

Rationalization of chirality transfer and fast conformational changes in a tris(2-pyridylmethyl)amine-based cage

ELECTRONIC SUPPORTING INFORMATION

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Computational details

The computational treatment combines two approaches: preliminary molecular dynamics calculations were performed to explore the potential energy surface of the neutral cage. Notably, the **E** conformation corresponds to an energy minimum extracted from several simulated annealing runs from the optimized experimental structure, using the Amber99 force field of the GROMACS 2020 program.^{1a} All the obtained structures were optimized with the MM2 force field implemented in CHEM 3D 19.0 program,^{1b} following the procedure specified in the next section.

Reported energies are obtained from Density Functional Theory calculations. All structures were fully optimized by using the functional PBE0,² in combination with the D3 dispersion empirical corrections (PBE0-D3).³ Calculations (optimizations and stationary point characterizations by frequency calculations) were performed by employing the def2-TZVP basis set.⁴ The RI-J technique (Resolution of Identity for Coulomb fitting) was employed to reduce the computational cost.⁵ DFT calculations were performed with the program package TURBOMOLE.⁶

1. (a) J. Wang, P. Cieplak and P. A. Kollman, *J. Comp. Chem.* 2000, **21**, 1049-1074; (b) N. L. Allinger, *J. Am. Chem. Soc.* 1977, **99**, 8127-8134.
2. (a) P. A. M. Dirac, *Proc. Royal Soc. Lond. A*, 1929, **123**, 714-733; (b) J. C. Slater, *Phys. Rev.*, 1951, **81**, 385-390; (c) J. P. Perdew and Y. Wang, *Phys. Rev. B*, 1992, **45**, 13244; (d) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865; (e) J. P. Perdew, M. Ernzerhof and K. Burke, *J. Chem. Phys.*, 1996, **105**, 9982-9985.
3. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
4. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
5. K. Eichkorn, F. Weigend, O. Treutler and R. Ahlrichs, *Theor. Chem. Acc.*, 1997, **97**, 119-124.
6. TURBOMOLE V7.2 2017, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from <http://www.turbomole.com>.

Molecular dynamics simulations

Starting from the experimental conformation, several molecular dynamics runs of simulated annealing with 100 cycles were carried out under pressure condition close to zero and a final temperature equal to 298K, starting from the following temperatures: 400, 500, 600, 700, 800, 900 et 1000K. The GROMACS 2020 program was used with the Amber99 force field. 900 conformations were generated and optimized using the MM2 force field implemented in the CHEM 3D program.

An average "pyridine twist" for each optimized conformation was calculated using the following formula:

$$\varphi = \frac{\varphi_1 + \varphi_2 + \varphi_3}{3}$$

where the φ_1 , φ_2 et φ_3 are the three O-C-C-N torsion angles. The variation of the energy as a function of the "pyridine twist" is shown in Figure S1. The **E** conformation corresponds to a minimum extracted from the steric energy plotted against the "pyridine twist".

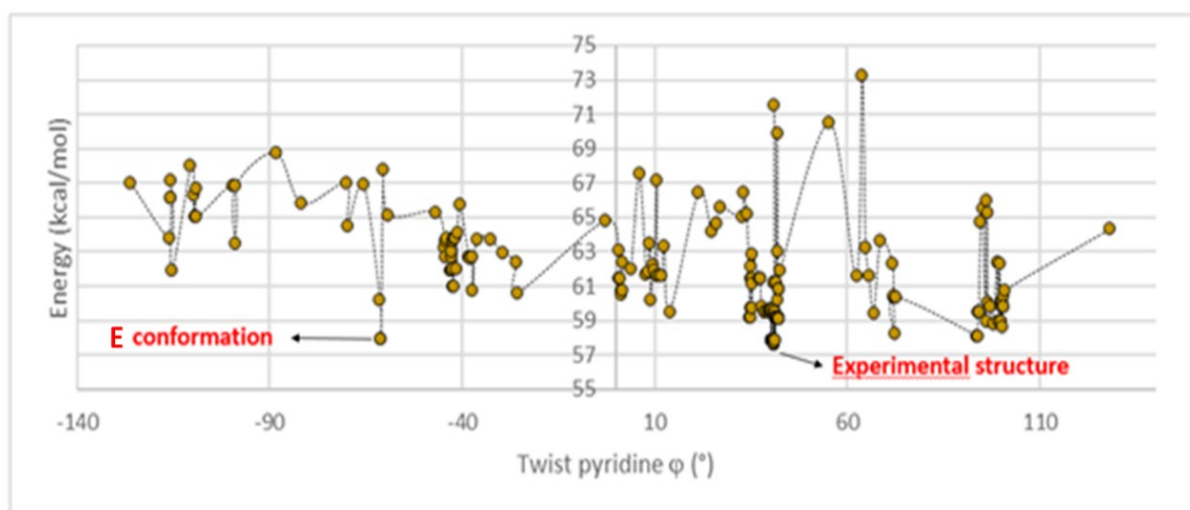


Figure S1. Variation of the energy as a function of the "pyridine twist" from molecular dynamics simulations.

Conversion from **II** to the **P/P** structure

The transition state (xyz coordinates: TsII_PP.xyz) that leads from **II** to a *P/P* structure implies a rotation of the pyridine connected to the carbon atom C(78) (torsion angle $\theta = \text{N}(91)\text{-C}(78)\text{-C}(76)\text{-N}(94)$), resulting into intermediate **1e** (a *P/P* structure that is also an intermediate in Path **AE**), as depicted here below. The latter can convert into **A** as shown in Figure 6 of the main article.

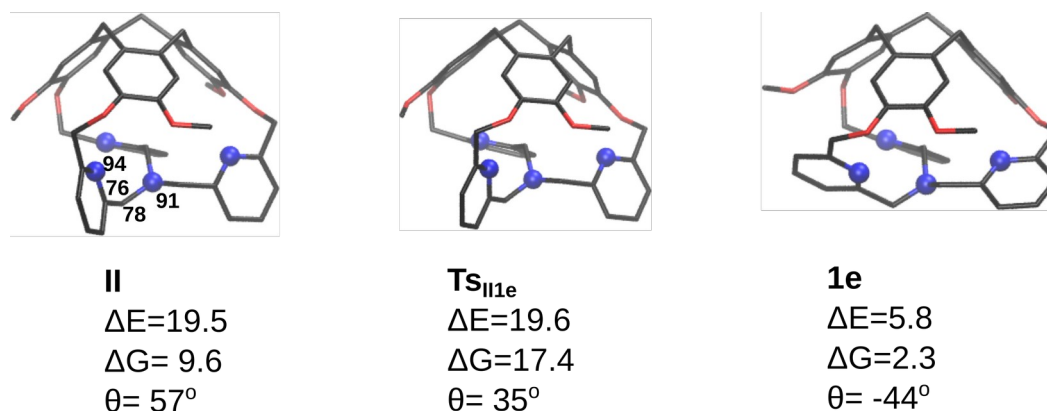


Figure S2. Computed structures for the conversion of **II** to **1e**. ΔE (including ZPE) and ΔG (kJ/mol) are relative to *P/P*-**1** (Figure 2 of the main article). θ is the torsion angle: $\theta = \text{N}(91)\text{-C}(78)\text{-C}(76)\text{-N}(94)$.

Structure of a TPA-based hemicryptophane

For the TPA-based hemicryptophane of Figure S2, owning phenyl linkages, no chirality transfer was observed between the CTV and the southern TPA unit while the phenyl linkers were helically arranged (see reference: S. A. Ikbāl, C. Colombar, D. Zhang, M. Delecluse, T. Brotin, V. Dufaud, J. P. Dutasta, A. B. Sorokin and A. Martinez, *Inorg. Chem.*, 2019, **58**, 7220-7228).

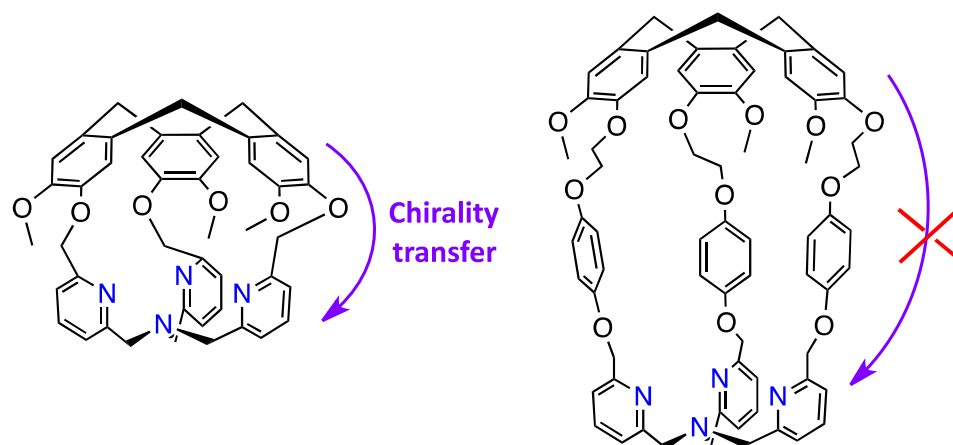


Figure S3. Schematic representation of cage-1 from this work and a bigger TPA-based hemicryptophane, owning phenyl linkages.

Paths AB, AC, AD

We present here the detailed pathways for the **AB** (Figure S4), **AC**, and **AD** paths (relative ΔG values in kJ/mol, def2-TZVP/D3-PBE0 level).

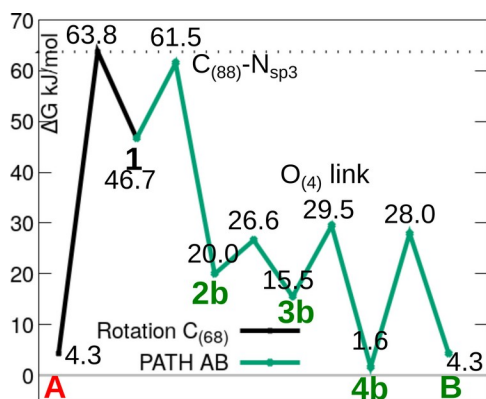


Figure S4. Computed Path **AB**, relative ΔG (kJ/mol) are indicated for all intermediates and transition states.

For Path **AC** (Figure S5), intermediates **2c** and **4c** are depicted: from **1**, the rotation of the $C_{(78)}-N_{sp3}$ arm is accomplished in a two-step mechanism: firstly the pyridine ring connected to $C_{(78)}$ undergoes a rotation, leading to **2c**, which readily converts into **3c** through the rotation of the $C_{(78)}-N_{sp3}$ arm. In the next step a rotation occurs that adjusts simultaneously the positions of the pyridine rings and the oxygen link of the new inside arm ($O_{(51)}$). From there, the following steps are rearrangements to reorient the OMe groups and the oxygen link $O_{(2)}$.

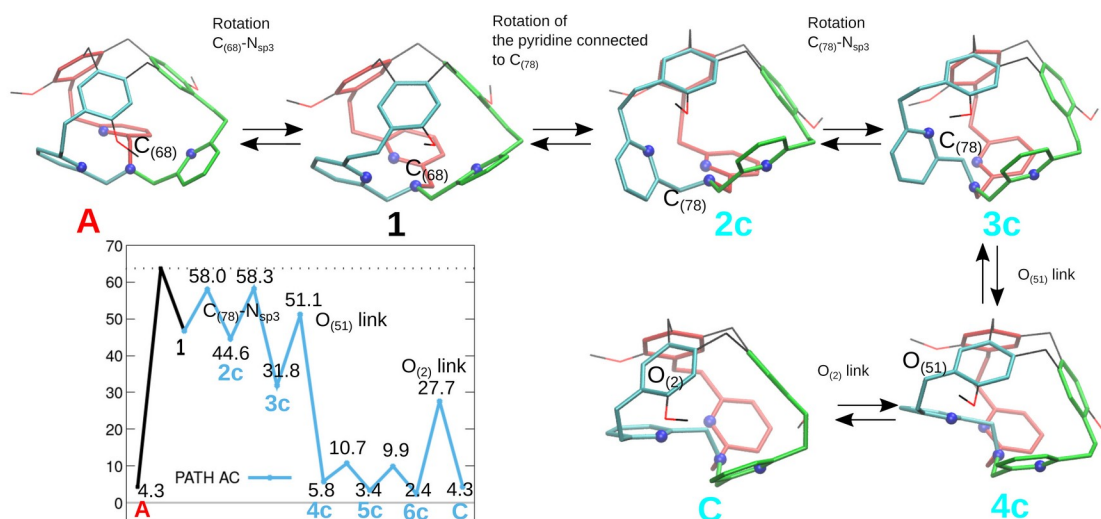


Figure S5. Computed Path **AC**, relative ΔG (kJ/mol) are indicated for all intermediates and transition states.

