5.90698400	0.29826600	0.68786300
H	4.68250400	2.15606900	-0.18533500
H	4.33201300	1.43394400	2.09278500
Si	3.62092600	-1.91370700	0.90792800
H	4.59989600	-2.67887100	0.09856900
H	4.19340000	-1.72943600	2.26495500
H	2.39764600	-2.73711000	1.05258300
Si	3.36833700	-0.33459400	-1.76777300
H	2.77388100	0.86840400	-2.39939600
H	4.79614000	-0.38587800	-2.17267000
H	2.70134100	-1.53550100	-2.31405900
N	1.59432100	2.16998300	0.47512200
C	0.71767500	2.53627500	-0.35258900
C	-1.11342600	0.52230100	3.21951600
H	-1.86759000	0.50638000	4.01890000

H	-0.32015000	-0.17401600	3.49843300
H	-0.67520800	1.52453100	3.19754300
C	-2.71591400	2.49703000	1.31431600
H	-3.56721400	2.67104900	1.98698700
H	-1.83637600	2.95199900	1.77930700
H	-2.92597600	3.03207800	0.38325100
C	-4.16136700	0.75459900	-0.94098300
H	-5.17745100	0.68351500	-0.52922300
H	-3.98559500	1.80173200	-1.20446200
H	-4.13983400	0.17390300	-1.86697900
C	-3.36668700	-2.31134300	-0.47674400
H	-4.28060900	-2.65324700	0.02864600
H	-3.63066800	-2.06534600	-1.50928400
H	-2.66957900	-3.15307000	-0.50831800
C	-1.40422800	-2.44416600	2.05511200
H	-2.12596100	-2.78267700	2.81130000
H	-1.26864200	-3.25637600	1.33635500
H	-0.44574400	-2.28600200	2.55715200
C	0.43777100	3.93242100	-0.83300800
H	0.58127700	3.99644000	-1.91890700
H	-0.60220200	4.21349900	-0.62486700
H	1.11436200	4.62974100	-0.33223300

TS_{A1-10}

E= -877.716437

C	-3.11663500	-0.30822900	-0.5658380
C	-2.48893500	-1.55272700	-0.2054530
C	-2.06946400	-1.46478900	1.1667830
C	-2.42374700	-0.16279100	1.6511360
C	-3.06289700	0.55515900	0.5875140
W	-0.84660200	0.14151000	-0.1531040
C	-0.02634700	-0.43097200	-1.8504580
O	0.39725800	-0.78934700	-2.8796520
C	-0.62356900	1.91657600	-0.9800830
O	-0.51241800	2.98744800	-1.4416150
Si	1.30742300	-0.32638300	0.7692570
H	0.09773800	1.04221000	1.0295810
H	1.49066100	-0.52604900	2.2406350
C	3.00764200	-0.86283900	0.0859850
Si	4.30235800	-0.90802800	1.4717520
H	3.98906100	-1.99430300	2.4334110
H	5.64513200	-1.19067600	0.9052940
H	4.36877900	0.37165000	2.2078740
Si	2.75896600	-2.65791500	-0.4965880
H	1.92423400	-3.40521400	0.4792500
H	2.10809300	-2.73443400	-1.8198500
H	4.07306300	-3.34229500	-0.5689520
Si	3.68314900	0.17276600	-1.3513700
H	4.38009200	-0.70219000	-2.3269700
H	2.62657800	0.91680300	-2.0652570
H	4.68216200	1.14751800	-0.8490410
N	2.40492300	2.16576000	1.0626920
C	2.29225200	3.26173400	0.7014750
C	-2.26889900	0.31163800	3.0708360
H	-2.20087600	1.40150600	3.1287950
H	-3.13197600	0.00100100	3.6763140
H	-1.37180700	-0.10160500	3.5406270
C	-3.71901500	1.90511100	0.7038930

H	-4.76312500	1.80267300	1.0310200
H	-3.20575800	2.54210600	1.4298930
H	-3.72391000	2.43431600	-0.2531310
C	-1.54061500	-2.59946800	2.0024280
H	-0.88098400	-2.24615600	2.8001280
H	-2.36984100	-3.14307200	2.4775740
H	-0.97876500	-3.31904000	1.4005110
C	-3.86717100	-0.03143200	-1.8410330
H	-4.91702200	-0.34599200	-1.7525010
H	-3.86263600	1.03382200	-2.0892050
H	-3.43283100	-0.56687300	-2.6897770
C	-2.44288700	-2.79323500	-1.0574090
H	-1.56519700	-3.40540100	-0.8320500
H	-3.33489300	-3.41218200	-0.8877500
H	-2.40759800	-2.54976800	-2.1227930
C	2.11315800	4.62790600	0.2211070
H	1.93792500	5.30543600	1.0624330
H	3.00475500	4.95759000	-0.3210380
H	1.25056600	4.65575000	-0.4520660

10A

E= -877.722593

C	-2.95345900	-0.59985000	-0.76632200
C	-2.13957800	-1.71703800	-0.35279800
C	-1.90157900	-1.59865200	1.05857500
C	-2.56233400	-0.40970600	1.51570800
C	-3.20968500	0.20691500	0.39626200
W	-0.88264400	0.26832000	-0.07779200
C	0.04346200	0.06303800	-1.81094900
O	0.52495200	-0.07619800	-2.86884300
C	-0.84944400	2.15139600	-0.61254500
O	-0.81455500	3.29398600	-0.89297000
Si	1.40447600	-0.00820400	0.78964800
H	-0.30060200	1.13196800	1.31115600
H	1.62599500	-0.23498800	2.25243300
C	3.00063900	-0.84320100	0.06198900
Si	4.24572100	-1.08667100	1.46613400
H	3.77091300	-2.11171200	2.42724200
H	5.56301800	-1.53468800	0.94536900
H	4.46463400	0.18109700	2.20370700
Si	2.53210200	-2.54959300	-0.60910400
H	1.66017800	-3.27346300	0.34931500
H	1.83412100	-2.46763600	-1.90946900
H	3.75513500	-3.37156900	-0.78826400
Si	3.86299100	0.13681900	-1.30808500
H	4.57203500	-0.76878000	-2.24481500
H	2.93554400	0.98047000	-2.08970400
H	4.88483300	1.04141900	-0.71650800
N	2.14930400	1.84123500	0.86043400
C	2.24539000	2.98150300	0.69734000
C	-1.27207800	-2.63818000	1.94577500
H	-0.76858100	-2.18825400	2.80651900
H	-2.03774000	-3.32446000	2.33587900
H	-0.53515200	-3.24132700	1.40924200
C	-2.67621000	0.02742000	2.95102700
H	-3.53809100	-0.45577000	3.43296500
H	-1.78482300	-0.23804700	3.52608300
H	-2.81440800	1.10886600	3.03518100

C	-4.12356300	1.40130700	0.45721500
H	-5.15541200	1.09086100	0.67386700
H	-3.81813500	2.10264600	1.23906700
H	-4.13522500	1.94903400	-0.48928700
C	-3.58698000	-0.42509700	-2.12107600
H	-4.54870900	-0.95569300	-2.17433600
H	-3.77795500	0.62861000	-2.34435800
H	-2.94985700	-0.81785400	-2.91869900
C	-1.77076200	-2.89636900	-1.21261600
H	-2.57186500	-3.64907900	-1.20244000
H	-1.60655200	-2.60287500	-2.25325300
H	-0.85583900	-3.38008500	-0.86042400
C	2.28939400	4.41423900	0.45327400
H	1.35816400	4.70536000	-0.04422500
H	2.38715800	4.95385600	1.40026800
H	3.14124400	4.65618000	-0.18988200

TS_{A10-9}
E= -877.695625

C	-2.84729200	-1.10197500	0.07906400
C	-2.04287000	-1.29743000	1.26057400
C	-1.85902900	-0.01698700	1.89170200
C	-2.53230400	0.96320100	1.09685000
C	-3.13572400	0.30443300	-0.02575100
W	-0.80747500	-0.04758700	-0.29341200
C	0.09615000	-1.66712200	-0.94208000
O	0.55509800	-2.67600500	-1.32130700
C	-0.85292500	0.27350100	-2.23976100
O	-0.93648200	0.47389100	-3.38815600
Si	1.49341800	0.25476700	0.78145700
H	-0.17112400	1.62930400	-0.46840000
H	1.64713000	0.04137200	2.25632300
C	3.21581300	-0.27046100	0.12216600
Si	4.59776100	0.78852600	0.87105400
H	5.90821300	0.10874300	0.71617200
H	4.70090500	2.09992400	0.18546500
H	4.37228600	1.02600200	2.31598800
Si	3.51699600	-2.05154700	0.71198900
H	4.29637400	-2.81965400	-0.28704900
H	4.28071300	-2.04265900	1.98487700
H	2.24749400	-2.76838100	0.97148700
Si	3.34591800	-0.14123200	-1.76349600
H	2.84159300	1.17402600	-2.22966500
H	4.77534800	-0.22476400	-2.15927500
H	2.61457600	-1.21358200	-2.46616500
N	1.74646500	2.17482400	0.76354500
C	0.99204700	2.76784700	0.06307000
C	-1.25403700	0.21442400	3.24856100
H	-2.01452100	0.08534500	4.03167600
H	-0.44218600	-0.48616700	3.45901700
H	-0.84736200	1.22519700	3.34973400
C	-2.68893900	2.41710500	1.44795400
H	-3.57719800	2.56875000	2.07716100
H	-1.82715600	2.79513900	2.00646400
H	-2.81586700	3.03718400	0.55526800
C	-4.06614100	0.93894000	-1.02524000
H	-5.10329400	0.91144000	-0.66281900
H	-3.81034400	1.98642800	-1.21124700

H	-4.03878500	0.42002200	-1.98718900
C	-3.44463800	-2.18921200	-0.77398700
H	-4.41574000	-2.51073300	-0.37134000
H	-3.60679200	-1.85091100	-1.80143800
H	-2.79736100	-3.06952600	-0.81835600
C	-1.64778500	-2.62649900	1.84732900
H	-2.43463100	-3.00511000	2.51482300
H	-1.48274400	-3.37728200	1.06986400
H	-0.72575900	-2.55158300	2.43112300
C	0.49125900	3.96375600	-0.62417100
H	0.50245000	3.79428400	-1.70461400
H	-0.53576000	4.17201600	-0.31318100
H	1.13973200	4.81143600	-0.37306500