For Path **AD** (Figure S6), the intermediate **2d** is shown, resulting from a rotation of the organic link containing O₍₅₁₎.

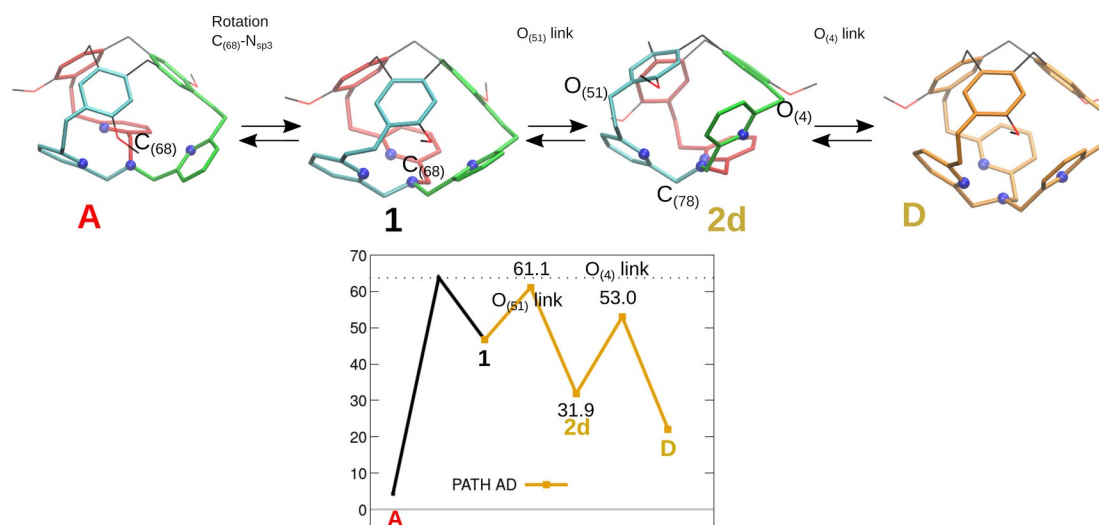


Figure S6. Computed Path **AD**, relative ΔG (kJ/mol) are indicated for all intermediates and transition states.

Energies and xyz coordinates

Total energies E and ZPE (in a.u.), chemical potentials, relative $\Delta(E+ZPE)$ and relative ΔG (in kJ/mol) are reported for optimized structures at the def2-TZVP/D3-PBE0 level.

Ts0.xyz specifies the transition state that allows for the transformation between the conformations *P/P-1* and **A** of Figure 2 of the main article.

Table 1: Total electronic energies, ZPE, chemical potentials, relative $\Delta(E+ZPE)$ and relative ΔG energies of all computed stationary points (D3-PBE0/def2-TZVP).

	E(a.u.)	ZPE (a.u.)	chem. pot. (kJ/mol)	$\Delta(E+ZPE)$ (kJ/mol)	ΔG (kJ/mol)
PP.xyz	-2408.550969421	0.79678	1881.56	0.00	0.00
Ts0.xyz	-2408.540602033	0.7962914	1882.32	25.94	27.98
A.xyz	-2408.550733909	0.7972846	1885.25	1.94	4.31
I_PM.xyz	-2408.530661445	0.7954453	1868.86	49.81	40.62
II.xyz	-2408.543085789	0.7963329	1870.43	19.52	9.57
TsII_PP.xyz	-2408.54297489	0.7962586	1877.99	19.62	17.42
PATHS AB-AC-AD					
TsA1.xyz	-2408.525902531	0.7956418	1879.55	62.82	63.80
1.xyz	-2408.531080471	0.7957705	1876.04	49.57	46.70
PATH AC					
Ts12c.xyz	-2408.527154865	0.7955677	1877.02	59.34	57.99
2c.xyz	-2408.52911292	0.7954695	1868.79	53.94	44.61
Ts23c.xyz	-2408.526649213	0.7953925	1875.97	60.21	58.26
3c.xyz	-2408.536049071	0.7961888	1874.21	37.62	31.82
Ts34c.xyz	-2408.526626904	0.7944626	1868.77	57.83	51.12
4c.xyz	-2408.547952054	0.7966723	1879.47	7.64	5.83
Ts45c.xyz	-2408.545940667	0.7957578	1879.02	10.52	10.66
5c.xyz	-2408.548048874	0.7961243	1877.26	5.95	3.37
Ts56c.xyz	-2408.546345	0.7958591	1879.32	9.72	9.90
6c.xyz	-2408.550596753	0.7969584	1883.00	1.45	2.42
Ts67c.xyz	-2408.54151349	0.7965054	1884.39	24.11	27.66
PATH AB					
Ts12b.xyz	-2408.52527294	0.7951039	1875.59	63.07	61.50
2b.xyz	-2408.543613005	0.7964666	1882.22	18.49	19.97
Ts23b.xyz	-2408.541995141	0.7962915	1884.63	22.28	26.63
3b.xyz	-2408.546681657	0.7969833	1885.81	11.79	15.51
Ts34b.xyz	-2408.541540524	0.7967564	1886.3	24.69	29.50
4b.xyz	-2408.55094563	0.7971505	1883.12	1.04	1.62
PATH AD					
Ts12d.xyz	-2408.525942458	0.7951185	1876.97	61.35	61.12
2d.xyz	-2408.536069800	0.7953959	1874.31	35.48	31.87

	E(a.u.)	ZPE (a.u.)	chem. pot. (kJ/mol)	$\Delta(E+ZPE)$ (kJ/mol)	ΔG (kJ/mol)
Ts2d_D.xyz	-2408.528847693	0.7951513	1876.47	53.80	52.99
D.xyz	-2408.539011941	0.795235	1872.28	27.34	22.11
PATH AE					
TsA1e.xyz	-2408.535280372	0.795757	1877.83	38.51	37.46
1e.xyz	-2408.548554988	0.7965729	1877.52	5.80	2.30
Ts12e.xyz	-2408.539085765	0.7957821	1879.66	28.58	29.30
2e.xyz	-2408.54429861	0.7963851	1877.76	16.48	13.71
Ts2e_E.xyz	-2408.533074267	0.7955977	1872.96	43.88	38.38
E.xyz	-2408.536928941	0.7956952	1869.29	34.02	24.59

Table 3 reports the values of some selected dihedral angles of the DFT optimized structures. The angles are defined in Table 2:

Table 2: Definition of the dihedral angles

Name	Atom numbers
Orientation of the (TPA) bottom CH ₂	
α_1	69 68 91 78
α_2	68 91 78 80
α_3	68 91 88 89
Orientation of the pyridines	
β_1	69 68 66 92
β_2	79 78 76 94
β_3	89 88 83 93
Orientation of the CH ₂ O links	
γ_1	92 67 29 2
γ_2	94 77 6 51
γ_3	93 82 32 4

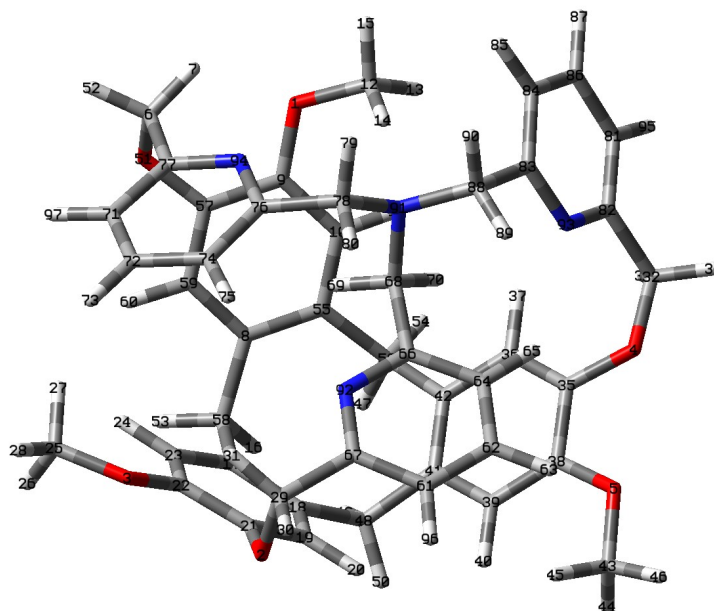


Table 3: Selected dihedral angles, as defined in Table 2.

	α_1	α_2	α_3	β_1	β_2	β_3	γ_1	γ_2	γ_3
PP.xyz	59.71	64.94	-54.19	-25.39	65.97	37.18	92.55	104.99	9.58
Ts0.xyz	59.1	61.91	-55.45	-26.1	63.38	31.61	87.94	94.81	18.5

	α_1	α_2	α_3	β_1	β_2	β_3	γ_1	γ_2	γ_3
A.xyz	62.04	66	-57.98	-24.76	73.69	27.7	88.06	22.21	23.64
I_PM.xyz	-169.1	-169.1	-169.1	-113.74	-113.74	-113.74	-143.6	-143.6	-143.6
II.xyz	46.74	29.97	156.73	-17.58	-179.9	-156.49	82.84	-79.15	-76.74
TsII_PP.xyz	50.92	34.49	152.57	-15.49	158.81	-162.38	81.38	-59.18	-68.18
PATHS AB-AC-AD									
TsA1.xyz	139.02	7.14	-59.52	-80.09	76.38	60.26	91.89	24.49	29.87
1.xyz	-168.72	-22.64	-52.97	-143.41	76.66	85.74	114.73	25.55	26.56
PATH AC									
Ts12c.xyz	-167.75	-65.89	-44.67	-156.94	172.13	77.43	106.35	-56.47	29.29
2c.xyz	-163.06	-58.35	-41.4	-158.61	-159.34	71.87	129.12	-96.12	32.6
Ts23c.xyz	-170.76	-97.93	-51.35	-178.25	-139.1	111.22	112.83	-73.11	15.02
3c.xyz	174.49	-100.7	-3.32	134.16	-72.28	36.63	133.49	-74.19	51.31
Ts34c.xyz	-167.36	-146.81	32.51	131.24	-78.41	48.37	124.54	-13.94	37.09
4c.xyz	-178.67	-169.27	48.39	142.23	-141.77	65.23	110.63	82.36	30.78
Ts45c.xyz	178.46	-167.44	45.84	135.14	-139.83	65.05	117.76	81.14	30.39
5c.xyz	178.26	-167.22	45.49	134.56	-139.86	65.13	118.41	81.09	30.71
Ts56c.xyz	178.52	-167.29	45.02	134.72	-139.89	65.78	118.55	79.9	29.69
6c.xyz	179.67	-168.46	52.29	137.58	-140.36	70.78	115.02	85.52	23.76
Ts67c.xyz	-178.05	-167.82	52.06	132.04	-140.48	70.85	74.13	85.57	22.05
PATH AB									
Ts12b.xyz	-169.79	-22.18	-114.1	-134.37	69.7	170.22	110.71	22.28	-19.19
2b.xyz	-69.56	-40.13	173.21	175.83	41.19	-133.61	110.15	10.09	8.55
Ts23b.xyz	-69.65	-40.19	173.3	175.69	41.47	-133.26	110.21	9.77	8.17
3b.xyz	-70	-41.45	173.44	175.49	41.9	131.99	110.01	10.99	5.27
Ts34b.xyz	-68.63	-40.52	173.01	177.75	39.18	138.95	108.16	9.12	49.91

	α_1	α_2	α_3	β_1	β_2	β_3	γ_1	γ_2	γ_3
4b.xyz	-67.32	-40.55	175.8	-178.38	37.18	141.88	104.95	9.72	92.49
PATH AD									
Ts12d.xyz	-162.04	-28.49	-46.66	-165.95	65.22	84.29	120.55	74	28.94
2d.xyz	-163.54	-25.94	-38.04	-164.55	68.99	70.51	127.78	127.33	37.39
Ts2d_D.xyz	-161.15	-28	-38.9	-166.83	67.31	67.31	125.76	126.48	81.41
D.xyz	-155.06	-22.34	-37.3	-175.78	68.25	68.21	138.14	138.2	138.17
PATH AE									
TsA1e.xyz	51.36	49.68	-114.36	-22.21	105.01	63.46	78.28	1.85	25.41
1e.xyz	58.63	66.73	154.32	-15.2	78.24	167.61	79.99	19.91	-25.44
Ts12e.xyz	52.33	66.13	155.09	-9.86	76.2	165.36	37.6	23.54	-24.99
2e.xyz	57.8	66.54	153.54	2.08	66.38	178.01	-18.05	30.71	-30.57
Ts2e_E.xyz	57.87	-13.81	170.31	-7.19	-153.24	-143.3	-31.3	-76.72	-72.57
E.xyz	-29.45	102.87	-32.07	-54.27	-25.68	-14.93	96.59	27.97	-71.91

Cartesian coordinates of all intermediates and transition states at the optimizing level follow.

Coordinates

PP.xyz

97

Energy = -2408.550969421

O	1.4106427	-4.1231829	0.8969154
O	0.8726216	4.6870841	0.7790665
O	2.9746934	3.5365066	2.0737769
O	-3.5357818	-0.6457278	-3.1453106
O	-3.3913624	1.9225760	-3.3589258
C	2.8895164	-2.9950186	3.1217383
H	2.1832876	-3.8191086	3.0295487
C	3.0640387	-0.8419319	-1.0620954
C	1.9026242	-3.0372038	0.2560369
C	1.3865154	-2.5512246	-0.9365900
H	0.5288407	-3.0514408	-1.3712628
C	0.0190650	-4.3418999	0.7969542
H	-0.2697496	-4.6984212	-0.1978349
H	-0.5290049	-3.4283129	1.0439576
H	-0.2208506	-5.1163513	1.5256019
H	3.6831497	0.3906406	-2.7226418
C	3.0004173	1.6396898	-1.0987568
C	1.9735836	2.2928456	-1.7727706
C	1.2969588	3.3176797	-1.1110280
H	0.4665429	3.8231527	-1.5912528
C	1.6044825	3.7020714	0.1739215
C	2.6808273	3.0889553	0.8290690
C	3.3575050	2.0717142	0.1810397
H	4.1699043	1.5649349	0.6853453
C	4.1665828	3.0758440	2.6600761
H	5.0347775	3.3162946	2.0362521
H	4.1427397	1.9950874	2.8355618

H	4.2564196	3.5922230	3.6150982
C	-0.0185455	4.2152942	1.7968826
H	-0.4971258	5.1147207	2.1865629
H	0.5483985	3.7256335	2.5930332
C	-3.7002132	-2.0316283	-3.1224991
H	-3.0442102	-2.5231583	-3.8537721
H	-4.7299378	-2.2017229	-3.4506760
C	-2.2837188	-0.1275193	-3.1202328
C	-1.1103074	-0.8497495	-3.0077910
H	-1.1590120	-1.9278924	-2.9085818
C	-2.2121811	1.2685858	-3.2543272
C	-0.9714998	1.8713441	-3.2766111
H	-0.9065459	2.9449300	-3.3952922
C	0.2155049	1.1443853	-3.1596106
C	0.1501529	-0.2388598	-3.0258534
C	-3.3447324	3.3102497	-3.5766892
H	-2.8261153	3.5533831	-4.5112539
H	-2.8526132	3.8336035	-2.7489888
H	-4.3799548	3.6414776	-3.6452617
H	2.1632023	-0.6736181	-3.5910909
C	1.5092784	1.9195179	-3.1607320
H	2.2854659	1.3691620	-3.6911284
H	1.3560506	2.8406871	-3.7298488
O	3.6651266	-2.8501290	1.9287158
H	3.6286765	-3.2257241	3.8909298
H	4.7453043	0.4343858	-1.3395308
H	1.1258594	-2.0605644	-3.4749462
C	1.9500936	-1.4749524	-1.6200754
C	1.3792247	-1.1195594	-2.9778839
C	3.0309038	-2.4143202	0.8015255

C	3.6930434	0.4074917	-1.6335572	H	-3.6567596	-0.5438012	1.4864284
C	3.5779822	-1.3361639	0.1337727	H	-3.3985746	-1.9192763	2.5625261
H	4.4468602	-0.8711508	0.5864336	N	-1.6321050	-1.1645453	1.8147746
C	-2.1823058	3.7041175	0.6024935	N	-0.6988403	1.9662897	1.2857226
C	-3.0078823	2.7732004	-0.0057878	N	-3.4189328	-1.8641168	-0.7142599
H	-3.9175512	3.0822743	-0.5084703	N	0.8339108	-1.7390893	3.2181255
C	-2.6440350	1.4376274	0.0119640	H	-3.5701140	-4.6772395	-2.5369003
H	-3.2337429	0.6839575	-0.4968648	H	-2.4136530	4.7630969	0.5809454
C	-1.4764740	1.0699454	0.6778977	H	3.8773084	-0.6706713	4.1415113
C	-1.0265076	3.2552469	1.2308833				
C	-1.0277582	-0.3686016	0.7472134	Ts0.xyz			
H	0.0543403	-0.3822593	0.8858520	97			
H	-1.2408792	-0.8549958	-0.2044046	Energy = -2408.540602033			
C	2.8099458	-0.6231541	3.9575052	O	-4.5768279	1.2125126	0.3548152
C	2.0857577	0.5296933	4.1980793	O	4.7620568	1.0990408	-0.0526956
H	2.5669694	1.4182418	4.5897867	O	3.5550124	3.5517252	-0.0355367
C	0.7309742	0.5368594	3.9157216	O	-0.5941094	-4.7753718	0.5101801
H	0.1372371	1.4329340	4.0401634	O	1.9713535	-4.7283826	0.8118614
C	0.1409995	-0.6227362	3.4320753	C	-3.0860296	4.0880087	-0.9814243
C	2.1411073	-1.7374623	3.4598563	H	-3.8530746	3.5844099	-1.5721788
C	-1.3359411	-0.6714094	3.1446010	C	-0.9935603	1.7208104	2.4213639
H	-1.7936849	-1.3634290	3.8600945	C	-3.3529397	1.4030805	0.9174628
H	-1.7675050	0.3246018	3.3368234	C	-2.7990641	0.3557395	1.6392565
C	-3.4933725	-4.0537287	-1.6527313	H	-3.3483794	-0.5802397	1.6350305
C	-3.5174538	-2.6677966	-1.7634055	C	-4.6596808	1.1424483	-1.0600749
C	-3.2686381	-2.3980175	0.4975602	H	-3.6708432	1.1244662	-1.5247672
C	-3.2621804	-3.7726136	0.7028140	H	-5.2266679	1.9978440	-1.4388997
H	-3.1457655	-4.1704997	1.7036982	H	-5.2008417	0.2289622	-1.3165916
C	-3.3805291	-4.6118790	-0.3918819	H	0.2281910	1.4390272	4.1677442
H	-3.3732975	-5.6886554	-0.2647197	C	1.5227343	1.7582600	2.4768729
C	-3.0474696	-1.4477228	1.6411972	C	2.2223796	0.5554173	2.5346130

C	3.3094266	0.3837164	1.6796324	H	2.7600287	-1.0176855	3.8547305
H	3.8523537	-0.5546573	1.6663923	O	-3.2453446	3.7794220	0.4045090
C	3.7207110	1.3565241	0.7956093	H	-3.2507678	5.1655721	-1.0387314
C	3.0737249	2.5974256	0.8020012	H	0.2169800	3.0622026	3.5350247
C	1.9829874	2.7718152	1.6343789	H	-2.1104215	-1.2384713	3.5396961
H	1.4494712	3.7141360	1.6210780	C	-1.6415011	0.4800919	2.4018977
C	3.2734849	4.8903805	0.2945088	C	-1.2055632	-0.7056184	3.2349299
H	3.5776750	5.1132838	1.3228800	C	-2.7001726	2.6400503	0.9319079
H	2.2113653	5.1314187	0.1820891	C	0.2452461	2.0101989	3.2399321
H	3.8501829	5.5046188	-0.3963877	C	-1.5351369	2.7607533	1.6729188
C	4.3722059	0.9200113	-1.4210996	H	-1.0759977	3.7429298	1.7038774
H	5.3022712	0.7122258	-1.9512292	C	3.8111087	-1.5250247	-1.7216452
H	3.9288478	1.8431244	-1.8042650	C	2.8561910	-2.5291970	-1.7075732
C	-1.9770468	-4.8957056	0.3438605	H	3.1413209	-3.5678765	-1.8318075
H	-2.4939441	-4.8856784	1.3130505	C	1.5292670	-2.1942353	-1.5013251
H	-2.1221998	-5.8887244	-0.0910896	H	0.7586862	-2.9534284	-1.4311475
C	-0.1099858	-3.7401763	1.2369627	C	1.1923758	-0.8492463	-1.3580808
C	-0.8645349	-2.7451950	1.8291389	C	3.3922789	-0.2105779	-1.5577123
H	-1.9418696	-2.7561643	1.7152706	C	-0.2352415	-0.4100427	-1.1482085
C	1.2853060	-3.7234401	1.4018564	H	-0.2246419	0.5477304	-0.6246628
C	1.8553729	-2.7053915	2.1369512	H	-0.7441820	-1.1271051	-0.5042871
H	2.9288046	-2.6869183	2.2714399	C	-0.6481822	4.5714999	-1.4423044
C	1.0959855	-1.6866047	2.7186537	C	0.5608113	4.1522815	-1.9696110
C	-0.2866189	-1.7104824	2.5753079	H	1.4385835	4.7847723	-1.9196864
C	3.3572023	-4.7858203	1.0388027	C	0.6401180	2.9004344	-2.5538806
H	3.5852811	-4.8914189	2.1056856	H	1.5786344	2.5146911	-2.9291005
H	3.8682113	-3.8975216	0.6504227	C	-0.5072011	2.1219317	-2.6240929
H	3.7153412	-5.6663148	0.5071960	C	-1.7448221	3.7232802	-1.5467858
H	-0.7510075	-0.3528923	4.1614289	C	-0.4968049	0.7601412	-3.2656668
C	1.8417512	-0.5925165	3.4404088	H	-1.1532473	0.7968556	-4.1416244
H	1.2693373	-0.2332386	4.2948458	H	0.5196905	0.5404240	-3.6298098

C	-3.9679809	-3.6467792	-0.5336910	H	0.2448301	-3.3623588	-1.7372192
C	-2.5965963	-3.8652080	-0.5717345	C	0.3084175	-4.6092382	1.8228408
C	-2.3071709	-2.2993364	-2.2157301	H	-0.0045774	-3.6522849	2.2465533
C	-3.6706109	-2.0341632	-2.2612595	H	1.1261764	-5.0176564	2.4176412
H	-4.0501495	-1.2824107	-2.9417190	H	-0.5221719	-5.3165872	1.8241315
C	-4.5137002	-2.7237550	-1.4090890	H	3.5343672	0.0673345	-2.5905644
H	-5.5810797	-2.5331903	-1.4128141	C	2.8426782	1.4084051	-1.0530621
C	-1.3472420	-1.4951051	-3.0478089	C	1.9145347	2.1227842	-1.8069179
H	-0.4692881	-2.1137687	-3.2893909	C	1.2996711	3.2273129	-1.2193288
H	-1.8299303	-1.2330031	-3.9931009	H	0.5353371	3.7780515	-1.7557095
N	-1.0168644	-0.2530552	-2.3726912	C	1.5861998	3.6438124	0.0612800
N	2.1097862	0.1161827	-1.4094685	C	2.5975490	2.9928277	0.7771102
N	-1.7893668	-3.2163844	-1.4009863	C	3.1978479	1.8815339	0.2124094
N	-1.6746000	2.5371494	-2.1418471	H	3.9514647	1.3425355	0.7728090
H	-4.5913810	-4.1880734	0.1695385	C	4.1306876	3.1017008	2.5645057
H	4.8646146	-1.7502374	-1.8433109	H	4.9624330	3.2888529	1.8762411
H	-0.7503351	5.5368057	-0.9593899	H	4.1298001	2.0435260	2.8436484

A.xyz

97

Energy = -2408.550733909

O	0.6840352	-4.4635836	0.4600832	C	-3.8624495	-1.9767047	-3.1134152
O	0.8916773	4.6905230	0.6020879	H	-3.3632949	-2.4889571	-3.9469799
O	2.9060924	3.4961284	1.9980084	H	-4.9402396	-2.0997126	-3.2522674
O	-3.6497512	-0.5947439	-3.1765419	C	-2.3767677	-0.1334177	-3.2086562
O	-3.3915259	1.9717171	-3.3831968	C	-1.2360238	-0.9114457	-3.1599242
C	3.2103894	-2.3998480	2.9975684	H	-1.3301390	-1.9879350	-3.0902293
H	3.3607799	-3.0525824	3.8624031	C	-2.2424733	1.2609707	-3.3179171
C	2.6565228	-1.1000079	-1.0114134	C	-0.9759556	1.8058540	-3.3474900
C	1.3266038	-3.3360807	0.0695569	H	-0.8639599	2.8785651	-3.4330114
C	1.0206529	-2.8406521	-1.1867139	C	0.1786163	1.0224900	-3.2610798