TS_{A4-9}
E= -877.693339

W	-0.76982700	-0.05228500	-0.2706100
C	-2.57876500	1.07538200	0.9519180
C	-3.11426100	0.31667700	-0.1420300
C	-2.83058000	-1.07383100	0.1078030
C	-2.08867300	-1.15455300	1.3392130
C	-1.93484200	0.18017200	1.8599660
Si	1.49079200	0.11044000	0.8217370
H	1.65555900	-0.12334600	2.2991110
C	0.11812900	-1.79040100	-0.6002710
O	0.58017700	-2.84494900	-0.8157260
C	-0.69552700	-0.13828300	-2.2517700
O	-0.71702000	-0.21043700	-3.4134320
H	1.45528600	2.00095800	0.6156520
C	3.24931300	-0.23980500	0.1686140
Si	4.43803300	1.08684200	0.8118740
H	4.16805100	1.40509700	2.2340030
H	5.84536400	0.63068900	0.6994430
H	4.30176400	2.33609800	0.0226670
Si	3.82700500	-1.89679000	0.9006280
H	2.71843500	-2.87207400	0.9919590
H	4.89929700	-2.48406700	0.0609720
H	4.36828100	-1.68796200	2.2660520
Si	3.33901000	-0.26205800	-1.7257430
H	2.72631500	-1.48384300	-2.2879940
H	2.67348000	0.93190800	-2.2938320
H	4.76396100	-0.22878800	-2.1416590
N	-0.23130800	1.95335200	-0.6217090
C	0.69979600	2.62679600	-0.1873350
C	-1.37788400	0.52854000	3.2122260
H	-1.01082600	1.55807900	3.2502180
H	-2.15348700	0.42710800	3.9842060
H	-0.54928000	-0.12758600	3.4926250
C	-2.73765100	2.55722400	1.1281930
H	-3.74747600	2.79007600	1.4920220
H	-2.02359000	2.95680400	1.8530950
H	-2.58626700	3.08936800	0.1850590
C	-3.97932500	0.86765700	-1.2435570
H	-5.02434600	0.95105400	-0.9137990
H	-3.64812800	1.86331700	-1.5528330
H	-3.96246200	0.22496300	-2.1279540
C	-3.37700500	-2.23837100	-0.6740690

H	-4.37032000	-2.52270400	-0.2996460
H	-3.47994200	-1.99776000	-1.7360660
H	-2.73031600	-3.11691700	-0.5977620
C	-1.72462400	-2.41902100	2.0709210
H	-2.54958800	-2.73459500	2.7244090
H	-1.51277800	-3.24156900	1.3827140
H	-0.83987800	-2.27950800	2.6991930
C	1.19942300	4.02214500	-0.4093640
H	0.52351700	4.55690100	-1.0824550
H	1.27590800	4.56121800	0.5424930
H	2.20162300	3.99574300	-0.8532130

TS_{A11-2}
E= -877.680047

C	-2.48504600	1.22700200	0.78974400
C	-1.96412300	1.77238400	-0.43084700
C	-2.29404100	0.87264900	-1.49833500
C	-3.02468600	-0.22807200	-0.94508100
C	-3.14645400	-0.01495600	0.47536500
W	-0.86514700	-0.32389800	0.03977200
C	-0.82334100	-2.28318800	-0.16006200
O	-0.89085800	-3.43922300	-0.30347800
Si	1.42959800	0.40963900	0.01970900
C	3.07093500	-0.53255500	-0.23994000
C	-0.29318700	-0.76344200	1.87557400
O	-0.01867000	-1.00903600	2.98558900
H	0.17344300	-0.63741200	-1.33306300
H	1.70080900	1.73381900	-0.93487600
Si	2.74585600	-2.29121200	-0.91138800
H	4.06174500	-2.88239800	-1.26043600
H	2.11602300	-3.14661100	0.11451900
H	1.92200600	-2.27182300	-2.13746900
Si	3.97486000	-0.74422300	1.42653400
H	4.93308700	-1.87011000	1.30992800
H	4.75011500	0.47012600	1.77225000
H	3.02291900	-1.04495600	2.51523000
Si	4.23939400	0.31748400	-1.45610900
H	5.54308600	-0.38500600	-1.51903800
H	3.66087300	0.35187200	-2.82118200
H	4.52075400	1.71681300	-1.04986700
N	2.03949100	1.76041500	1.32849800
C	2.14533800	2.51364800	0.38777100
C	-1.34161500	3.13129600	-0.59234400
H	-0.62514900	3.15097200	-1.41979600
H	-2.10956300	3.88820900	-0.80608000
H	-0.82240200	3.44343100	0.31884200
C	-2.03189500	1.11112000	-2.96076400
H	-2.84815700	1.69429800	-3.41002400
H	-1.10257900	1.66538600	-3.12097100
H	-1.95364600	0.17144000	-3.51393000
C	-2.50308800	1.91508300	2.12897500
H	-1.64885700	2.58735300	2.25098100
H	-3.41731700	2.51408100	2.24511300
H	-2.47180800	1.19703000	2.95298600
C	-3.98929600	-0.82994500	1.42002500
H	-3.61545900	-0.77131000	2.44622800
H	-5.02885800	-0.47207100	1.42462100
H	-4.00477200	-1.88643500	1.13750200

C	-3.68814400	-1.32901200	-1.72787400
H	-4.70921100	-1.03878300	-2.01207700
H	-3.14083600	-1.55780200	-2.64675500
H	-3.75653500	-2.25369100	-1.14826200
C	2.48555900	3.86643300	-0.10416900
H	2.79020000	4.47762500	0.75273400
H	3.30478400	3.81135200	-0.82595700
H	1.61856200	4.32189700	-0.59134400

TS_{A3-1}
E= -883.96223

C	2.82470900	1.08712600	0.0163760
C	2.98867400	-0.13182900	0.7731920
C	2.79407400	-1.23836700	-0.1271340
C	2.50252100	-0.70526200	-1.4286880
C	2.51330300	0.72013100	-1.3374090
W	0.75878100	-0.03893400	0.2074860
Si	-1.70440900	-0.27677400	-1.0270220
Si	-0.84232800	-2.58348000	-1.1517940
C	0.26185300	-1.42820900	1.5245750
O	0.07842800	-2.23759600	2.3429680
C	0.34191800	1.06352200	1.7677080
O	0.19828700	1.75426000	2.6980500
H	-1.83234700	-0.08030200	-2.4956190
H	-2.36461400	-1.82832700	-1.3030500
H	-1.52515200	-3.52619500	-0.2317220
H	-0.99252300	-2.87788100	-2.6033540
H	0.58710000	-2.95832700	-0.9279330
C	-3.31839800	0.03150000	-0.0182120
Si	-3.79784000	1.83576700	0.2996460
H	-5.03382700	1.88102900	1.1170300
H	-2.75622000	2.59089000	1.0315790
H	-4.08131300	2.55350600	-0.9695560
Si	-4.74127800	-0.75908300	-1.0120890
H	-4.90074300	-2.19916200	-0.7051110
H	-6.02122000	-0.09083800	-0.6603290
H	-4.53976700	-0.59468500	-2.4701470
Si	-3.31652400	-0.82102300	1.6793630
H	-2.82276100	-2.20895300	1.5851760
H	-2.50346400	-0.07003900	2.6619200
H	-4.71054600	-0.86862100	2.1892180
N	-0.65978800	1.23600100	-0.7366020
C	-0.85607300	2.43504800	-1.1366340
H	-1.73944000	2.63406700	-1.7573020
C	2.40168900	-1.48787500	-2.7067100
H	1.81208000	-0.95981100	-3.4612040
H	3.40509100	-1.65222700	-3.1249550
H	1.94915300	-2.46976600	-2.5495690
C	2.36763300	1.64313800	-2.5164250
H	3.19831200	1.49409800	-3.2183390
H	1.43843500	1.46487000	-3.0680620
H	2.38052800	2.69216000	-2.2137000
C	3.20587900	2.45270100	0.5258530
H	4.29594900	2.51516500	0.6449010
H	2.91222700	3.24616800	-0.1650040
H	2.75674500	2.67272600	1.4990380
C	3.53671200	-0.21768600	2.1734850
H	4.63564500	-0.22259000	2.1592080

H	3.21679700	0.63160700	2.7838730
H	3.20826800	-1.12892600	2.6809250
C	3.10708800	-2.67482600	0.1929020
H	4.18079500	-2.86160500	0.0527250
H	2.86051000	-2.92460100	1.2284240
H	2.55963000	-3.36521100	-0.4518680
C	-0.03231700	3.64442400	-0.8084060
H	0.74426600	3.41914100	-0.0777310
H	0.42421800	4.07093400	-1.7115040
H	-0.68909400	4.42057100	-0.3941830

TS_{A2-1}
E=-883.979757

C	-2.76679600	0.02395900	-1.3740900
C	-3.23678100	-0.20549000	-0.0304660
C	-2.78273800	0.88782900	0.7843220
C	-2.03269200	1.78446000	-0.0512110
C	-2.02798800	1.25110200	-1.3829760
W	-0.89471900	-0.36711500	0.0211290
Si	1.45552700	0.41674900	0.0003100
Si	0.81642800	0.94400500	2.5542380
C	-0.66594800	-1.44601300	1.6567440
O	-0.65120100	-2.10171900	2.6256240
C	-0.80472000	-2.19255400	-0.7166340
O	-0.84179700	-3.25531100	-1.1928540
H	0.33514100	-0.41341800	-1.2245080
H	2.03251200	1.06450600	1.4142570
H	-0.58061200	0.91911700	3.0492690
H	1.57613700	-0.06661900	3.3130030
H	1.23664900	2.33417400	2.9005080
C	2.99234200	-0.70206900	-0.2032950
Si	3.35419300	-0.91663300	-2.0601550
H	4.19427700	-2.12702600	-2.2403750
H	2.11841500	-1.10078900	-2.8525460
H	4.10905300	0.23662700	-2.6031520
Si	4.52894100	0.07828000	0.5835150
H	4.51424100	-0.09120100	2.0569960
H	5.76248800	-0.56353900	0.0662710
H	4.61701500	1.52749000	0.2867580
Si	2.77965300	-2.43163400	0.5547830
H	2.23264200	-2.36144000	1.9255750
H	1.92002300	-3.29795300	-0.2783970
H	4.11995500	-3.06475400	0.6370480
N	1.80283200	1.75808600	-1.0521030
C	2.16105900	2.97112800	-1.0611100
H	2.35224500	3.43745800	-2.0422960
C	-1.53431200	3.14884800	0.3403270
H	-0.65581700	3.43942800	-0.2416260
H	-2.31177100	3.90527700	0.1621660
H	-1.26900900	3.19957200	1.3999470
C	-1.47017100	1.93576900	-2.6006250
H	-2.19152300	2.66676400	-2.9919710
H	-0.54033800	2.46441100	-2.3789970
H	-1.25668800	1.22136900	-3.3999460
C	-3.13853700	-0.79030400	-2.5846750
H	-4.07823600	-0.42373000	-3.0198540
H	-2.36941100	-0.73536900	-3.3600570
H	-3.27814400	-1.84580300	-2.3365300

C	-3.21997400	1.14568800	2.2005120
H	-2.55034200	1.83563200	2.7187340
H	-4.22392600	1.59211900	2.2106850
H	-3.26210300	0.22374600	2.7880770
C	-4.20043800	-1.27950800	0.3977000
H	-4.07233900	-1.53892300	1.4523670
H	-5.23879600	-0.94556800	0.2616050
H	-4.06991600	-2.19604000	-0.1844690
C	2.38230100	3.90836500	0.1005930
H	3.41953600	4.26864500	0.0839470
H	1.74349300	4.79522100	-0.0075090
H	2.18447300	3.43876000	1.0656870

TS_{A6-1}
E=-884.002014

W	-1.52993000	-0.34385800	-0.0419720
C	0.73919400	-0.99562000	-0.4234090
Si	-1.36096900	-1.50663000	2.3333260
H	-0.15911600	-0.73832200	0.9593950
C	-2.27205300	1.62344600	1.1586740
C	-1.06548400	1.96616800	0.4550260
C	-1.31895700	1.84765200	-0.9512200
C	-2.68590500	1.41893200	-1.1170080
C	-3.26912500	1.28164600	0.1843650
H	-0.52301900	-0.73547400	3.2918560
H	-0.80725500	-2.88243100	2.3192930
H	-2.70075800	-1.59120700	2.9731030
Si	3.23556900	-0.17038400	-1.2436440
H	3.33944700	0.92689300	-2.2365320
H	3.54690100	-1.44110600	-1.9523220
C	4.56976800	0.10177600	0.0763540
N	1.59899700	-0.08515400	-0.6287290
C	1.00961500	-2.48901200	-0.4776770
H	2.07396300	-2.71308500	-0.3497090
H	0.43820300	-3.02247000	0.2851750
H	0.69401700	-2.88142300	-1.4510420
C	-2.83761500	-1.78672300	0.1885890
C	-1.41874800	-1.35125500	-1.7385580
O	-3.67856200	-2.59265800	0.2991390
O	-1.38869700	-1.89340100	-2.7697920
Si	6.16668800	0.57599100	-0.8354460
H	6.14314200	2.00652900	-1.2222990
H	7.34448000	0.34542800	0.0343050
H	6.32852300	-0.23777500	-2.0638720
Si	4.13465700	1.50113700	1.2737520
H	3.60511300	2.67763500	0.5456730
H	3.13080200	1.06268100	2.2704930
H	5.35137900	1.92744700	2.0077940
Si	4.88379700	-1.48261900	1.0656260
H	5.53688500	-2.50804800	0.2169410
H	5.76840600	-1.20288400	2.2217010
H	3.61503000	-2.04542600	1.5835930
C	0.19208900	2.51519600	1.0643800
H	0.29183000	2.23015500	2.1154460
H	1.07041000	2.14808300	0.5301060
H	0.19457600	3.61286800	1.0151400
C	-0.36872700	2.25574500	-2.0414510
H	-0.32100600	3.35051600	-2.1198360

H	0.63967900	1.88513700	-1.8375990
H	-0.68338600	1.86802500	-3.0144470
C	-3.42322900	1.30643300	-2.4249550
H	-3.84316300	2.28049900	-2.7104630
H	-2.76817200	0.97845300	-3.2364080
H	-4.25136700	0.59497300	-2.3615980
C	-4.71358400	0.98217200	0.4821440
H	-5.29205500	1.91411400	0.5421870
H	-5.16782500	0.36022600	-0.2936270
H	-4.83124600	0.45828300	1.4348380
C	-2.51755800	1.80239400	2.6321390
H	-2.89330400	2.81578600	2.8301390
H	-3.26127200	1.09632500	3.0117500
H	-1.60441300	1.67101400	3.2181560

TS_{B1-4}

E= -938.1051022

C	-1.29019300	-1.76825000	1.5903220
C	-2.19034700	-0.66250600	1.6131960
C	-2.88709100	-0.60848100	0.3578100
C	-2.43441900	-1.71833000	-0.4469180
C	-1.42655100	-2.41993600	0.3080980
W	-0.62188000	-0.32157200	-0.2393300
C	-1.01053000	0.80008800	-1.8176410
O	-1.28064200	1.43962300	-2.7577620
Si	1.59700000	0.13375600	0.8432430
C	0.51762400	-1.18268900	-1.5555110
O	1.13347300	-1.79168300	-2.3449660
O	-1.49434700	2.60317700	0.6755700
C	-1.38834100	3.75242900	0.2682800
H	1.74761800	-0.24535100	2.2821270
H	1.09589200	1.56432900	0.8724240
C	3.40865300	0.19276000	0.2053660
Si	4.45580600	0.96604700	1.5801980
H	4.60931400	0.02526500	2.7164660
H	5.81497100	1.30492400	1.0873490
H	3.83359200	2.21138700	2.0918460
Si	4.07090700	-1.55529000	-0.1061360
H	3.80960200	-2.01245800	-1.4872880
H	5.53777900	-1.60063800	0.1210750
H	3.44652100	-2.52105400	0.8336670
Si	3.57650000	1.23785300	-1.3573700
H	3.34547800	2.67171600	-1.0415180
H	4.94708600	1.12230300	-1.9155710
H	2.61595900	0.83500000	-2.4060930
C	-4.02963600	0.31811600	0.0381830
H	-4.96728700	-0.05499400	0.4736430
H	-3.84870100	1.32067100	0.4348390
H	-4.18144200	0.40903800	-1.0411030
C	-3.04018700	-2.17250700	-1.7474210
H	-3.90907600	-2.82052400	-1.5649600
H	-3.37866100	-1.32700700	-2.3534140
H	-2.32372500	-2.73964800	-2.3477360
C	-0.79604200	-3.73255500	-0.0700030
H	-1.40647500	-4.56943900	0.2958660
H	-0.69978400	-3.83767500	-1.1535080
H	0.20482900	-3.83745300	0.3582540
C	-0.47900800	-2.28101700	2.7470130

H	-1.08900500	-2.94684000	3.3734890
H	0.38970000	-2.84998800	2.4058800
H	-0.10867600	-1.47155700	3.3816060
C	-2.41766400	0.26855300	2.7703720
H	-3.34305100	-0.00119900	3.2982260
H	-1.59840000	0.21799600	3.4929320
H	-2.50872900	1.30452300	2.4346180
C	-2.36338800	4.82770000	0.7009000
H	-3.16289500	4.39981800	1.3090600
H	-1.83359600	5.59441500	1.2809460
H	-2.78858500	5.33257600	-0.1755360
C	-0.30235300	4.15752000	-0.7058100
H	-0.65077700	3.93253700	-1.7223300
H	-0.07715400	5.22682400	-0.6531010
H	0.60275400	3.57138700	-0.5310320

4B

E= -938.1283908

C	-1.61799300	-1.04337400	1.80740400
C	-2.61253800	-0.10060900	1.41133800
C	-3.09570700	-0.45145100	0.11053200
C	-2.41360700	-1.65219400	-0.30283400
C	-1.48629000	-2.01000300	0.74264400
W	-0.77664700	-0.02610900	-0.25188500
C	-1.11449800	0.71341800	-2.04058400
O	-1.39505000	1.09131600	-3.11384800
Si	1.58812100	0.21469700	0.86323600
C	0.36559900	-1.12418100	-1.39923300
O	0.95778300	-1.84991600	-2.10096500
O	-0.79670000	2.04041700	0.42596600
C	-0.39171200	3.18417000	0.16371900
H	1.62245700	-0.54076100	2.15500100
H	1.74916400	1.64077000	1.31365600
C	3.35291800	-0.19768100	0.16063700
Si	4.58338800	0.65720000	1.31981600
H	4.22280500	0.44933500	2.74201500
H	5.95929700	0.13232200	1.12075600
H	4.62687200	2.11838800	1.06024200
Si	3.69846600	-2.05324600	0.26985100
H	4.75897700	-2.46280100	-0.68476100
H	4.16910500	-2.40431400	1.63479500
H	2.49896600	-2.87602400	-0.00115400
Si	3.69476800	0.46661900	-1.57099900
H	3.22443400	1.87034300	-1.69262600
H	5.15748500	0.49005300	-1.83048500
H	3.06021700	-0.32416100	-2.64477000
C	-0.70790200	-3.29476800	0.83269400
H	0.21262900	-3.16771300	1.40905900
H	-1.30825500	-4.07076700	1.32761100
H	-0.42771200	-3.67042800	-0.15471600
C	-1.01319100	-1.14930800	3.17834800
H	-1.67889100	-1.71707900	3.84388900
H	-0.04799200	-1.65914600	3.16059100
H	-0.85424100	-0.16605300	3.63170700
C	-3.09529200	1.05053100	2.24455900
H	-3.90843600	0.72837000	2.90922800
H	-2.29558800	1.45380600	2.87224700
H	-3.48009100	1.86500700	1.62455900

C	-4.24025100	0.20449200	-0.61532500
H	-5.19663200	-0.25460400	-0.32906000
H	-4.30735400	1.27225100	-0.38506100
H	-4.13870800	0.10770800	-1.69962000
C	-2.76000700	-2.49015000	-1.50485500
H	-3.56700600	-3.19663600	-1.26563100
H	-3.09607600	-1.87240500	-2.34276100
H	-1.90101100	-3.07133500	-1.85114300
C	0.45423700	3.47190600	-1.03968000
H	-0.14053000	3.29853900	-1.94546700
H	0.82021700	4.50129600	-1.04536300
H	1.29762200	2.77626200	-1.08499900
C	-0.78699000	4.31958300	1.06685100
H	0.11375800	4.76677200	1.50720400
H	-1.28092400	5.11114100	0.48842300
H	-1.44802200	3.97333200	1.86295700