C	0.0501010	-0.3590119	-3.1818334	H	2.3725321	1.8133808	4.8013159
C	-3.2828756	3.3594548	-3.5760957	C	0.6475109	0.7912084	4.0384503
H	-2.7673853	3.5954874	-4.5142689	H	-0.0436923	1.6007966	4.2345955
H	-2.7546175	3.8433467	-2.7466656	C	0.1964708	-0.3781732	3.4390408
H	-4.3022758	3.7401297	-3.6223311	C	2.3103998	-1.2496447	3.3874769
H	2.0762871	-0.8640859	-3.6659804	C	-1.2648495	-0.5589998	3.1199013
C	1.5030647	1.7418030	-3.2106785	H	-1.6848807	-1.2594826	3.8518790
H	2.2826524	1.1512588	-3.6903663	H	-1.7763733	0.4056828	3.2756425
H	1.4194949	2.6595433	-3.7996539	C	-3.1618058	-3.9801359	-1.7757434
O	2.6771969	-3.2367576	2.0071849	C	-3.4569365	-2.6232621	-1.8090230
H	4.1991606	-2.0157549	2.7139818	C	-3.0474661	-2.3939145	0.4301655
H	4.4580211	0.0237740	-1.1143493	C	-2.7592481	-3.7468035	0.5581151
H	0.9642814	-2.2010811	-3.6984998	H	-2.4678191	-4.1432454	1.5212010
C	1.6579239	-1.7380267	-1.7507555	C	-2.8186812	-4.5527630	-0.5628983
C	1.2314960	-1.3030246	-3.1347674	H	-2.5772467	-5.6074599	-0.4986374
C	2.3274114	-2.6920190	0.8080365	C	-2.8926184	-1.4741475	1.6097029
C	3.4396124	0.0977446	-1.5056258	H	-3.5544302	-0.6040558	1.4785332
C	2.9587376	-1.5904355	0.2576004	H	-3.2216975	-1.9975892	2.5123495
H	3.7399523	-1.1008142	0.8269308	N	-1.4980906	-1.1149975	1.8049792
C	-2.2067729	3.7076960	0.4978806	N	-0.6644866	2.0305947	1.2010172
C	-3.0151239	2.7368011	-0.0714985	N	-3.4108303	-1.8514343	-0.7300791
H	-3.9409971	3.0055670	-0.5675075	N	1.0154604	-1.3821221	3.1405265
C	-2.6103478	1.4139549	-0.0303857	H	-3.1913571	-4.5704915	-2.6850447
H	-3.1873282	0.6317089	-0.5104262	H	-2.4702704	4.7584712	0.4532156
C	-1.4207967	1.0973273	0.6238442	H	3.9136378	-0.0560418	4.1863128
C	-1.0288678	3.3087004	1.1171838				
C	-0.9209325	-0.3230879	0.7191452	I_PM.xyz			
H	0.1608900	-0.2969543	0.8538646	97			
H	-1.1154827	-0.8409393	-0.2201053	Energy = -2408.530661445			
C	2.8474445	-0.1227038	3.9971458	C	-0.8154020	-4.4338323	-0.6985120
C	1.9917487	0.9099352	4.3391123	H	-1.1241743	-5.2186120	-0.0025852

H	-0.7231033	-4.9158637	-1.6707562	H	-1.8026532	-0.3348133	-4.1055818
C	0.5182097	-3.8874409	-0.2425975	C	0.1659096	0.4178145	-4.0258293
C	1.5077005	-3.4517335	-1.1220967	C	1.5129485	0.1325842	-3.7772301
C	2.6735128	-2.9121477	-0.5820246	C	1.8489834	-1.1491210	-3.3705392
H	3.4707723	-2.5824038	-1.2396757	H	2.8875419	-1.3878441	-3.1818217
C	2.8667134	-2.7553924	0.7736173	C	0.8922369	-2.1460332	-3.1719400
C	1.8801727	-3.2018883	1.6595841	C	3.7063303	0.9502367	-3.4801919
C	0.7330478	-3.7734920	1.1319563	H	4.2399455	0.1731807	-4.0392404
H	-0.0355727	-4.1314952	1.8044463	H	4.2189340	1.9008974	-3.6201566
C	1.0529110	-3.2471428	3.8689700	H	3.7051469	0.6957210	-2.4143335
H	0.7343884	-4.2954008	3.8968327	C	-0.9159679	2.4227736	-3.4752767
H	1.4205975	-2.9636662	4.8541546	H	-1.5376986	3.1253266	-4.0389977
H	0.1977125	-2.6136440	3.6081852	H	-1.5725623	1.7884724	-2.8728374
C	4.1337878	-0.8015716	1.0390915	C	1.1399709	3.8079392	-3.0246438
H	5.2066932	-0.5870332	1.0121472	C	1.8763398	4.5823302	-2.1506136
H	3.6993312	-0.5067227	0.0795056	H	2.7708818	5.0952795	-2.4864064
C	3.5882931	-0.3665058	3.4601276	C	1.4483734	4.7023272	-0.8367652
C	3.0648065	0.4736816	4.4223235	H	1.9909516	5.3191576	-0.1296294
H	3.1365677	0.2208834	5.4744683	C	0.3071616	4.0199036	-0.4351116
C	2.4531365	1.6526110	4.0226167	C	-0.0124854	3.1921322	-2.5460888
H	2.0504643	2.3451586	4.7527599	C	-0.1987185	4.0809575	0.9796576
C	2.3640194	1.9389364	2.6663694	H	-1.2838027	4.0007259	0.9221597
C	3.4890534	0.0188377	2.1266993	H	0.0443712	5.0661141	1.4228518
C	1.6904711	3.1843237	2.1597781	C	-1.5768723	-2.8392668	-3.2054990
H	2.2168342	3.4703895	1.2496419	H	-1.2321587	-3.8659904	-3.3205506
H	1.8155028	4.0034992	2.8942094	H	-2.3275694	-2.6856724	-3.9854664
C	1.3684504	-3.4729728	-2.6263855	C	-2.2374515	-2.6433633	-1.8600233
H	2.3471548	-3.6947548	-3.0604902	C	-1.8876939	-3.3697233	-0.7231764
H	0.7102697	-4.2801252	-2.9449371	C	-2.5259445	-3.0584743	0.4758370
C	-0.4471298	-1.8619415	-3.4321342	H	-2.2902499	-3.6192013	1.3741027
C	-0.7714946	-0.5813188	-3.8756781	C	-3.4500782	-2.0422173	0.5890775

C	-3.8119394	-1.3186463	-0.5524640
C	-3.2087676	-1.6461397	-1.7566532
H	-3.4842767	-1.1015509	-2.6503665
C	-4.9275713	0.5511333	-1.4616811
H	-5.3684206	0.0606339	-2.3369659
H	-5.6177691	1.3110042	-1.0978845
H	-3.9846356	1.0297199	-1.7492105
C	-3.1722090	-1.1362585	2.7328483
H	-3.5625006	-1.3994753	3.7209333
H	-2.1495929	-1.5163272	2.6540740
C	-4.2951251	1.0801490	2.3151269
C	-3.1352471	0.3642075	2.5952888
C	-1.8862158	2.2747782	2.7781751
C	-3.0019392	3.0690846	2.5466350
H	-2.9138603	4.1493042	2.5623449
C	-4.2224948	2.4586518	2.2988908
H	-5.1062255	3.0560047	2.1033277
C	-0.5265664	2.8674479	3.0258300
H	-0.0130914	2.1869411	3.7044659
H	-0.6306366	3.8426777	3.5398153
N	0.2857480	2.9982261	1.8243160
O	2.1236208	-3.0488948	2.9792503
O	4.0238293	-2.2003087	1.2501887
O	2.3981511	1.1359792	-3.9610472
O	-0.2104080	1.6653063	-4.4455270
O	-4.7385204	-0.3482369	-0.3975124
O	-4.0328404	-1.7651162	1.7964050
N	2.8874460	1.1355954	1.7389996
N	-1.9619720	0.9434474	2.8129578
N	-0.4142123	3.2880672	-1.2856059
H	-5.2161628	0.5498169	2.1132252

H	4.0619705	-1.3058704	3.7121943
H	1.4346172	3.6652757	-4.0557219

II.xyz

97

Energy = -2408.543085789

O	-1.7829303	3.3057567	2.2430942
O	4.1936063	-2.2742320	-1.8752385
O	4.7146764	0.3680382	-1.3259028
O	-3.2550432	-3.1533116	0.4272432
O	-1.4723933	-4.8061428	-0.4566194
C	1.5556526	4.6187458	0.9423609
H	1.9575388	5.6048114	1.1825774
C	1.4683909	0.8043766	2.9609910
C	-0.7584598	2.4589905	2.4970438
C	-0.9088041	1.1488362	2.9226636
H	-1.9048814	0.7553773	3.0770684
C	-3.0857630	2.8502380	2.5177451
H	-3.7529442	3.6709173	2.2583690
H	-3.2080330	2.6077589	3.5797990
H	-3.3466770	1.9704280	1.9178113
H	2.5860287	-0.7681489	3.9162450
C	3.1300878	-0.7004365	1.8331429
C	2.8627596	-2.0326416	1.5290659
C	3.2680520	-2.5178169	0.2851512
H	3.0594133	-3.5444715	0.0054053
C	3.8758809	-1.7262954	-0.6642225
C	4.1354243	-0.3837164	-0.3611339
C	3.7737288	0.0950563	0.8839567
H	3.9700535	1.1307436	1.1288135
C	4.6254548	1.7670347	-1.1926359

H	5.2485369	2.1377510	-0.3704732	C	0.5373778	2.9618098	2.3240575
H	3.5871750	2.0810863	-1.0357123	C	2.7141327	-0.0318888	3.1238627
H	4.9954072	2.1866155	-2.1273479	C	1.6136469	2.1347006	2.5726404
C	3.4807266	-1.7497401	-3.0049632	H	2.6118090	2.5473892	2.4768301
H	3.7846321	-2.3840294	-3.8382226	C	1.2292452	-2.8708237	-3.2294346
H	3.7879916	-0.7194058	-3.1941696	C	-0.1249710	-2.8860845	-2.9215171
C	-4.2968697	-2.2636509	0.7828049	H	-0.7595539	-3.7024025	-3.2473186
H	-4.1759495	-1.8782204	1.7976100	C	-0.6484982	-1.8560048	-2.1674678
H	-5.2091595	-2.8627626	0.7556239	H	-1.6936086	-1.8429492	-1.8828682
C	-2.0169497	-3.0269934	0.9698525	C	0.1962716	-0.8255484	-1.7564968
C	-1.6470455	-2.1304739	1.9501651	C	1.9969626	-1.8025649	-2.7919408
H	-2.3682144	-1.4085017	2.3074749	C	-0.3359954	0.3067533	-0.9242833
C	-1.0564298	-3.9372673	0.4939933	H	0.4977207	0.8397873	-0.4544341
C	0.2223584	-3.8909372	1.0124360	H	-0.9564103	-0.1114857	-0.1288378
H	0.9677434	-4.5814956	0.6406952	C	0.3711806	5.8541903	-0.9041267
C	0.5994837	-2.9763081	2.0003000	C	-0.3509589	5.8206989	-2.0836148
C	-0.3581580	-2.0965894	2.4912413	H	-0.7076109	6.7372892	-2.5402546
C	-0.5480853	-5.7653493	-0.9039841	C	-0.6219341	4.5925403	-2.6614276
H	-0.2118143	-6.4118571	-0.0851569	H	-1.1976464	4.5224632	-3.5773903
H	0.3250797	-5.2973716	-1.3724868	C	-0.1472055	3.4348426	-2.0502769
H	-1.0714697	-6.3691427	-1.6442537	C	0.8099608	4.6519636	-0.3611966
H	0.7170080	-1.4621083	4.2338600	C	-0.4671796	2.0749135	-2.6232349
C	2.0529424	-2.9512529	2.4159659	H	-1.0538545	2.2153529	-3.5389927
H	2.1531789	-2.6719799	3.4643697	H	0.4631522	1.5792244	-2.9149851
H	2.4571833	-3.9636395	2.3334674	C	-5.3565199	-1.1693229	-1.2086886
O	0.6811645	4.2802950	2.0082041	C	-4.3923842	-1.1401513	-0.2112963
H	2.3833146	3.9089164	0.8664518	C	-3.4509241	0.7719154	-1.0581344
H	3.5281312	0.6211679	3.4509114	C	-4.3878628	0.8174712	-2.0895596
H	-0.9802631	-1.0850144	4.2460037	H	-4.3384363	1.6093139	-2.8276846
C	0.1807052	0.3067648	3.1488446	C	-5.3621383	-0.1582777	-2.1570346
C	-0.0961426	-1.1059952	3.6022584	H	-6.1081130	-0.1429470	-2.9437272