TS_{B4-5}

E= -938.1100043

C	1.55656400	-1.53664800	1.48947200
C	1.78054900	-2.06033100	0.16251800
C	2.70333600	-1.18218600	-0.50977100
C	3.04437800	-0.11717400	0.40598100
C	2.34615700	-0.35478700	1.63178200
W	0.74393300	-0.02451500	-0.23280500
C	1.14353300	1.24722400	-1.67423600
O	1.47659200	1.94885100	-2.55555900
Si	-1.62078900	-0.80794300	0.61904000
O	0.00467700	1.72854500	1.11600500
C	0.23259700	2.79630500	0.50785900
C	-0.15400500	-0.88969500	-1.72809500
O	-0.59289600	-1.49247900	-2.63153400
H	-1.63099600	-0.63306200	2.10586400
H	-1.73140400	-2.28942700	0.43928700
C	-3.39028700	-0.16747200	0.13413800
Si	-3.63684300	0.33111300	-1.66902200
H	-5.07046200	0.62914400	-1.91744900
H	-2.87876100	1.55899600	-2.01333700
H	-3.22825100	-0.74096300	-2.59941700
Si	-4.56451900	-1.61641200	0.48341000
H	-4.29816000	-2.21069300	1.81435400
H	-5.97983000	-1.16134200	0.47194200
H	-4.42166900	-2.67338400	-0.54560800
Si	-3.91074100	1.23996100	1.28040300
H	-4.18259700	0.73604800	2.64885100
H	-2.87266400	2.29073000	1.39281200
H	-5.14808200	1.89741600	0.78771400
C	2.44130000	0.45276500	2.89563700
H	3.09248900	1.32208600	2.77112200
H	1.45920900	0.80961200	3.22262300
H	2.86175000	-0.15651200	3.70586100
C	0.84159400	-2.23681100	2.61032000
H	1.53526600	-2.90819100	3.13636300
H	0.44517500	-1.52795500	3.34217500
H	0.00582800	-2.84268400	2.25146500
C	1.32177000	-3.40633600	-0.32957000
H	2.04849500	-4.18074600	-0.04847900
H	0.35553000	-3.68231900	0.10038400

H	1.21506000	-3.42642100	-1.41720300
C	3.37399500	-1.44840700	-1.83120300
H	4.31198000	-2.00222400	-1.68489200
H	2.73673600	-2.04386300	-2.49065100
H	3.61324000	-0.51991100	-2.35761900
C	4.11094400	0.91761400	0.16196200
H	5.10596800	0.50429000	0.37711900
H	4.11423500	1.25557200	-0.87837900
H	3.98036600	1.79906300	0.79555600
C	1.45683600	3.61941100	0.82636500
H	2.11059700	3.64967300	-0.05387800
H	1.16652500	4.65493200	1.04177900
H	1.99923100	3.20094300	1.67466000
C	-0.74902200	3.40505100	-0.45591200
H	-1.23266800	4.25659400	0.04431400
H	-0.23283900	3.79700700	-1.33889200
H	-1.50823300	2.68716100	-0.75927100

5B

E= -938.1143167

C	1.58281800	-1.71709900	1.24329900
C	1.81788800	-2.03354500	-0.14306100
C	2.73768600	-1.06398600	-0.66175700
C	3.09023300	-0.15981200	0.40994100
C	2.38044300	-0.57550400	1.57839700
W	0.76887700	0.07691400	-0.19162100
C	1.19541700	1.46397800	-1.50446700
O	1.54418200	2.24964100	-2.30022100
Si	-1.63926700	-0.87524700	0.44143300
O	-0.11163700	1.33323000	1.33193100
C	0.28807600	2.34412400	0.60851400
C	-0.28829700	-0.54497300	-1.70857600
O	-0.83105500	-0.97965000	-2.65475400
H	-1.54340400	-0.95834600	1.92331000
H	-1.72606100	-2.29375600	-0.01794300
C	-3.40009700	-0.16217000	0.12519600
Si	-3.77416800	0.46721200	-1.62183500
H	-5.09058800	1.15486300	-1.61511700
H	-2.76502900	1.44361400	-2.08704700
H	-3.85082200	-0.64352300	-2.59659000
Si	-4.57308400	-1.62955000	0.43872000
H	-4.41201500	-2.14272600	1.82138400
H	-5.98555600	-1.20501700	0.27495500
H	-4.31497000	-2.73765800	-0.50762800
Si	-3.87367200	1.17682800	1.38393900
H	-3.37017400	0.84761200	2.73665000
H	-3.36786700	2.51530700	1.00737400
H	-5.35198000	1.28681900	1.46189600
C	0.84939200	-2.57362500	2.23695000
H	0.05358400	-3.15753000	1.76813100
H	1.54696500	-3.28262800	2.70501600
H	0.39796400	-1.97567300	3.03296400
C	2.45208400	0.02741400	2.95330300
H	1.49557100	0.48047000	3.23779300
H	2.69531800	-0.74106100	3.69675500
H	3.22384500	0.79932800	3.01600000
C	1.34390800	-3.27518600	-0.84777700
H	2.02236000	-4.11212800	-0.63396300

H	0.34114500	-3.56716200	-0.52483800
H	1.31409500	-3.13941700	-1.93183600
C	3.39431900	-1.10245400	-2.01665100
H	4.32715900	-1.68153500	-1.97557000
H	2.74757600	-1.56900000	-2.76453100
H	3.64150700	-0.09980500	-2.37676400
C	4.18735200	0.86799100	0.32382400
H	5.16864300	0.37530100	0.35303300
H	4.13757700	1.44220600	-0.60626400
H	4.15453600	1.57840000	1.15302700
C	-0.73413000	3.16388200	-0.15046500
H	-1.19058700	3.87890300	0.54912800
H	-0.26521700	3.73604500	-0.95649000
H	-1.51933400	2.53649600	-0.56767000
C	1.50733600	3.12830100	1.06038900
H	2.05948800	3.54424500	0.21189600
H	1.15970600	3.97489000	1.67103500
H	2.17386300	2.52162300	1.67227400

TS_{B5-6}

E= -938.0989685

W	-0.90614300	-0.14777500	-0.2381940
C	-2.49527300	1.61362400	-0.4129590
C	-3.20857100	0.39068200	-0.2115310
C	-2.92260100	-0.09076900	1.1205810
C	-2.00109100	0.81835600	1.7179960
C	-1.72003400	1.87051900	0.7690790
Si	1.64993700	0.82766000	0.2448340
C	-0.02212900	0.45504400	-1.8541500
O	0.39090700	0.88515100	-2.8685600
C	-1.28538500	-1.62685500	-1.4772860
O	-1.53971500	-2.51517500	-2.1879350
O	0.78755000	-0.71463200	1.0118540
C	0.25549900	-1.91057600	0.5452670
C	3.45727400	0.23657900	0.0903760
H	1.48745900	1.46235300	1.5729970
H	1.67706100	2.00337300	-0.6902100
C	1.14220500	-2.74942800	-0.3507930
H	1.97670000	-3.17514500	0.2216480
H	0.56619200	-3.57983200	-0.7711570
H	1.54169600	-2.17182900	-1.1858970
C	-0.37780300	-2.69967500	1.6782020
H	-1.08701900	-3.43585400	1.2853370
H	0.39749400	-3.24490000	2.2373780
H	-0.90096500	-2.04711400	2.3789810
C	-1.46179200	0.77284500	3.1219230
C	-3.63658800	-1.23578600	1.7869220
C	-4.24604900	-0.18880000	-1.1365950
C	-2.62553400	2.54501800	-1.5868840
C	-0.99060000	3.15278100	1.0657190
Si	4.06698900	-0.74316900	1.5894730
Si	3.97348200	-0.63496500	-1.5144850
Si	4.40675100	1.89631600	0.0637310
H	-1.79808700	1.64888900	3.6908040
H	-0.36644200	0.76768800	3.1370490
H	-1.80606400	-0.11580200	3.6575430
H	-3.10668900	-1.59118400	2.6736730
H	-4.63935600	-0.92295100	2.1093700

H	-3.76248500	-2.08908900	1.1135360
H	-4.30909800	-1.27698100	-1.0469020
H	-5.23798600	0.22109700	-0.9029610
H	-4.02950800	0.04374300	-2.1828300
H	-2.96967800	2.02098300	-2.4824240
H	-3.35268300	3.33844300	-1.3655830
H	-1.67363900	3.02401300	-1.8321560
H	-0.45323900	3.53031700	0.1905990
H	-1.70230100	3.93026700	1.3773930
H	-0.26296200	3.02768200	1.8709430
H	5.49841900	-1.09520200	1.4206790
H	3.32591400	-2.00782800	1.7914330
H	3.94019900	0.06842900	2.8249950
H	3.99554300	-2.10702300	-1.3497310
H	5.35257000	-0.22701500	-1.8816740
H	3.07199700	-0.29168900	-2.6357140
H	4.38702100	2.50793300	-1.2837900
H	5.82015500	1.65311500	0.4417200
H	3.83503600	2.86056100	1.0334580

6B

E= -938.1376733

C	3.11391700	0.77798400	0.7605180
C	3.22063800	0.54025300	-0.6535070
C	2.25185700	1.36691200	-1.3258630
C	1.51238500	2.06842900	-0.3314880
C	2.02527000	1.70010200	0.9624240
W	1.17562100	-0.33953500	0.1108240
C	-0.34203800	-1.08942500	-1.2873250
O	-1.00343700	-0.19618600	-0.2980050
Si	-2.28069300	-0.40252800	0.8161420
C	1.91816400	-2.13808600	-0.0067020
O	2.40366200	-3.20079600	-0.0893980
C	0.84414500	-1.05582100	1.8928740
O	0.72676700	-1.45133000	2.9927930
H	-1.90771400	0.47572900	1.9434020
H	-2.36236600	-1.80844500	1.2561230
C	-3.94082600	0.17154600	0.1323040
Si	-5.03644100	0.50707000	1.6541590
H	-4.71910500	1.82949200	2.2416180
H	-6.46524000	0.48743900	1.2655930
H	-4.81517000	-0.53149500	2.6885030
Si	-3.77721900	1.79058600	-0.8393960
H	-2.85609900	2.72287400	-0.1502740
H	-3.27316800	1.54479000	-2.2097430
H	-5.10356200	2.44483600	-0.9453730
Si	-4.80974700	-1.12826600	-0.9395280
H	-3.94370000	-1.57023300	-2.0556420
H	-5.17387700	-2.31215400	-0.1259500
H	-6.04759900	-0.55549300	-1.5185640
C	4.07262100	0.29911500	1.8176870
H	4.54932800	-0.64216100	1.5297910
H	4.86968800	1.03761900	1.9844630
H	3.56982000	0.13080700	2.7743290
C	4.31343900	-0.23707400	-1.3387840
H	5.18273000	0.40726900	-1.5308220
H	4.65261000	-1.08032400	-0.7315180
H	3.98043300	-0.63860700	-2.3006500

C	2.19523400	1.57913600	-2.8132160
H	3.02723900	2.22195600	-3.1335120
H	2.27866800	0.64002400	-3.3685170
H	1.26988400	2.07054900	-3.1251460
C	0.44099400	3.09352400	-0.5795030
H	0.87586900	4.10066600	-0.6436970
H	-0.09621900	2.90849200	-1.5144140
H	-0.29725900	3.10957400	0.2274320
C	1.64490100	2.33632200	2.2737110
H	2.23280500	3.24788600	2.4520710
H	0.58750300	2.61737600	2.2976700
H	1.82178900	1.65879700	3.1134650
C	-0.53354600	-0.48997300	-2.6687120
H	0.16788600	-0.95469700	-3.3710900
H	-1.55095900	-0.66772700	-3.0511500
H	-0.35369600	0.58640500	-2.6712180
C	-0.83896600	-2.52264000	-1.2273810
H	-1.85764900	-2.63197300	-1.6316280
H	-0.17843200	-3.14133700	-1.8452980
H	-0.80809900	-2.93376400	-0.2158440

TS_{B6-7}

E= -938.1055708

C	-2.94306300	1.00348400	-0.41358600
C	-3.01107300	0.21888800	0.80083000
C	-2.08023900	0.78258400	1.74658000
C	-1.44496500	1.89687100	1.11654700
C	-1.95295900	2.02595700	-0.21250300
W	-0.98293900	-0.20158700	-0.23282000
C	-1.83079800	-1.65454300	-1.19733700
O	-2.43505100	-2.47295000	-1.77571200
C	-0.39986600	0.07843500	-2.08383000
O	-0.12888100	0.28664500	-3.20300900
Si	2.03236100	0.02551000	0.80812800
O	1.46047600	-1.48980100	0.46808600
C	0.08044000	-1.96201500	0.74874900
H	1.00897700	0.98123700	0.25130400
H	2.13804400	0.33176500	2.25912200
C	3.68847400	0.25839900	-0.02652600
Si	3.90278000	2.07768200	-0.50802700
H	3.42256700	2.96358700	0.58199800
H	5.33249200	2.38179900	-0.74934000
H	3.13308900	2.39371300	-1.73376300
Si	3.82750700	-0.82533500	-1.58706200
H	4.08178400	-2.23637800	-1.22451100
H	2.61409000	-0.72419100	-2.42196900
H	4.98333900	-0.33822400	-2.38063300
Si	5.06700200	-0.22128600	1.18779100
H	6.33957300	-0.42828100	0.45761600
H	5.27342500	0.85191200	2.19029500
H	4.72394900	-1.47107400	1.90475000
C	-0.48722600	2.84450200	1.78155000
H	0.10970200	2.35050800	2.55358300
H	0.20092300	3.30226700	1.06513100
H	-1.04089700	3.65995700	2.26724700
C	-1.62777700	3.13505300	-1.17708400
H	-2.29478400	3.99409600	-1.02047200
H	-0.60000200	3.49036500	-1.05694300

H	-1.74244000	2.81340000	-2.21554600
C	-3.89537400	0.91427200	-1.57651900
H	-4.78996000	1.52545500	-1.39299300
H	-3.43368700	1.27092000	-2.50189300
H	-4.22458500	-0.11344400	-1.75247800
C	-4.04715800	-0.82678300	1.11565400
H	-4.94303300	-0.36144100	1.55002100
H	-4.35614200	-1.37171400	0.21985700
H	-3.67282300	-1.56133800	1.83497200
C	-2.02584000	0.46608800	3.21610100
H	-2.75674900	1.08189300	3.75960300
H	-2.26437800	-0.57975500	3.42139400
H	-1.04267700	0.67384500	3.64858300
C	0.04502900	-3.35355600	0.11942800
H	0.26774100	-3.31496300	-0.95000400
H	0.78814900	-4.00699000	0.60062000
H	-0.94147200	-3.81230600	0.24666300
C	-0.07089700	-2.11327000	2.26338900
H	-1.07920100	-2.47032200	2.50347300
H	0.64676200	-2.85173000	2.65287700
H	0.08803500	-1.17649600	2.80492000

7B

E= -938.1149557

C	3.01811000	-0.81976800	-0.0671820
C	2.72889100	-0.11629000	1.1657550
C	1.65764600	-0.81259700	1.8277270
C	1.29946000	-1.93794500	1.0076370
C	2.13261300	-1.94398200	-0.1495440
W	0.91538300	0.14683600	-0.2906480
C	1.78840800	1.68619700	-1.1255290
O	2.42127000	2.54590600	-1.5983770
C	0.65774900	-0.22382500	-2.2021060
O	0.57674400	-0.48907700	-3.3376490
Si	-1.80538900	0.05267300	0.6487070
O	-1.59118900	1.61755600	1.0783680
C	-0.25188100	2.05634000	0.5710080
H	-0.88976400	-0.29014000	-0.5855970
H	-1.60099100	-0.92108600	1.7449770
C	-3.51564700	-0.29345400	-0.0552450
Si	-3.47861600	-1.84351200	-1.1433370
H	-2.59323100	-2.87350100	-0.5444790
H	-4.83742400	-2.42187200	-1.2652780
H	-2.97080900	-1.52538500	-2.4972680
Si	-4.17636700	1.16689900	-1.0743480
H	-4.60253900	2.27950800	-0.1972630
H	-3.15871600	1.64955600	-2.0320580
H	-5.35642000	0.70944400	-1.8485580
Si	-4.68543800	-0.61038100	1.4077690
H	-6.09492800	-0.48231800	0.9688900
H	-4.48667500	-1.97795500	1.9462240
H	-4.44043500	0.36046500	2.4992120
C	0.35389000	-3.04030600	1.3967970
H	-0.39533000	-2.70429400	2.1165730
H	-0.17127300	-3.45853300	0.5327830
H	0.91505700	-3.86025900	1.8664640
C	2.16821700	-3.01799000	-1.2026070
H	2.89107100	-3.79866100	-0.9283440

H	1.19369800	-3.49927700	-1.3241580
H	2.46340700	-2.62220000	-2.1778010
C	4.19651600	-0.56232400	-0.9689910
H	5.09062500	-1.07667700	-0.5905470
H	4.01095600	-0.92460400	-1.9842430
H	4.43179400	0.50304500	-1.0397730
C	3.59374800	0.96341900	1.7586820
H	4.45321500	0.51677600	2.2779870
H	3.98653300	1.63467800	0.9899760
H	3.04961900	1.57265200	2.4833430
C	1.19553500	-0.60907100	3.2453810
H	1.63656100	-1.37478700	3.8987420
H	1.50144800	0.36345000	3.6362580
H	0.10836400	-0.68215000	3.3461280
C	-0.60235300	3.14856400	-0.4437820
H	-1.08373800	2.73941500	-1.3368450
H	-1.29509700	3.86529500	0.0214120
H	0.28601600	3.69939200	-0.7655140
C	0.44167900	2.69300900	1.7719380
H	1.42759900	3.07821900	1.4914550
H	-0.15956700	3.53488300	2.1478580
H	0.56388400	1.98664600	2.5959450

TS_{B7-8}

E= -938.1130403

C	2.92088800	-0.89329000	-0.0626290
C	2.74102000	0.00320700	1.0573330
C	1.68756800	-0.52997700	1.8756770
C	1.22572800	-1.74945800	1.2684150
C	1.98861600	-1.97402700	0.0844490
W	0.80926300	0.10933900	-0.3147660
C	1.65074700	1.54681300	-1.3614730
O	2.29551500	2.33735500	-1.9228400
C	0.49376200	-0.67323200	-2.1020790
O	0.35241600	-1.15610100	-3.1511730
Si	-1.61097700	0.22000500	0.6827310
O	-1.53853000	1.84948600	0.9869080
C	-0.24753500	2.22808900	0.3886740
H	-0.86517400	0.21585800	-0.9113810
H	-1.52065600	-0.55828300	1.9544560
C	-3.30438500	-0.29879600	-0.0072940
Si	-3.19461900	-1.96642100	-0.8912850
H	-2.30480900	-2.89942300	-0.1558330
H	-4.53326600	-2.59820900	-0.9775460
H	-2.66035200	-1.81297800	-2.2641880
Si	-4.02467300	0.97535600	-1.2105540
H	-4.53273200	2.16879700	-0.4976200
H	-3.01548200	1.39497800	-2.2083890
H	-5.15945100	0.36513700	-1.9472180
Si	-4.48007200	-0.48621000	1.4706380
H	-5.88953700	-0.50794600	1.0087670
H	-4.21615300	-1.75570100	2.1916230
H	-4.32028600	0.63483800	2.4252180
C	0.30171600	-2.74542400	1.9097710
H	-0.41214800	-2.26702100	2.5832020
H	-0.26625100	-3.31647900	1.1700470
H	0.88663100	-3.46209100	2.5035370
C	1.92898400	-3.21227200	-0.7688490

H	2.61138900	-3.97651900	-0.3725830
H	0.92411400	-3.64342000	-0.7867400
H	2.22216200	-3.01410500	-1.8029730
C	4.04403400	-0.82577600	-1.0637840
H	4.94494700	-1.30923100	-0.6619090
H	3.78591600	-1.33494700	-1.9968090
H	4.30688700	0.20570100	-1.3140000
C	3.67098700	1.13354400	1.4078350
H	4.57374800	0.74537400	1.8991330
H	3.99101400	1.68546500	0.5190980
H	3.20506800	1.84858400	2.0890070
C	1.29935100	-0.08017300	3.2579590
H	1.61419600	-0.83132500	3.9947490
H	1.78254100	0.86074900	3.5287190
H	0.21759000	0.04982700	3.3673690
C	-0.60186900	3.20782200	-0.7314400
H	-1.12720500	2.71778900	-1.5556100
H	-1.26624400	3.98017800	-0.3173560
H	0.28168900	3.70726700	-1.1382540
C	0.55085700	2.95006400	1.4668400
H	1.51783000	3.29147200	1.0822150
H	-0.01335900	3.83478700	1.7997830
H	0.71869200	2.32299000	2.3431540

8B

E= -938.115446

C	2.95369100	-0.82647300	-0.01973400
C	2.74427200	0.14594500	1.02873800
C	1.69628200	-0.34509700	1.87669100
C	1.25594300	-1.61268300	1.35133700
C	2.04950400	-1.91252100	0.20027100
W	0.76556900	0.09986800	-0.33072900
C	1.64801400	1.29471000	-1.66846600
O	2.25524900	1.93915300	-2.41484000
C	0.23792200	-1.09068800	-1.82678400
O	-0.03249400	-1.78724800	-2.71446500
Si	-1.55883300	0.26472600	0.72342100
O	-1.52408600	1.94188100	0.81259100
C	-0.21701400	2.26062600	0.25438600
H	-0.55943500	0.59134000	-1.32431200
H	-1.60803900	-0.28208900	2.12154100
C	-3.25026000	-0.28190300	0.02195900
Si	-3.24240200	-2.09540000	-0.49698400
H	-2.42696400	-2.91302300	0.43626500
H	-4.61798100	-2.65162600	-0.48449500
H	-2.69174400	-2.27470900	-1.85952700
Si	-3.81609700	0.77787100	-1.43777200
H	-4.30058500	2.10536200	-0.99632400
H	-2.72764700	0.97130400	-2.42473300
H	-4.93482100	0.09947300	-2.14019700
Si	-4.50611200	-0.08746800	1.43177500
H	-5.89234900	-0.09666700	0.90004500
H	-4.38732800	-1.20967900	2.39552900
H	-4.30010200	1.18293000	2.16317000
C	1.32035100	0.15698500	3.24483400
H	0.24059300	0.28990200	3.36168600
H	1.64303700	-0.57299200	3.99940100
H	1.80949200	1.10366700	3.48159800