C	-2.3100047	1.7530748	-1.0282407
H	-2.6152309	2.6694487	-1.5391238
H	-2.0637605	2.0283404	0.0037477
N	-1.1742018	1.1835633	-1.7288788
N	1.4817456	-0.7913936	-2.0871513
N	-3.4770600	-0.1734233	-0.1214502
N	0.5678373	3.4735446	-0.9274394
H	-6.0818818	-1.9734615	-1.2419408
H	1.6867375	-3.6746031	-3.7951394
H	0.5891344	6.7903355	-0.4041077

TsII_PP.xyz

97

Energy = -2408.542974890

O	-4.2502021	1.1945780	0.4411371
O	4.9991329	0.9902267	0.4388494
O	3.5619356	3.3278173	0.2821171
O	-0.5426611	-4.4610200	0.1505274
O	2.0184837	-4.5700936	0.5029929
C	-2.1401775	4.4339147	-0.0609728
H	-2.6523951	5.3974139	-0.0223488
C	-0.8654039	1.5216812	2.8406482
C	-3.1543217	1.2507646	1.2336288
C	-2.6798394	0.1975326	1.9951917
H	-3.2051075	-0.7480947	1.9720602
C	-4.9653050	-0.0161028	0.4081599
H	-5.7885873	0.1384004	-0.2877112
H	-5.3708189	-0.2696992	1.3946458
H	-4.3426893	-0.8456754	0.0527383
H	0.3714296	1.1327691	4.5561883
C	1.6546591	1.5094811	2.8693409

C	2.3992589	0.3342979	2.9344395
C	3.5294073	0.2258247	2.1234047
H	4.1202580	-0.6834068	2.1295163
C	3.9113036	1.2084006	1.2368213
C	3.1633266	2.3906006	1.1736725
C	2.0633266	2.5223153	2.0000909
H	1.4781956	3.4317741	1.9589699
C	2.6353086	4.3315420	-0.0561632
H	2.4645365	5.0248926	0.7756429
H	1.6801192	3.8949512	-0.3695287
H	3.0726927	4.8837742	-0.8870230
C	4.7359783	0.9047416	-0.9696830
H	5.6891978	0.6077459	-1.4079889
H	4.4428596	1.8840700	-1.3531924
C	-1.9339556	-4.5281741	-0.0882137
H	-2.5083146	-4.2309033	0.7934106
H	-2.1456493	-5.5812727	-0.2847183
C	-0.0370555	-3.5882777	1.0589628
C	-0.7623324	-2.6888657	1.8111056
H	-1.8294713	-2.6097108	1.6564666
C	1.3558229	-3.6509304	1.2430616
C	1.9495585	-2.7875374	2.1417399
H	3.0233445	-2.8170341	2.2710303
C	1.2162530	-1.8601817	2.8885346
C	-0.1652588	-1.8329812	2.7418905
C	3.4032242	-4.6889567	0.7099627
H	3.6323571	-4.9660960	1.7454733
H	3.9297827	-3.7602647	0.4625785
H	3.7427793	-5.4814781	0.0442776
H	-0.5982001	-0.6399655	4.4721178
C	1.9885527	-0.8783230	3.7399303

H	1.4158030	-0.5880343	4.6201726
H	2.8897564	-1.3709602	4.1145212
O	-2.9996470	3.4992588	0.5550723
H	-1.1957213	4.5350242	0.4809542
H	0.3870547	2.7837472	4.0032098
H	-1.9616746	-1.5002456	3.8188898
C	-1.5347488	0.3027913	2.7868966
C	-1.0762807	-0.9238154	3.5352232
C	-2.4674534	2.4727094	1.2715311
C	0.3859203	1.7464289	3.6562277
C	-1.3616639	2.5873363	2.0892184
H	-0.8609696	3.5453141	2.1616947
C	3.9499389	-1.4068904	-1.6215347
C	2.8960794	-2.2928997	-1.8068900
H	3.0806500	-3.3246506	-2.0836734
C	1.6061488	-1.8477463	-1.6023754
H	0.7572563	-2.5125322	-1.7061177
C	1.4038941	-0.5172984	-1.2375139
C	3.6610610	-0.0970622	-1.2715305
C	0.0170167	0.0015078	-0.9836650
H	0.0787509	0.9612251	-0.4589380
H	-0.4999293	-0.7052518	-0.3311933
C	-2.1544511	4.9274823	-2.5293942
C	-1.8490186	4.5384311	-3.8242418
H	-2.0799846	5.1851427	-4.6635216
C	-1.2653340	3.3027602	-4.0270964
H	-1.0280886	2.9549254	-5.0262812
C	-0.9901665	2.4943033	-2.9243892
C	-1.8462419	4.0613431	-1.4896327
C	-0.3427216	1.1391786	-3.1230579
H	-0.5279552	0.8267970	-4.1583355

H	0.7425298	1.2628689	-3.0354173
C	-2.7331471	-4.3169141	-2.4601235
C	-2.3225027	-3.7027680	-1.2849082
C	-2.4490009	-1.6153105	-2.2297842
C	-2.8758344	-2.1526400	-3.4429401
H	-3.0741578	-1.4979352	-4.2834160
C	-3.0316593	-3.5207158	-3.5546225
H	-3.3661900	-3.9653491	-4.4853018
C	-2.1640319	-0.1424595	-2.0977360
H	-2.6830148	0.3953724	-2.8948345
H	-2.5556168	0.2416683	-1.1511319
N	-0.7367820	0.0884402	-2.2241873
N	2.4093921	0.3400380	-1.1076189
N	-2.2101272	-2.3803029	-1.1665348
N	-1.2723737	2.8766717	-1.6841130
H	-2.8105638	-5.3963235	-2.5145234
H	4.9795534	-1.7245149	-1.7419893
H	-2.6333991	5.8783154	-2.3275521

PATHS AB, AC, AD

TsA1.xyz

97

Energy = -2408.525902531

O	-4.7562945	1.0870026	0.2255658
O	4.7553431	1.0295435	-0.1653575
O	3.6096120	3.4645539	-0.4877112
O	-1.1565977	-4.5347096	1.1737467
O	1.4350253	-4.5344697	1.1857282
C	-2.2397472	3.8094209	-1.5421000
H	-2.8389892	4.2221649	-2.3586374
C	-1.1081734	1.8865451	2.0524197

C	-3.5280513	1.3299427	0.7738327	H	2.5820084	-2.3894300	2.3230609
C	-3.0884862	0.5632309	1.8321292	C	0.8280097	-1.3088487	2.8899634
H	-3.7379649	-0.2374369	2.1689804	C	-0.5610917	-1.3186018	2.9180250
C	-5.6939322	2.1335225	0.3989725	C	2.8337658	-4.6213355	1.2889156
H	-5.3639385	3.0537616	-0.0895975	H	3.1577794	-4.6369289	2.3361023
H	-5.8660775	2.3272735	1.4638955	H	3.3313346	-3.7948433	0.7700656
H	-6.6241482	1.7968751	-0.0595808	H	3.1149691	-5.5597679	0.8125797
H	0.1110937	1.9999588	3.8141350	H	-0.8540099	0.3007152	4.3051077
C	1.4193887	2.0121624	2.1098112	C	1.6745209	-0.1738394	3.4110141
C	2.0939160	0.8166037	2.3491939	H	1.1668089	0.3413161	4.2259332
C	3.2047590	0.5212754	1.5617478	H	2.5823339	-0.5982898	3.8491828
H	3.7420848	-0.4108267	1.6960361	O	-3.1034071	2.9210675	-0.8871334
C	3.6671425	1.3756507	0.5850545	H	-1.9664135	4.6474603	-0.8869182
C	3.0514557	2.6210653	0.4164081	H	0.0596515	3.4575736	2.8639938
C	1.9304305	2.9111681	1.1726567	H	-2.2796862	-0.6459346	3.9774171
H	1.4287565	3.8614275	1.0396062	C	-1.8634031	0.7875028	2.4615605
C	3.2290541	4.8166367	-0.4279166	C	-1.3996005	-0.2007798	3.5055666
H	3.3827619	5.2264053	0.5765077	C	-2.6798131	2.3104380	0.2463972
H	2.1825292	4.9595958	-0.7156070	C	0.1245933	2.3682671	2.7891417
H	3.8672966	5.3455105	-1.1349682	C	-1.5119636	2.6063548	0.9272567
C	4.4452967	0.7445022	-1.5303673	H	-0.8730730	3.4046099	0.5705273
H	5.4037867	0.7648700	-2.0514704	C	4.5737219	-1.7429167	-1.8116570
H	3.7953451	1.5203525	-1.9402722	C	3.9390677	-2.9662855	-1.9300703
C	-2.5510859	-4.5361179	1.0215711	H	4.5119088	-3.8793696	-2.0503556
H	-3.0518688	-4.5166702	1.9990656	C	2.5571975	-3.0030478	-1.9049195
H	-2.7775863	-5.4982765	0.5546424	H	2.0238072	-3.9413883	-1.9967002
C	-0.5710693	-3.4629227	1.7555435	C	1.8426469	-1.8149251	-1.7477173
C	-1.2339955	-2.4066417	2.3499616	C	3.7917553	-0.6015856	-1.6778592
H	-2.3163444	-2.3993138	2.3614471	C	0.3466066	-1.9127580	-1.6183009
C	0.8349823	-3.4637471	1.7544998	H	0.1288249	-1.8996027	-0.5433567
C	1.4999564	-2.3964379	2.3216026	H	0.0609184	-2.9206674	-1.9459389

C	0.1059865	4.0235503	-2.3700463	O	-4.0066604	2.7889690	0.1701016
C	1.2270559	3.4766069	-2.9682804	O	4.7034549	-1.0494293	0.3642404
H	2.0996953	4.0861960	-3.1731763	O	4.6211177	1.6621282	0.4878423
C	1.2252670	2.1280340	-3.2704145	O	-2.6671563	-3.7673580	-0.2212596
H	2.0921997	1.6516616	-3.7112796	O	-0.4461414	-4.9975496	0.3238762
C	0.0968268	1.3719395	-2.9755177	C	-0.4694728	4.7095672	-0.6442759
C	-0.9839755	3.1954961	-2.1241983	H	-0.7566038	5.4878040	-1.3570937
C	0.0600470	-0.0986170	-3.3205267	C	-0.6269290	1.7309432	2.3547338
H	-0.5339790	-0.2038072	-4.2390309	C	-2.8700452	2.4282330	0.8377785
H	1.0688452	-0.4129652	-3.5889308	C	-2.8936733	1.3440845	1.6889729
C	-4.3538241	-2.9019879	0.3904603	H	-3.8280620	0.7994633	1.7731401
C	-3.0826573	-3.4145445	0.1595850	C	-4.5443660	4.0390592	0.5603466
C	-2.6921018	-1.9289966	-1.5361872	H	-3.8462815	4.8564074	0.3622715
C	-3.9313179	-1.3307581	-1.3489679	H	-4.8066351	4.0333362	1.6245276
H	-4.2106503	-0.4583763	-1.9248100	H	-5.4482675	4.1872722	-0.0311226
C	-4.7840637	-1.8437192	-0.3872069	H	0.2642063	1.0163991	4.1693564
H	-5.7520246	-1.3889020	-0.2196436	C	1.7182611	0.7912887	2.6021112
C	-1.7940716	-1.4609616	-2.6517128	C	1.8608124	-0.5946672	2.6428282
H	-1.6779659	-2.3160304	-3.3493015	C	2.8673578	-1.1743756	1.8720067
H	-2.3262311	-0.6728979	-3.1839082	H	2.9869014	-2.2515188	1.8473942
N	-0.5014769	-0.9229064	-2.2739453	C	3.7410692	-0.4285410	1.1108875
N	2.4598905	-0.6381762	-1.6390146	C	3.6702927	0.9683171	1.1637796
N	-2.2904476	-2.9646008	-0.8005261	C	2.6507611	1.5512511	1.8942593
N	-0.9939546	1.9056971	-2.4290165	H	2.5664010	2.6306601	1.9189303
H	-4.9761852	-3.3091040	1.1802486	C	4.8627010	2.9836171	0.9051619
H	5.6542811	-1.6627913	-1.8285986	H	5.0511397	3.0266131	1.9834687
H	0.0693977	5.0733508	-2.0981122	H	4.0298751	3.6513678	0.6629816
				H	5.7505795	3.3170830	0.3686000
				C	4.4511771	-0.9938538	-1.0398897
				H	5.3856434	-1.3119975	-1.5072812
				H	4.2249152	0.0285237	-1.3508968

1.xyz

97

Energy = -2408.531080471

C	-3.9253656	-3.2122799	-0.4861572	H	2.4416278	-5.1543869	-1.5963027
H	-4.5602441	-3.2491005	0.4096532	C	1.2280865	-3.4770873	-2.1529583
H	-4.3708030	-3.8771011	-1.2314690	H	0.3596034	-4.0697785	-2.4144141
C	-1.9078540	-3.2108394	0.7510560	C	1.1877440	-2.0894538	-2.2784703
C	-2.2494798	-2.1062074	1.5063628	C	3.3196584	-1.9006718	-1.4469184
H	-3.2074021	-1.6280558	1.3473101	C	-0.0490011	-1.4802871	-2.8919175
C	-0.6847362	-3.8525829	1.0077406	H	-0.9081395	-2.0363837	-2.5154459
C	0.1798637	-3.2907618	1.9229855	H	-0.0042727	-1.6766292	-3.9844644
H	1.1385589	-3.7600505	2.1016483	C	1.9133951	4.2252412	-1.2085310
C	-0.1290630	-2.1200765	2.6224342	C	2.8662378	3.4537186	-1.8491442
C	-1.3824244	-1.5470472	2.4503486	H	3.9151115	3.7239904	-1.8143438
C	0.6122223	-5.8021145	0.7772246	C	2.4591502	2.3125266	-2.5119740
H	0.4863320	-6.0651385	1.8339639	H	3.1768189	1.6610110	-2.9945906
H	1.5838985	-5.3141473	0.6470825	C	1.1054596	1.9919840	-2.5399633
H	0.5868257	-6.7087326	0.1734187	C	0.5827483	3.8303467	-1.2847788
H	-1.3200712	-0.2467886	4.1608850	C	0.6637082	0.7788590	-3.3136655
C	0.9651834	-1.5040342	3.4554960	H	0.2536833	1.1171780	-4.2831209
H	0.5557815	-0.9682069	4.3112656	H	1.5559305	0.2001574	-3.5378009
H	1.5838002	-2.3045492	3.8708542	C	-5.0223092	-0.9913064	-0.8216304
O	-1.6727111	4.0720568	-0.3151621	C	-3.9122140	-1.8002916	-1.0270035
H	-0.0396818	5.2149316	0.2309090	C	-2.8031465	-0.1537786	-2.1662822
H	0.9277245	2.5090270	3.5676092	C	-3.8651568	0.7277850	-1.9891603
H	-2.9087915	-0.5005341	3.4940360	H	-3.7868385	1.7495891	-2.3363384
C	-1.7781681	0.9459776	2.4258156	C	-4.9939145	0.2983086	-1.3192269
C	-1.8633321	-0.3335550	3.2198036	H	-5.8212920	0.9768595	-1.1516154
C	-1.6633785	3.1082783	0.6387616	C	-1.6363444	0.3240113	-2.9928018
C	0.5740885	1.5221779	3.2556042	H	-1.8481256	0.0378109	-4.0455472
C	-0.5798998	2.7806888	1.4364957	H	-1.6551905	1.4130776	-2.9571774
H	0.3434008	3.3379197	1.3380819	N	-0.2903380	-0.0787284	-2.6231906
C	3.4495285	-3.2761323	-1.3141067	N	2.2181352	-1.3242708	-1.9259235
C	2.3798426	-4.0753147	-1.6798477	N	-2.8403963	-1.3996955	-1.6973083

N	0.1858222	2.7514063	-1.9459272
H	-5.8757776	-1.3607525	-0.2635218
H	4.3695650	-3.6995615	-0.9283974
H	2.1899543	5.1183979	-0.6580245

PATH AC

Ts12c.xyz

97

Energy = -2408.527154865

O	-1.9877230	4.3606897	0.5609700
O	3.4936523	-3.5595412	0.9070101
O	4.4599203	-0.9964948	1.0187706
O	-3.8055896	-1.9093620	-1.1891589
O	-2.7605277	-4.2174101	-0.5583866
C	2.1049031	4.3892612	0.6588673
H	2.4529246	5.4228719	0.7079955
C	-0.0948206	1.4233971	2.8169043
C	-1.3381141	3.3889831	1.2720401
C	-2.0576565	2.3350869	1.8022618
H	-3.1264644	2.3221983	1.6167164
C	-2.0367769	5.6209846	1.2040623
H	-1.0350372	6.0252140	1.3716048
H	-2.5641805	5.5475564	2.1621169
H	-2.5878880	6.2886931	0.5410969
H	-0.0341635	0.0497021	4.4620432
C	1.3476054	-0.6528103	2.9744189
C	0.8441013	-1.9460880	2.8642195
C	1.5982158	-2.8849247	2.1588346
H	1.2422250	-3.9036989	2.0525345
C	2.7951411	-2.5744900	1.5478424
C	3.2862504	-1.2653921	1.6391872

C	2.5613092	-0.3389316	2.3637791
H	2.9431124	0.6680955	2.4619982
C	4.8432706	0.3536685	0.9117966
H	5.0990499	0.7796758	1.8889811
H	4.0534064	0.9564526	0.4492058
H	5.7296272	0.3688476	0.2790160
C	3.6245915	-3.3957673	-0.5071152
H	4.2279407	-4.2475592	-0.8259652
H	4.1496518	-2.4696298	-0.7436933
C	-4.5530577	-0.7605870	-1.4867121
H	-5.3132126	-0.5869716	-0.7131687
H	-5.0769513	-1.0045407	-2.4150583
C	-3.1409293	-1.9630185	-0.0100682
C	-3.0482178	-0.9348685	0.9065339
H	-3.5608998	-0.0015230	0.7132445
C	-2.5269162	-3.1894508	0.2948071
C	-1.7376049	-3.2748918	1.4229161
H	-1.2173774	-4.2005894	1.6334599
C	-1.5644941	-2.2010153	2.3016271
C	-2.2819240	-1.0325296	2.0717192
C	-2.4725373	-5.5102568	-0.0887910
H	-2.9842810	-5.7095656	0.8597144
H	-1.3979300	-5.6698335	0.0508609
H	-2.8367874	-6.1999712	-0.8496707
H	-1.9966730	-0.1565692	4.0118347
C	-0.5187059	-2.3537489	3.3817360
H	-0.7835590	-1.7856698	4.2732666
H	-0.4778793	-3.4017056	3.6903542
O	0.7081407	4.4491379	0.8424097
H	2.5998555	3.8447583	1.4672940
H	1.3939527	1.0243187	4.2700086

H	-3.3326762	0.4929060	3.1041063
C	-1.4597796	1.3207383	2.5469565
C	-2.2962781	0.1555185	3.0111443
C	0.0491219	3.4206008	1.4405689
C	0.6424619	0.4574145	3.7127537
C	0.6339288	2.4616736	2.2470229
H	1.6966014	2.5015653	2.4421409
C	1.5689436	-4.5850512	-1.3080674
C	0.3108578	-4.5346346	-1.8809127
H	-0.2843960	-5.4328310	-1.9949630
C	-0.1807429	-3.3157039	-2.3054284
H	-1.1783485	-3.2351083	-2.7193340
C	0.6214123	-2.1817911	-2.1882619
C	2.2867344	-3.4027808	-1.1883553
C	0.1105015	-0.9187370	-2.8263576
H	-0.9762224	-0.9795328	-2.8247397
H	0.4281159	-0.9558374	-3.8922117
C	3.3099384	4.5244111	-1.5275153
C	3.6657284	3.9577298	-2.7391604
H	4.2996189	4.4934328	-3.4369283
C	3.1730804	2.7063906	-3.0527975
H	3.4068235	2.2401036	-4.0023490
C	2.3537610	2.0412773	-2.1384973
C	2.4926059	3.7963656	-0.6720831
C	1.8716121	0.6585380	-2.4891433
H	2.1309306	0.4853368	-3.5516490
H	2.4417545	-0.0745905	-1.9130052
C	-4.3453732	1.7336860	-1.3992122
C	-3.7550077	0.5089276	-1.6888283
C	-1.7873016	1.5020454	-2.3122485
C	-2.2929810	2.7643173	-2.0245692

H	-1.6617608	3.6393543	-2.1100112
C	-3.5962456	2.8812341	-1.5775886
H	-4.0017892	3.8537355	-1.3281633
C	-0.3863135	1.3917356	-2.8641301
H	-0.4582277	1.2479873	-3.9616050
H	0.0840443	2.3628582	-2.7151415
N	0.4622971	0.3748514	-2.2610465
N	1.8298149	-2.2335364	-1.6333319
N	-2.5203658	0.4001897	-2.1558807
N	2.0362362	2.5796966	-0.9619317
H	-5.3595314	1.7782761	-1.0172953
H	1.9936230	-5.5155102	-0.9494284
H	3.6480415	5.5163673	-1.2514189

2c.xyz

97

Energy = -2408.529112920

O	-1.3642915	3.7568355	0.5460832
O	3.9486236	-2.9694060	0.0227528
O	4.9371653	-0.6027913	0.8503411
O	-3.7111711	-2.4750910	-0.8818969
O	-2.3344994	-4.6697921	-0.5608377
C	2.3110580	4.0200964	0.6542054
H	2.9879041	4.8638840	0.8024450
C	0.4315948	1.0414317	3.1513413
C	-0.7678933	2.9045822	1.4298896
C	-1.4427377	1.7660863	1.8391994
H	-2.4490192	1.6228467	1.4605127
C	-1.6743812	5.0378122	1.0620450
H	-0.7771223	5.5649778	1.3945651
H	-2.3810959	4.9585848	1.8964038

H	-2.1407899	5.5957436	0.2492282	H	-2.2612326	-6.6337903	-0.9569406
H	0.5627074	-0.5251361	4.6361287	H	-1.3611043	-0.7446831	4.0619493
C	1.9674134	-0.8852685	3.0316092	C	0.2331686	-2.7670976	3.1678629
C	1.4995564	-2.1335593	2.6350478	H	-0.0340391	-2.3402049	4.1342947
C	2.1999428	-2.8125023	1.6347109	H	0.4293855	-3.8270104	3.3526075
H	1.8438951	-3.7720185	1.2777749	O	1.2177569	4.2488881	1.5420876
C	3.3177765	-2.2875806	1.0268679	H	2.8245340	3.0908064	0.9153688
C	3.8163880	-1.0509434	1.4614771	H	1.9239831	0.5672315	4.5975887
C	3.1373404	-0.3785351	2.4589139	H	-2.7192370	-0.0411127	3.2360675
H	3.4969417	0.5862249	2.7910762	C	-0.8673624	0.8180606	2.6821982
C	5.3824190	0.6908923	1.1704438	C	-1.6911051	-0.3838342	3.0876254
H	5.6692037	0.7715299	2.2252248	C	0.5235059	3.1237545	1.9036659
H	4.6165670	1.4419697	0.9458770	C	1.2108692	0.0338071	3.9636123
H	6.2576846	0.8741606	0.5491853	C	1.0862656	2.2065531	2.7698986
C	3.7234908	-2.4026346	-1.2679687	H	2.0839445	2.4124429	3.1431208
H	4.4551353	-2.8839746	-1.9216728	C	1.8195407	-3.9598593	-1.7429559
H	3.9096299	-1.3268591	-1.2648549	C	0.5181699	-4.1607516	-2.1604854
C	-4.6963700	-1.4762441	-0.9163928	H	0.0809741	-5.1517923	-2.1622837
H	-5.2862470	-1.4911161	0.0097289	C	-0.2279012	-3.0720368	-2.5716500
H	-5.3573587	-1.7670038	-1.7375137	H	-1.2663123	-3.1891587	-2.8570698
C	-2.8420804	-2.4918420	0.1580139	C	0.3686538	-1.8147038	-2.5986679
C	-2.6845448	-1.4786589	1.0842612	C	2.3236801	-2.6649123	-1.7565174
H	-3.3107844	-0.5995089	1.0182608	C	-0.4313870	-0.6857731	-3.1927664
C	-2.0733949	-3.6574877	0.3025120	H	-1.4801803	-0.9568877	-3.0853412
C	-1.1225706	-3.7089470	1.3031241	H	-0.2171397	-0.6698680	-4.2827125
H	-0.5130876	-4.5977579	1.4067271	C	1.6742962	5.1172949	-1.5069246
C	-0.9139517	-2.6534951	2.1943449	C	1.2607408	5.0156845	-2.8212035
C	-1.7357285	-1.5344518	2.1071090	H	1.1191103	5.9016901	-3.4300510
C	-1.8556050	-5.9452708	-0.2165190	C	1.0368094	3.7544454	-3.3461220
H	-2.1963835	-6.2408604	0.7822885	H	0.7158991	3.6293140	-4.3739554
H	-0.7615265	-5.9987359	-0.2434564	C	1.2242587	2.6328384	-2.5411292