C	0.35630100	-2.57843600	2.06802800
H	0.94009800	-3.15502000	2.80010300
H	-0.44120000	-2.06676600	2.61065300
H	-0.10809400	-3.29094000	1.38165100
C	2.04465800	-3.21800000	-0.54792700
H	2.72197800	-3.92809900	-0.05502500
H	1.05117300	-3.67299700	-0.57278000
H	2.38381000	-3.10212800	-1.58045300
C	4.08226400	-0.80736100	-1.01572700
H	4.97726100	-1.27408900	-0.58238800
H	3.83100600	-1.35784500	-1.92677000
H	4.35340800	0.21043800	-1.30820500
C	3.66506000	1.30339500	1.30853800
H	4.58301500	0.94352900	1.79314400
H	3.96177000	1.82468200	0.39328100
H	3.20762300	2.03786300	1.97306100
C	-0.47116400	3.21837000	-0.91267400
H	-1.07764600	4.05803100	-0.54321900
H	0.46001400	3.62946800	-1.31638700
H	-1.02183000	2.74381800	-1.72921300
C	0.57446400	3.00195400	1.32835000
H	1.55935800	3.31002600	0.96178900
H	0.01872500	3.90985900	1.60924700
H	0.69839800	2.40728700	2.23251400

TS_{B8-9}

E= -938.1006977

C	2.96005800	-0.90562600	-0.1122840
C	2.82140500	0.00495700	1.0062450
C	1.77514700	-0.49266500	1.8476570
C	1.26810000	-1.70471400	1.2497240
C	2.00818300	-1.95846700	0.0522720
W	0.82880100	0.11730000	-0.3025270
C	1.74587800	1.33873600	-1.5914000
O	2.31660100	2.03637100	-2.3223500
C	0.04156900	-0.74745500	-1.8839730
O	-0.34031500	-1.32721100	-2.8195490
Si	-1.54314800	0.18163600	0.7257790
O	-1.59112200	1.88639100	0.8584590
C	-0.36101200	2.36460400	0.3569170
H	-0.24132300	1.32973900	-0.8891700
H	-1.59717200	-0.35696800	2.1258150
C	-3.24990000	-0.32873900	0.0260000
Si	-3.30821400	-2.13486300	-0.5205820
H	-2.53622900	-2.99790800	0.4089330
H	-4.70723300	-2.62962400	-0.5160530
H	-2.76037300	-2.32438800	-1.8815410
Si	-3.77989600	0.77849800	-1.4127650
H	-4.33605500	2.06473100	-0.9320930
H	-2.64949800	1.06719000	-2.3254030
H	-4.83746200	0.10313000	-2.2061770
Si	-4.50115100	-0.12156300	1.4383250
H	-5.88866300	-0.10427300	0.9097510
H	-4.39887100	-1.25221400	2.3941530
H	-4.27336200	1.14023100	2.1780680
C	1.44786600	-0.04389100	3.2460460
H	0.36954500	0.02802300	3.4184070
H	1.84761300	-0.76623600	3.9710880

H	1.89548100	0.92524900	3.4779290
C	0.33599900	-2.67633500	1.9165380
H	0.91459500	-3.37255800	2.5403520
H	-0.38534500	-2.17347000	2.5641910
H	-0.22340600	-3.27110200	1.1897850
C	1.89434900	-3.18760800	-0.8077590
H	2.56112800	-3.97595400	-0.4335370
H	0.87724700	-3.58859200	-0.8100670
H	2.17103200	-2.98548200	-1.8459600
C	4.05689300	-0.87292200	-1.1432980
H	4.93084500	-1.43305400	-0.7841440
H	3.73873200	-1.32550900	-2.0867370
H	4.38819400	0.14591400	-1.3609720
C	3.77339200	1.12558600	1.3282460
H	4.65370200	0.73842200	1.8598360
H	4.13142500	1.62849200	0.4250070
H	3.31177300	1.88263700	1.9666360
C	-0.61692100	3.44374200	-0.6978160
H	-1.14272000	4.27806100	-0.2135260
H	0.32032100	3.82270300	-1.1179240
H	-1.24618700	3.07852300	-1.5142930
C	0.50571500	2.93085000	1.4771860
H	1.49339800	3.23037500	1.1149230
H	0.00370800	3.82870400	1.8729730
H	0.61594100	2.22839500	2.3018480

9B

E= -938.1373111

C	2.79866500	-1.22553600	-0.2389210
C	3.14318300	-0.00829400	0.4574190
C	2.38079900	0.03412400	1.6729400
C	1.55723700	-1.12974000	1.7349820
C	1.79585700	-1.90585900	0.5409790
W	0.90005500	0.06680900	-0.2748710
C	1.39860500	1.03196700	-1.9323450
O	1.73233000	1.56226200	-2.9152660
C	-0.09635500	-0.90009500	-1.6388870
O	-0.60583900	-1.56033700	-2.4608320
Si	-1.53323900	0.24318900	0.6697830
O	-1.77509000	1.93344400	0.5004240
C	-0.62404300	2.70926300	0.2683670
H	0.29010100	2.02680000	0.0965230
H	-1.58337300	-0.03865800	2.1449830
C	-3.18814700	-0.49494300	0.0685220
Si	-3.14408500	-2.38182000	-0.0262430
H	-2.23684100	-2.93059200	1.0170770
H	-4.49295500	-2.94194800	0.2385020
H	-2.69053600	-2.89061500	-1.3365870
Si	-3.74142500	0.26723100	-1.5759450
H	-4.51187700	1.51211800	-1.3413780
H	-2.60074600	0.59172700	-2.4591740
H	-4.63233200	-0.67338100	-2.3008290
Si	-4.48998100	-0.05958900	1.3817080
H	-5.85659100	-0.28095900	0.8454630
H	-4.33395100	-0.92503900	2.5772240
H	-4.38466200	1.35314200	1.8088590
C	2.49555400	1.08196100	2.7448580
H	1.56447300	1.18776400	3.3091260

H	3.28398400	0.81218300	3.4611720
H	2.75358900	2.06192700	2.3327400
C	0.74460400	-1.57299000	2.9172090
H	1.37685000	-2.14547500	3.6104290
H	0.32581200	-0.72786000	3.4693980
H	-0.08845800	-2.21577000	2.6220140
C	1.26451300	-3.28908500	0.2813630
H	1.89745100	-4.04236100	0.7702080
H	0.24750700	-3.40676000	0.6650040
H	1.23942100	-3.51651300	-0.7873680
C	3.50591300	-1.77859400	-1.4467380
H	4.39489300	-2.34947000	-1.1443580
H	2.85997100	-2.44951100	-2.0192110
H	3.83610300	-0.98417600	-2.1223340
C	4.25482300	0.93580300	0.0817590
H	5.20844500	0.59946600	0.5116600
H	4.38499400	0.99690400	-1.0021150
H	4.06867200	1.94954900	0.4489120
C	-0.79281300	3.54889800	-0.9934610
H	-1.63223600	4.23808900	-0.8451480
H	0.10777900	4.13457100	-1.2073090
H	-1.01703800	2.91422800	-1.8539960
C	-0.27946400	3.54327000	1.5013550
H	0.62759100	4.13748100	1.3436930
H	-1.11266300	4.22467000	1.7076650
H	-0.14001500	2.90459500	2.3783820

TS_{B1-10}

E= -938.1185262

C	-3.30268600	-0.25215400	-0.2852690
C	-2.70623700	-1.29207700	0.5134280
C	-2.15860400	-0.68671000	1.6992180
C	-2.41002600	0.72435500	1.6279310
C	-3.10722200	0.99491500	0.4078250
W	-0.98288500	0.11255800	-0.2310870
C	-0.45837700	-1.04706700	-1.7295660
O	-0.22100000	-1.74672500	-2.6369740
C	-0.71651800	1.47718900	-1.6328380
O	-0.60263000	2.29767200	-2.4585060
Si	1.16703500	-0.39659000	0.6744940
O	2.68491400	1.73518700	0.7382150
C	2.99251500	2.83249000	0.2895830
H	0.24982900	1.17014300	0.4964530
H	1.40395300	-0.29100500	2.1463350
C	2.72308800	-1.33099300	0.0787780
Si	4.10088200	-1.31353300	1.3849060
H	3.70220100	-2.13232800	2.5568190
H	5.33583600	-1.91653200	0.8225690
H	4.42746900	0.04844100	1.8532670
Si	2.18367300	-3.15242000	-0.0808420
H	1.29207300	-3.52640400	1.0466740
H	1.48253800	-3.42648800	-1.3497550
H	3.38312700	-4.02181000	-0.0001220
Si	3.42094900	-0.74736700	-1.5791850
H	4.07704100	-1.87439500	-2.2870860
H	2.38104000	-0.18191400	-2.4626810
H	4.45952800	0.29162300	-1.3617370
C	-2.10150900	1.72257000	2.7107090

H	-2.91711800	1.75753200	3.4466770
H	-1.18397000	1.46675000	3.2482780
H	-1.97928300	2.73152800	2.3070010
C	-3.67607900	2.32505200	-0.0079630
H	-4.69690600	2.44647100	0.3802290
H	-3.07744400	3.15850100	0.3706260
H	-3.72373400	2.42148900	-1.0961610
C	-4.14980600	-0.45852300	-1.5124480
H	-5.19883800	-0.63871500	-1.2366310
H	-4.12810600	0.41449100	-2.1712420
H	-3.81095200	-1.31829100	-2.0974280
C	-2.81549400	-2.77054600	0.2500670
H	-3.76312100	-3.16438500	0.6438250
H	-2.78311400	-2.99524300	-0.8198820
H	-2.00293100	-3.32617200	0.7266200
C	-1.61449400	-1.41916200	2.8954310
H	-2.42169200	-1.65077900	3.6048500
H	-1.14433500	-2.36415900	2.6100700
H	-0.86644500	-0.82761200	3.4310960
C	2.66355700	3.25459800	-1.1238870
H	2.49943100	4.33466400	-1.1944370
H	3.52380000	3.01285000	-1.7634760
H	1.79352600	2.71808000	-1.5047870
C	3.75517800	3.82016100	1.1466680
H	4.63424200	4.19785100	0.6103700
H	3.11701600	4.68788900	1.3595510
H	4.05928200	3.35373200	2.0854350