C	1.8615683	3.9472269	-0.7777890	H	-3.2707675	5.2546521	0.9844754
C	0.9751377	1.2549488	-3.0897086	C	-1.0365994	0.8795732	2.9024016
H	1.0041016	1.3090671	-4.1956047	C	-3.2662360	0.9374509	1.2165296
H	1.7776575	0.5927668	-2.7652616	C	-2.6907289	-0.2630948	1.6013504
C	-4.8635920	1.0049773	-0.5891496	H	-3.1422863	-1.1730703	1.2196500
C	-4.1942848	-0.0712405	-1.1617587	C	-5.5672777	1.2507370	0.8851630
C	-2.6408164	1.2980348	-2.1379708	H	-5.5719014	2.2588652	1.3074188
C	-3.2391816	2.4283054	-1.5905425	H	-5.8440329	0.5291477	1.6626406
H	-2.7946675	3.4029441	-1.7415546	H	-6.2911379	1.1954176	0.0714725
C	-4.3760672	2.2790252	-0.8179678	H	0.2356495	0.1407024	4.4724746
H	-4.8570047	3.1432835	-0.3736755	C	1.4730242	0.9005361	2.8822146
C	-1.4253076	1.4630210	-3.0145281	C	2.2955214	-0.2154200	2.7684891
H	-1.7202265	1.2810392	-4.0666609	C	3.4229302	-0.1228387	1.9505492
H	-1.1391290	2.5122411	-2.9557095	H	4.0832908	-0.9749555	1.8361712
N	-0.2769840	0.6511166	-2.6412181	C	3.7385656	1.0103354	1.2339590
N	1.6229470	-1.6222816	-2.1924313	C	2.8941081	2.1279370	1.3300668
N	-3.1281160	0.0756235	-1.9344909	C	1.7875910	2.0520651	2.1574666
N	1.6450287	2.7355901	-1.2804445	H	1.1247713	2.9037488	2.2362584
H	-5.7320919	0.8400864	0.0389569	C	2.3434266	4.3126569	0.6193040
H	2.4414683	-4.7761155	-1.3951018	H	2.2804264	4.7655917	1.6157222
H	1.8612115	6.0808190	-1.0471674	H	1.3399601	4.0173841	0.2935389

Ts23c.xyz

97

Energy = -2408.526649213

O	-4.3063755	0.9280716	0.3290019	C	-1.3926864	-4.4522790	-1.4269449
O	4.8937289	1.0261073	0.5029006	H	-1.8746632	-4.9974235	-0.6034674
O	3.2332694	3.2211566	0.6076407	H	-1.4262413	-5.0986231	-2.3089153
O	-0.0301822	-4.2809787	-1.1588975	C	0.3344636	-3.7120264	0.0164161
O	2.4298291	-4.6927090	-0.3886445	C	-0.5058915	-3.0132878	0.8596031
C	-2.6082743	4.3894420	0.9418024	H	-1.5566354	-2.9343364	0.6149850

C	1.6766352	-3.8786936	0.3913729	H	0.1513429	-1.1711634	-3.3637896
C	2.1408162	-3.2175994	1.5110020	H	0.8612108	0.3321500	-3.9836959
H	3.1859610	-3.2995632	1.7804511	C	-2.6938811	4.7791692	-1.5532556
C	1.3107833	-2.4236561	2.3060228	C	-2.2174417	4.4613377	-2.8169891
C	-0.0464046	-2.3657232	2.0075547	H	-2.6192535	4.9514486	-3.6967691
C	3.6936142	-5.0598716	0.1025541	C	-1.2284335	3.5041860	-2.9357141
H	3.6179003	-5.5230712	1.0929018	H	-0.8381874	3.2211898	-3.9062387
H	4.3752484	-4.2034779	0.1652229	C	-0.7328581	2.8916637	-1.7833376
H	4.0975047	-5.7837384	-0.6044978	C	-2.1252217	4.1464031	-0.4581496
H	-0.6864442	-1.6002592	3.9002173	C	0.3105521	1.8164531	-1.8556638
C	1.9657826	-1.5668844	3.3622798	H	1.0395995	2.1019071	-2.6224095
H	1.3374378	-1.4705723	4.2469902	H	0.8487750	1.7973599	-0.9069643
H	2.8896483	-2.0485217	3.6930183	C	-3.5785525	-3.2885305	-1.6634844
O	-3.3911452	3.2966486	1.4041572	C	-2.1940813	-3.1994038	-1.7104131
H	-1.7547949	4.5716672	1.6015156	C	-2.2595526	-0.9712423	-2.2110747
H	0.2191279	1.8742246	4.2982946	C	-3.6537922	-0.9723306	-2.1949988
H	-1.9355139	-2.3423133	2.9487225	H	-4.1952620	-0.0474068	-2.3505584
C	-1.5821719	-0.3241974	2.4393654	C	-4.3207768	-2.1485866	-1.9230927
C	-1.0699485	-1.6763339	2.8822845	H	-5.4040717	-2.1732142	-1.8852669
C	-2.7479789	2.1302888	1.7164347	C	-1.5854992	0.3541164	-2.4923627
C	0.2213047	0.9390011	3.7316079	H	-1.7949473	0.6046447	-3.5533419
C	-1.6476533	2.0776634	2.5543388	H	-2.1451335	1.0850455	-1.9068689
H	-1.2424457	3.0041311	2.9448882	N	-0.1933979	0.4636867	-2.1536288
C	4.4628435	-1.2837906	-1.4962464	N	2.7813989	0.3198392	-2.0183667
C	3.6626687	-2.2948375	-1.9934598	N	-1.5485623	-2.0714959	-1.9897532
H	4.0045961	-3.3216609	-2.0045698	N	-1.1560807	3.2398202	-0.5725745
C	2.3977345	-1.9849610	-2.4660298	H	-4.0604127	-4.2282180	-1.4161805
H	1.7236697	-2.7636023	-2.8013989	H	5.4498247	-1.4854643	-1.0955342
C	1.9990070	-0.6552842	-2.4807558	H	-3.4871025	5.5049713	-1.4178840
C	3.9686180	0.0163222	-1.5090269				
C	0.6685042	-0.2608491	-3.0674419				

3c.xyz

97

Energy = -2408.536049071

O	-2.1032566	4.1777318	0.7887169
O	3.4678952	-3.6155587	0.7746735
O	4.2815159	-0.9471768	0.6740343
O	-3.4287605	-2.3972552	-1.0816538
O	-2.5046121	-4.6741353	-0.2342122
C	1.8307954	4.5800209	0.8867291
H	2.2158138	5.5977042	0.9612792
C	-0.0331267	1.3257796	3.0092844
C	-1.3997018	3.2641940	1.5235150
C	-2.0288584	2.1015582	1.9385875
H	-3.0773386	1.9867545	1.6852413
C	-2.3728829	5.3987142	1.4558891
H	-1.4507263	5.9186442	1.7252760
H	-2.9697641	5.2224847	2.3580226
H	-2.9456735	6.0131227	0.7609280
H	0.1363587	-0.1024196	4.5993402
C	1.4227662	-0.7459609	3.0022348
C	0.9975493	-2.0710975	2.9814331
C	1.7234743	-2.9815233	2.2145327
H	1.4204277	-4.0219134	2.1777800
C	2.8122116	-2.6241436	1.4461191
C	3.2153492	-1.2790631	1.4388154
C	2.5203650	-0.3769315	2.2255007
H	2.8299667	0.6599110	2.2359450
C	4.5586876	0.4221600	0.4958650
H	4.9190241	0.8824021	1.4233111
H	3.6770134	0.9687220	0.1427227
H	5.3449297	0.4762823	-0.2554935
C	3.6697433	-3.4530889	-0.6279166

H	4.1119022	-4.4013694	-0.9439757
H	4.3707171	-2.6472282	-0.8414311
C	-4.1641300	-1.2736930	-1.5029737
H	-4.9392080	-1.0312712	-0.7651142
H	-4.6608987	-1.6030510	-2.4185435
C	-2.8451770	-2.3823418	0.1393651
C	-2.7797197	-1.2979406	0.9927749
H	-3.2687364	-0.3734760	0.7185416
C	-2.2787870	-3.5989725	0.5596686
C	-1.5296067	-3.6195467	1.7176710
H	-1.0282184	-4.5332783	2.0099663
C	-1.3681631	-2.4875732	2.5225515
C	-2.0657365	-1.3309709	2.1947114
C	-2.0060594	-5.9154430	0.1966924
H	-2.4008483	-6.1868433	1.1821040
H	-0.9103966	-5.9212621	0.2392172
H	-2.3365147	-6.6475638	-0.5384527
H	-1.8452189	-0.3921947	4.1055083
C	-0.3043720	-2.5414456	3.5941695
H	-0.5749850	-1.9483323	4.4668547
H	-0.1903614	-3.5708976	3.9429903
O	0.5312039	4.6302109	1.4601335
H	2.4895189	3.9186495	1.4563800
H	1.5473413	0.8856841	4.3520602
H	-3.1948331	0.1671502	3.1655620
C	-1.3715522	1.1110002	2.6601556
C	-2.1398285	-0.1139684	3.0931393
C	-0.0563697	3.4578641	1.8408291
C	0.7623815	0.3372674	3.8235281
C	0.5914849	2.4973722	2.6004339
H	1.6213202	2.6690151	2.8917597

C	1.2549351	-3.9535812	-1.1599466
C	0.1025737	-3.6466313	-1.8627905
H	-0.8141222	-4.1999517	-1.7058823
C	0.1279530	-2.5990647	-2.7654547
H	-0.7709172	-2.2965649	-3.2892662
C	1.3193993	-1.9107457	-2.9508151
C	2.3950872	-3.1935057	-1.3835093
C	1.4178170	-0.7408112	-3.8989602
H	0.9738566	-1.0013405	-4.8623086
H	2.4854192	-0.5617230	-4.0684335
C	1.9505156	5.0297023	-1.5931194
C	1.8945340	4.5445410	-2.8900075
H	2.0379485	5.2111544	-3.7333008
C	1.6470780	3.1985697	-3.0938671
H	1.6027268	2.7670505	-4.0857498
C	1.4605358	2.3773918	-1.9858155
C	1.7862920	4.1312104	-0.5466058
C	1.1655519	0.9058514	-2.1114309
H	2.0697873	0.3606346	-1.8221672
H	0.4229888	0.6547418	-1.3397327
C	-3.7680750	1.1873979	-1.2746209
C	-3.3616829	-0.0292198	-1.8101990
C	-1.6441197	0.9625091	-2.9490038
C	-1.9702896	2.2125163	-2.4318888
H	-1.3751152	3.0786298	-2.6959525
C	-3.0533358	2.3293982	-1.5822476
H	-3.3114222	3.2848930	-1.1449683
C	-0.5108358	0.8526823	-3.9444477
H	-0.8038455	0.1243611	-4.7022565
H	-0.4486181	1.8285297	-4.4492784
N	0.7910071	0.4767713	-3.4307510

N	2.4270203	-2.1991551	-2.2670463
N	-2.3252734	-0.1403065	-2.6370230
N	1.5522246	2.8371975	-0.7413438
H	-4.6235504	1.2292681	-0.6090698
H	1.2795292	-4.7546763	-0.4309943
H	2.1210879	6.0808067	-1.3925223