10B

E= -938.1240627

C	-3.13916100	-0.59905600	-0.4992260
C	-2.32917500	-1.67932800	0.0040600
C	-1.94782000	-1.36060000	1.3534970
C	-2.51655800	-0.08548000	1.6803120
C	-3.24710300	0.38749000	0.5429960
W	-0.98001800	0.25736700	-0.1558990
C	-0.19539500	-0.21054100	-1.9039690
O	0.20634200	-0.49385500	-2.9676280
C	-1.08812200	2.01387100	-1.0155970
O	-1.21169000	3.07307500	-1.5083040
Si	1.30268800	-0.12852400	0.6610390
O	2.36221500	1.53393100	1.0327480
C	2.58208900	2.64061500	0.5158640
H	-0.21971700	1.33116900	0.9873290
H	1.43661600	-0.45431200	2.1159670
C	2.83240900	-1.11588100	-0.0238940
Si	4.07821400	-1.39152000	1.3802370
H	3.55593700	-2.36949700	2.3646280
H	5.35759800	-1.92927000	0.8493760
H	4.38899700	-0.13054200	2.0922620
Si	2.21989100	-2.83282100	-0.5506020
H	1.28207500	-3.38984500	0.4538120
H	1.54940200	-2.81237100	-1.8678480
H	3.37357200	-3.76380800	-0.6297690
Si	3.74714400	-0.35435900	-1.4858930
H	4.63880900	-1.34853600	-2.1306770
H	2.83443300	0.18389600	-2.5160510
H	4.61144000	0.76787700	-1.0267300

C	-2.10431400	-2.99651100	-0.6899830
H	-1.19411700	-3.48945800	-0.3387300
H	-2.94503700	-3.67968800	-0.5028100
H	-2.01442800	-2.87315700	-1.7729210
C	-1.26678500	-2.27984700	2.3302050
H	-2.01115900	-2.84139400	2.9126140
H	-0.62677900	-3.00798100	1.8254170
H	-0.64181800	-1.72865500	3.0390840
C	-2.46807600	0.57237300	3.0326300
H	-3.29759700	0.22005500	3.6622010
H	-1.53624400	0.34744000	3.5589820
H	-2.55093600	1.65998600	2.9556860
C	-4.10780300	1.62155800	0.5000020
H	-5.12830500	1.39462800	0.8388880
H	-3.71263200	2.41143500	1.1454520
H	-4.17863200	2.02957600	-0.5121290
C	-3.89211300	-0.58972200	-1.8028670
H	-4.88761900	-1.04184900	-1.6853220
H	-4.03242400	0.42845500	-2.1774500
H	-3.36351500	-1.15252300	-2.5776280
C	3.37348400	3.63722000	1.3142470
H	4.35089500	3.78092500	0.8350660
H	2.87055400	4.61149300	1.3064710
H	3.51751300	3.28830200	2.3377210
C	2.09938700	3.04596300	-0.8401930
H	1.12621800	3.54229700	-0.7259660
H	2.78873300	3.76366700	-1.2947640
H	1.94379400	2.18972900	-1.4956320

TS_{B10-9}

E= -938.1082657

C	-2.92931800	-1.14319100	-0.1192540
C	-2.07748800	-1.64451500	0.9296030
C	-1.84417200	-0.57752900	1.8649530
C	-2.53241000	0.58158000	1.3882990
C	-3.19757400	0.24394300	0.1612910
W	-0.89860900	-0.01788700	-0.3064160
C	0.04543300	-1.40563700	-1.3280650
O	0.54618400	-2.27462300	-1.9346260
C	-1.03989800	0.73357300	-2.1189850
O	-1.16980200	1.20162500	-3.1840760
Si	1.43006800	0.13400700	0.6890770
O	1.76365200	1.96871000	0.8650740
C	1.13663100	2.80530300	0.1284960
H	-0.34262800	1.66632800	-0.1310810
H	1.53310200	-0.13420200	2.1603310
C	3.14932100	-0.54415400	0.1384480
Si	4.51857000	0.54062300	0.8751170
H	5.81821700	-0.17618700	0.8442880
H	4.68914800	1.79163000	0.0954260
H	4.23072600	0.90178100	2.2828870
Si	3.30796000	-2.24929100	0.9573470
H	4.38185100	-3.04504000	0.3173920
H	3.63712900	-2.11274100	2.3974750
H	2.04205400	-3.01468400	0.8508150
Si	3.50385700	-0.72345300	-1.7198700
H	2.67017400	0.18720300	-2.5373850
H	4.92212400	-0.36138900	-1.9781120

H	3.30992000	-2.10444800	-2.2056800
C	-1.66565600	-3.08049500	1.1176590
H	-0.70903900	-3.16069500	1.6420520
H	-2.41625100	-3.62585300	1.7067550
H	-1.55676800	-3.59660100	0.1599420
C	-3.57749400	-1.96586300	-1.2007470
H	-2.93741400	-2.79505000	-1.5153220
H	-4.52739400	-2.39369900	-0.8495310
H	-3.79334100	-1.36499200	-2.0888830
C	-4.15749700	1.12620200	-0.5920450
H	-4.19085500	0.86836100	-1.6541410
H	-5.17675200	1.02559000	-0.1934060
H	-3.87742100	2.18154700	-0.5206200
C	-2.65757600	1.88852900	2.1207390
H	-2.78903000	2.72837300	1.4326590
H	-3.52986400	1.87220300	2.7893640
H	-1.77823100	2.09201300	2.7393480
C	-1.15700400	-0.70709400	3.1946710
H	-0.68442700	0.22978600	3.5034940
H	-1.87987200	-0.98852500	3.9733790
H	-0.37685900	-1.47253100	3.1763720
C	0.44711100	3.94180100	0.8268700
H	1.20512800	4.71126300	1.0380000
H	-0.32486100	4.39048200	0.1979230
H	0.02615400	3.61029600	1.7770440
C	1.46559600	2.96737400	-1.3261140
H	0.61141600	3.33882500	-1.8956580
H	2.26707000	3.72229800	-1.3816250
H	1.82920400	2.04119800	-1.7679950

TS_{B4-9}

E= -938.1032815

W	-0.82604800	-0.01941300	-0.2903150
C	-2.62893000	0.58130300	1.3350450
C	-3.16937300	0.11018800	0.0913760
C	-2.76939100	-1.26475100	-0.0682640
C	-1.92087500	-1.60196300	1.0460780
C	-1.83388000	-0.44698000	1.9114720
Si	1.50433000	0.15473700	0.6877970
H	1.61928300	0.13220200	2.1873280
O	-0.51663600	2.04985200	-0.0238280
C	0.61471700	2.72448200	-0.0489060
C	0.05709800	-1.59650800	-1.0784060
O	0.53126600	-2.56132500	-1.5403660
C	-0.91782600	0.36657700	-2.2251070
O	-1.05336400	0.55682500	-3.3688740
H	1.51780800	1.87303100	0.4962610
C	3.26643900	-0.40192600	0.1896020
C	1.26575400	2.95533500	-1.4086230
H	0.65632200	3.68428500	-1.9589810
H	2.27931100	3.35631900	-1.3087210
H	1.29647300	2.02934800	-1.9855530
C	0.64378000	3.93367600	0.8792820
H	1.65620800	4.33732700	0.9791170
H	0.00109300	4.71997200	0.4622820
H	0.26119500	3.66500700	1.8675830
Si	4.52582200	0.83545500	0.8790120
Si	3.57436500	-2.06591600	1.0527530

Si	3.59577500	-0.59724200	-1.6704940
C	-4.15460200	0.86187500	-0.7640350
C	-3.30321700	-2.22186500	-1.0998920
C	-1.43260000	-2.98255500	1.3962900
C	-1.19191700	-0.41983300	3.2708170
C	-2.86402000	1.95010600	1.8984320
H	-5.17718900	0.75059900	-0.3763480
H	-3.92377900	1.93098500	-0.7908450
H	-4.15147200	0.49848600	-1.7953780
H	-4.23617600	-2.68533500	-0.7498550
H	-3.51886800	-1.71376500	-2.0442750
H	-2.59310300	-3.02539100	-1.3135160
H	-2.18128600	-3.50846500	2.0046960
H	-1.24418400	-3.58799000	0.5060450
H	-0.50328000	-2.94846400	1.9724350
H	-1.90304600	-0.74793300	4.0418610
H	-0.32447300	-1.08357900	3.3237920
H	-0.84892800	0.58294000	3.5411500
H	-2.51678100	2.02278400	2.9326520
H	-2.33153300	2.70379900	1.3073440
H	-3.93265900	2.19402900	1.8849170
H	4.17684000	1.24365700	2.2598570
H	4.57041400	2.05296300	0.0319090
H	5.88717200	0.24640900	0.8978570
H	5.06213000	-0.56235300	-1.9002210
H	2.99618600	0.50979800	-2.4468850
H	4.69247200	-2.78743800	0.3988310
H	3.08651600	-1.88256900	-2.1900350
H	3.92335000	-1.85962300	2.4793310
H	2.37041100	-2.92871600	0.9952910

TS_{B11-2}

E= -938.0910871

W	0.91156300	-0.14757400	-0.2930220
C	2.54661900	1.30706300	0.6287620
C	1.85825300	0.73993400	1.7546500
C	2.09693800	-0.67390700	1.7490690
C	2.93206000	-0.98613400	0.6267980
C	3.21516800	0.23997600	-0.0728930
C	0.96705800	-1.53598400	-1.6850760
O	1.09308400	-2.37963300	-2.4821410
Si	-1.47296000	0.32649900	0.0169310
O	-2.32089100	1.64461800	-0.9935770
C	-2.31464600	2.56069600	-0.0554710
C	-2.85897200	-0.98817400	0.1699400
C	0.55069200	1.01699300	-1.8490880
O	0.39049200	1.73621700	-2.7565390
H	-0.15728100	-1.38544500	0.2678050
H	-1.79677100	1.38494200	1.1903970
Si	-2.47056500	-2.06730400	1.6914070
H	-3.72572400	-2.67205300	2.2042780
H	-1.53025700	-3.16963600	1.3978170
H	-1.90866600	-1.24057700	2.7876980
Si	-2.77881100	-2.04846800	-1.4218670
H	-4.05407700	-2.79881400	-1.5514030
H	-2.64191400	-1.18179400	-2.6132750
H	-1.67522900	-3.02654700	-1.3861090
Si	-4.65496300	-0.42462500	0.3518850

H	-5.55239000	-1.59870400	0.4340810
H	-4.84731800	0.35803300	1.5993140
H	-5.10389500	0.40602200	-0.7892030
C	2.74246200	2.77412200	0.3500610
H	3.69825500	3.11919800	0.7685430
H	2.75714700	2.98940100	-0.7225870
H	1.95438800	3.38347700	0.8013740
C	4.19940700	0.40684200	-1.1999510
H	3.94157400	1.25719000	-1.8379210
H	5.21368800	0.57857000	-0.8118050
H	4.23523300	-0.48114700	-1.8375110
C	3.53969900	-2.33007800	0.3266360
H	3.69982700	-2.47248300	-0.7457640
H	4.51321100	-2.43405200	0.8255430
H	2.90036200	-3.14701500	0.6729850
C	1.66742200	-1.63904100	2.8196870
H	1.53177900	-2.64849600	2.4228270
H	2.42497300	-1.69234700	3.6143380
H	0.72369800	-1.33743800	3.2821710
C	1.15897600	1.49839400	2.8494140
H	0.32463200	0.92695200	3.2659710
H	1.85330900	1.71975700	3.6724340
H	0.76013300	2.45222100	2.4933400
C	-1.13278000	3.48714700	0.0024780
H	-1.14587400	4.07888300	-0.9238040
H	-1.17359800	4.16131900	0.8616640
H	-0.19841600	2.91872600	-0.0020650
C	-3.61448200	3.07871000	0.4928210
H	-3.48808800	3.49913400	1.4940030
H	-3.93437000	3.89543300	-0.1729840
H	-4.39655400	2.32337100	0.4955010

TS_{B3-1}

E= -944.3573495

C	-2.80713400	1.13322400	-0.1132130
C	-3.06858900	-0.16274000	-0.6968570
C	-2.89041200	-1.14923100	0.3321920
C	-2.55013200	-0.46418900	1.5513080
C	-2.49380300	0.93307100	1.2761580
W	-0.81317200	-0.13501500	-0.2215940
Si	1.63598300	-0.20059300	0.9402990
Si	0.55127500	-2.37272300	1.5434860
C	-0.38085100	-1.70896400	-1.3001290
O	-0.24109200	-2.65278500	-1.9751620
C	-0.52578000	0.60044500	-2.0206830
O	-0.47713500	1.03985100	-3.0986920
H	1.69723500	0.35814800	2.3144020
H	2.09237600	-1.61076400	1.6341660
H	1.30976800	-3.49213200	0.9326210
H	0.60239400	-2.29183000	3.0282380
H	-0.84397300	-2.84549700	1.3157690
C	3.27861800	-0.29582100	-0.0659840
Si	3.38042400	0.84774900	-1.5758590
H	4.69882400	0.64907800	-2.2296590
H	2.33903700	0.53546500	-2.5760490
H	3.30678300	2.28191700	-1.2239800
Si	4.69232700	0.13960500	1.1259780
H	4.59974400	-0.65656100	2.3718790

H	6.00317400	-0.14634900	0.4926620
H	4.67865400	1.57552500	1.4930600
Si	3.66868000	-2.05478800	-0.6828660
H	3.99239300	-2.95896200	0.4450600
H	2.54380800	-2.62707600	-1.4507520
H	4.85484800	-2.00778100	-1.5705410
C	-2.50667500	-1.07228200	2.9234990
H	-1.88292200	-0.49223200	3.6086020
H	-3.52217300	-1.10231200	3.3439300
H	-2.13087900	-2.09738600	2.9071910
C	-2.37626800	1.99855900	2.3322810
H	-3.30679000	2.04804800	2.9147270
H	-1.56343400	1.79686200	3.0371480
H	-2.21515100	2.98951100	1.9013120
C	-3.11103900	2.44906100	-0.7793300
H	-4.18959100	2.65413500	-0.7358500
H	-2.60053100	3.28424000	-0.2935630
H	-2.81924500	2.45002400	-1.8335000
C	-3.66863800	-0.41109700	-2.0551400
H	-4.76493800	-0.35395300	-2.0062040
H	-3.33044000	0.32391400	-2.7905920
H	-3.40433900	-1.40172800	-2.4347680
C	-3.29446100	-2.59400000	0.2043840
H	-4.38333500	-2.68605500	0.3178420
H	-3.02576300	-3.00613500	-0.7721090
H	-2.82542000	-3.22007000	0.9653010
C	1.93882800	3.14390300	1.4700660
H	1.74482900	4.16902700	1.8076420
H	2.14169200	2.53299800	2.3522380
H	2.83336400	3.16046800	0.8418250
O	0.90909500	1.29331100	0.1791130
C	0.72188700	2.64629800	0.6896970
H	-0.13417500	2.62894500	1.3687670
C	0.41931200	3.56508100	-0.4928790
H	-0.41674100	3.19370000	-1.0887170
H	0.16567700	4.56904900	-0.1313290
H	1.29220200	3.64645800	-1.1475770

TS_{B2-1}
E= -944.400203

C	-2.68196400	0.47137100	-1.4905200
C	-3.33323000	-0.02578600	-0.3041900
C	-2.94710600	0.81919300	0.7933030
C	-2.07464600	1.84087900	0.2852900
C	-1.90667300	1.62124600	-1.1201850
W	-1.02564700	-0.34633700	-0.0272880
Si	1.38279700	0.18502200	0.2188230
Si	0.67487100	0.52121000	2.7166810
C	-0.98897100	-1.66367100	1.4441160
O	-1.07085500	-2.45423800	2.3020470
C	-1.00392800	-2.04151900	-1.0210150
O	-1.08018400	-3.02401100	-1.6455180
O	1.74297400	1.71806600	-0.3702920
C	2.86495700	2.58600900	-0.1430420
H	2.01038900	0.49062400	1.7166190
H	0.29459200	-0.21991200	-1.1877680
H	3.60944200	2.06860400	0.4760700
H	1.10056900	-0.70636100	3.4104250

H	1.33323100	1.73066100	3.2892910
H	-0.75114400	0.76940700	3.0333330
C	2.77122300	-1.09628600	-0.1285080
Si	2.82774800	-1.44429600	-2.0040250
H	4.16396300	-1.99214400	-2.3449480
H	1.80735200	-2.43291400	-2.4138500
H	2.63373800	-0.20268100	-2.7865590
Si	4.52334300	-0.57661300	0.3944480
H	4.53105600	0.01950200	1.7520190
H	5.42004300	-1.75620400	0.4118920
H	5.11172800	0.40669100	-0.5453430
Si	2.45979900	-2.77522500	0.7217770
H	2.57991700	-2.63782600	2.1923940
H	1.14855600	-3.35209000	0.3830740
H	3.51088700	-3.71960800	0.2710080
C	-3.53019600	0.75926600	2.1794220
H	-2.84665300	1.16323300	2.9304460
H	-4.45782100	1.34601200	2.2284300
H	-3.77175300	-0.26652200	2.4712800
C	-4.37704900	-1.10936900	-0.2615920
H	-4.40454800	-1.60640400	0.7121030
H	-5.37645400	-0.69257400	-0.4500900
H	-4.19232100	-1.87832000	-1.0172220
C	-2.92594800	-0.01684700	-2.8939470
H	-3.12353600	-1.09189300	-2.9198370
H	-3.79481800	0.49189700	-3.3335490
H	-2.06655400	0.17360800	-3.5427560
C	-1.15524900	2.52760800	-2.0566160
H	-0.94438500	2.03191400	-3.0079800
H	-1.74523300	3.42855400	-2.2749990
H	-0.19916000	2.83581000	-1.6275640
C	-1.58474500	3.04694300	1.0366380
H	-0.61977200	3.39126800	0.6562360
H	-2.29913300	3.87576600	0.9305290
H	-1.47916200	2.84893700	2.1068040
C	2.39427300	3.82943400	0.6120450
H	1.94411900	3.56094400	1.5729340
H	3.23829400	4.50095600	0.8072250
H	1.65153600	4.37798500	0.0210300
C	3.48871400	2.93845600	-1.4916560
H	4.35019600	3.60234800	-1.3560510
H	3.82447600	2.03898100	-2.0155730
H	2.75422000	3.44921200	-2.1247450

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C	-3.31861700	1.23699700	0.3671600
C	-2.47262400	1.18622500	1.5309900
C	-1.19863300	1.73388600	1.1715930
C	-1.23939100	2.09719000	-0.2131530
C	-2.55897300	1.81256900	-0.7097960
W	-1.58622600	-0.26193700	-0.2061140
C	-2.76615000	-1.25206600	-1.4058850
O	-3.51904800	-1.77122500	-2.1371790
C	0.79806300	-1.32860000	0.6366550
C	-0.45529900	-0.59612400	-1.7695400
O	0.22000300	-0.74697700	-2.7145310
Si	-2.63802100	-2.33983300	1.0074470

O	1.72207900	-0.33998200	0.2674650
H	-2.42519000	-2.36018000	2.4840390
H	-0.93455100	-1.42401100	0.9027180
H	-2.18534000	-3.67070500	0.5304400
H	-4.11955400	-2.32705700	0.8528080
Si	2.91739800	-0.17844900	-0.9036200
H	2.56467700	0.99464800	-1.7333400
H	3.03787600	-1.38281300	-1.7497980
C	4.57256300	0.16579800	-0.0605400
Si	4.35960100	1.29800000	1.4410160
H	3.86934400	0.54753600	2.6197900
H	5.66209700	1.91104100	1.7978950
H	3.40592000	2.39356200	1.1454300
Si	5.40122300	-1.44892700	0.4792190
H	5.94614100	-2.17374700	-0.6932920
H	6.51543700	-1.17413200	1.4175540
H	4.43093700	-2.33640100	1.1638610
Si	5.69018400	1.03643800	-1.3240760
H	7.11062500	0.91926100	-0.9188970
H	5.53507900	0.42249100	-2.6646510
H	5.34559900	2.47430300	-1.4252560
C	-0.06662100	2.04666400	2.1084820
H	0.90170100	1.76765800	1.6858890
H	-0.04001400	3.12469200	2.3193370
H	-0.18073500	1.53382800	3.0671690
C	-0.15748800	2.83931100	-0.9491740
H	-0.27451900	3.92357800	-0.8137230
H	0.83487300	2.56419000	-0.5835240
H	-0.18287600	2.63540100	-2.0230990
C	-3.09786000	2.20064100	-2.0607130
H	-3.54456000	3.20400700	-2.0237370
H	-2.31007300	2.21741200	-2.8192990
H	-3.87014600	1.50686400	-2.4043970
C	-4.79024200	0.92341900	0.3339050
H	-5.37741100	1.80719700	0.6186650
H	-5.11440300	0.61679400	-0.6644330
H	-5.04960600	0.11581200	1.0237790
C	-2.91549600	0.82359400	2.9228420
H	-3.27780600	1.71556700	3.4525580
H	-3.73040800	0.09475300	2.9148900
H	-2.10112300	0.39661600	3.5149190
C	0.87407900	-1.45189000	2.1581110
H	1.89834200	-1.74255600	2.4316000
H	0.65106400	-0.50417200	2.6508640
H	0.18546600	-2.21329200	2.5357430
C	1.01706100	-2.67154700	-0.0423060
H	0.25816200	-3.38936000	0.2782920
H	0.98819600	-2.61252300	-1.1309780
H	2.00160100	-3.06506700	0.2549940