Ts34c.xyz

97

Energy = -2408.526626904

O	-4.3497483	1.2255047	0.2659381
O	5.0492294	0.9625678	0.9710362
O	3.4973712	3.2403483	0.9714159
O	-0.3841674	-4.4921552	-0.8566148
O	2.1170470	-4.7819623	-0.1731807
C	-3.1063218	4.3190885	0.1477742
H	-4.1180064	4.5748936	-0.1876232
C	-1.1067474	1.0493288	2.8790083
C	-3.3051205	1.1867523	1.1507684
C	-2.8024776	-0.0316746	1.5722281
H	-3.2990724	-0.9276519	1.2148802
C	-5.5809031	1.6266276	0.8406096
H	-5.5042549	2.6163297	1.2999292
H	-5.9097182	0.9054309	1.5977121
H	-6.3108827	1.6560730	0.0310384
H	0.0491623	0.2747546	4.5176715
C	1.4097795	0.9671664	3.0034244
C	2.1767647	-0.1917419	2.9297792
C	3.3796916	-0.1419562	2.2247763
H	4.0060819	-1.0242198	2.1572188
C	3.8247097	0.9910133	1.5776394

C	3.0315159	2.1479363	1.6206468	H	0.1137436	2.0044599	4.3275741
C	1.8480927	2.1133978	2.3380871	H	-2.2018203	-2.1089133	2.9963950
H	1.2347147	3.0034998	2.3938453	C	-1.7126194	-0.1313433	2.4361943
C	2.6350517	4.3454325	0.8502885	C	-1.2966108	-1.4978427	2.9337860
H	2.4334127	4.8089933	1.8226921	C	-2.7071427	2.3588321	1.6063881
H	1.6854481	4.0612507	0.3828212	C	0.1095534	1.0642829	3.7695156
H	3.1501186	5.0640661	0.2147574	C	-1.6321458	2.2692681	2.4680981
C	5.0650307	1.1677677	-0.4421686	H	-1.1990568	3.1976229	2.8248335
H	6.1195482	1.0858205	-0.7152960	C	4.4485765	-1.2128958	-0.9737060
H	4.7038501	2.1629503	-0.7024731	C	3.6016458	-2.1139141	-1.5974857
C	-1.7521614	-4.4960453	-1.1745743	H	3.7149297	-3.1810322	-1.4573268
H	-2.3438893	-4.8639604	-0.3258501	C	2.5844604	-1.6303191	-2.3968078
H	-1.8447867	-5.2219865	-1.9864487	H	1.8613891	-2.2966899	-2.8523926
C	0.0260764	-3.7854506	0.2219382	C	2.4794541	-0.2562768	-2.5790751
C	-0.7804087	-2.9879523	1.0108427	C	4.2396180	0.1449928	-1.1716410
H	-1.8343725	-2.9081400	0.7815254	C	1.3735546	0.3062878	-3.4342334
C	1.3793402	-3.9237768	0.5740661	H	1.3747778	-0.1977006	-4.4042914
C	1.8671587	-3.2027198	1.6452830	H	1.5963453	1.3678828	-3.6139441
H	2.9138480	-3.2911351	1.9077354	C	-2.4936578	4.4000534	-2.2562983
C	1.0608801	-2.3553072	2.4110011	C	-1.7660649	3.9249262	-3.3289871
C	-0.2932296	-2.2705883	2.1069078	H	-1.8226845	4.4195178	-4.2924079
C	3.3482423	-5.2021244	0.3586773	C	-0.9796068	2.7937513	-3.1672175
H	3.2255896	-5.6195765	1.3644137	H	-0.4147566	2.3881395	-3.9956597
H	4.0806852	-4.3873546	0.4054645	C	-0.9471958	2.1771808	-1.9236389
H	3.7228714	-5.9742674	-0.3121553	C	-2.3659808	3.7434810	-1.0320080
H	-0.9350432	-1.4128489	3.9590864	C	-0.2125054	0.8819612	-1.6587390
C	1.7324897	-1.5268565	3.4810470	H	0.7199723	1.1034426	-1.1289839
H	1.0784888	-1.3979670	4.3430863	H	-0.8219150	0.3169732	-0.9451667
H	2.6099415	-2.0677091	3.8450782	C	-3.5870940	-2.7754956	-1.2660763
O	-3.2452552	3.5887790	1.3495911	C	-2.3013283	-3.1649015	-1.6342336
H	-2.6158639	5.2650429	0.4130609	C	-1.9591212	-1.2249189	-2.7880493

C	-3.2171917	-0.7447108	-2.4501920	H	-5.2938396	-2.0579762	3.4714160
H	-3.5242181	0.2466104	-2.7610671	H	-6.1246334	-2.6762508	2.0214444
C	-4.0495857	-1.5410340	-1.6811975	H	0.1980717	1.5891806	4.0032394
H	-5.0275823	-1.1838250	-1.3821959	C	0.5615141	2.3660171	2.0378496
C	-1.0059120	-0.3952698	-3.6079253	C	1.8598793	1.8811963	1.8889172
H	-0.5985800	-1.0348300	-4.3946466	C	2.6526541	2.4180916	0.8737796
H	-1.5794727	0.4077237	-4.1008519	H	3.6766673	2.0837434	0.7485597
N	0.0939562	0.0767966	-2.8090667	C	2.2098551	3.4077076	0.0206044
N	3.2837879	0.6132017	-1.9738191	C	0.8998640	3.8868087	0.1635793
N	-1.5134095	-2.4145009	-2.3882068	C	0.1043241	3.3551692	1.1649315
N	-1.6062352	2.6767146	-0.8775127	H	-0.9013251	3.7323944	1.2983595
H	-4.1951599	-3.4195881	-0.6398693	C	-0.7245264	5.4989427	-0.4286663
H	5.2468179	-1.5439601	-0.3194710	H	-0.7497327	5.9506501	0.5692697
H	-3.1437294	5.2621715	-2.3568001	H	-1.5571477	4.7948909	-0.5258521
				H	-0.8263676	6.2808328	-1.1798731
4c.xyz				C	2.8337544	3.8118654	-2.2432191
97				H	3.5701992	4.4475286	-2.7384902
Energy = -2408.547952054				H	1.8307142	4.1578032	-2.4974377
O	-4.2695557	-1.9561732	1.6703026	C	0.8953712	-5.0819251	0.4075741
O	3.0970559	3.9765667	-0.8508871	H	0.6986551	-5.3977985	1.4411404
O	0.5136416	4.8775946	-0.6758346	H	1.1286468	-5.9794207	-0.1711812
O	2.0568524	-4.2979910	0.3302856	C	2.0686559	-3.1015377	0.9593171
O	4.0754468	-2.7560185	-0.1992221	C	1.1302736	-2.6687000	1.8751011
C	-4.7848981	0.4620223	-0.2266339	H	0.2941160	-3.3115064	2.1192184
H	-4.8331281	-0.6247119	-0.3374760	C	3.1616156	-2.2665359	0.6685744
C	-1.3658708	0.8406754	2.7409379	C	3.2406484	-1.0339606	1.2844914
C	-3.3380712	-1.0169300	2.0182866	H	4.0758261	-0.3828781	1.0602787
C	-2.1412000	-1.4254448	2.5768040	C	2.2774707	-0.5867218	2.1953276
H	-2.0041680	-2.4890766	2.7385548	C	1.2131433	-1.4229903	2.5076365
C	-5.4803780	-1.8852947	2.4058336	C	5.2716638	-2.0372523	-0.3474814
H	-5.9719736	-0.9176254	2.2772886	H	5.8004679	-1.9380545	0.6080617

H	5.0971842	-1.0385190	-0.7611129	C	-1.3714603	0.7296547	-1.4259994
H	5.8866667	-2.6090302	-1.0415538	C	-3.6126547	1.0013152	-0.9909411
H	0.5385830	-0.3888267	4.2634757	C	-0.1595820	-0.1578893	-1.2734701
C	2.4519184	0.8014848	2.7635736	H	0.7151277	0.4528304	-1.0434005
H	2.0393632	0.8584064	3.7707556	H	-0.3282095	-0.8157438	-0.4192625
H	3.5222488	0.9975623	2.8695126	C	-1.5913083	-4.6806849	0.3581267
O	-4.6767432	0.8046654	1.1652276	C	-0.3318574	-4.4114396	-0.1645264
H	-5.7233813	0.9113245	-0.5523127	C	-1.1761428	-2.9080357	-1.6613096
H	-0.9457530	2.7842409	3.4663551	C	-2.4690514	-3.0999476	-1.1915267
H	-0.1089386	-1.9910202	4.0650407	H	-3.2828240	-2.5084746	-1.5899366
C	-1.1359510	-0.5269418	2.9285122	C	-2.6804025	-4.0149829	-0.1753152
C	0.1412955	-1.0779117	3.5180003	H	-3.6729251	-4.1626625	0.2308359
C	-3.5405497	0.3410983	1.7758199	C	-0.8888938	-1.9361974	-2.7753723
C	-0.3756376	1.9122526	3.1349776	H	-0.5319808	-2.5109352	-3.6370196
C	-2.5687944	1.2418341	2.1678063	H	-1.8320396	-1.4519751	-3.0792116
H	-2.7650972	2.2928641	1.9853637	N	0.1495068	-0.9879997	-2.4323911
C	4.2288571	1.7541479	-2.6436488	N	1.8730047	1.7338900	-2.9992838
C	4.2974026	0.4064402	-2.9529137	N	-0.1336176	-3.5655684	-1.1636867
H	5.2509389	-0.1093757	-2.9592315	N	-2.5139991	0.2512804	-0.9392453
C	3.1298283	-0.2742936	-3.2517471	H	-1.7079278	-5.3739086	1.1844202
H	3.1317013	-1.3388588	-3.4523007	H	5.1150011	2.3192721	-2.3792149
C	1.9339359	0.4332487	-3.2801360	H	-4.5545152	2.8253576	-1.6314653
C	2.9878711	2.3779490	-2.6641876				
C	0.6367086	-0.2617408	-3.5871955	Ts45c.xyz			
H	0.8043468	-0.9938099	-4.3826496	97			
H	-0.0772694	0.4830361	-3.9755798	Energy = -2408.545940667			
C	-3.6383822	2.2465333	-1.6035228	O	-4.7582655	1.1484776	0.5827326
C	-2.4625191	2.7276725	-2.1590186	O	5.0517230	1.2086470	0.5021534
H	-2.4431425	3.6912419	-2.6569238	O	3.5777761	3.5069105	0.5513816
C	-1.3054190	1.9765155	-2.0484025	O	-1.1032581	-4.5656083	-0.5428035
H	-0.3547532	2.3337482	-2.4274987	O	1.5549435	-4.4385369	-0.6093007

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O	-4.7582655	1.1484776	0.5827326
O	5.0517230	1.2086470	0.5021534
O	3.5777761	3.5069105	0.5513816
O	-1.1032581	-4.5656083	-0.5428035
O	1.5549435	-4.4385369	-0.6093007

C	-3.2233766	3.5441380	-0.6960969	H	-2.2623489	-2.9120698	1.2497234
H	-3.9135497	2.7865463	-1.0775272	C	0.8881526	-3.6821967	0.3114754
C	-1.1301752	1.2613586	2.6384660	C	1.5515701	-2.8705050	1.2079922
C	-3.5712051	1.2176188	1.2580472	H	2.6357154	-2.8546255	1.1743973
C	-3.0515078	0.0709606	1.8298093	C	0.8852691	-2.0693355	2.1350495
H	-3.6328498	-0.8396709	1.7348319	C	-0.5090420	-2.0836238	2.1377092
C	-5.8113876	1.9020799	1.1617625	C	2.3790359	-5.4506702	-0.0741541
H	-5.5677906	2.9667774	1.2033515	H	1.7963134	-6.1533094	0.5317804
H	-6.0317482	1.5419365	2.1725498	H	3.1880184	-5.0410685	0.5417959
H	-6.6858609	1.7516101	0.5284935	H	2.8129085	-5.9823282	-0.9213886
H	0.2000098	0.6710370	4.2140537	H	-0.8100068	-1.0789814	4.0133254
C	1.4286109	1.2673744	2.5626769	C	1.7220103	-1.2234296	3.0670279
C	2.1588355	0.0850874	2.4559943	H	1.1936126	-1.0527046	4.0047899
C	3.3489972	0.1065061	1.7294595	H	2.6173415	-1.7926955	3.3306705
H	3.9584472	-0.7870940	1.6581111	O	-3.2649390	3.5601861	0.7411856
C	3.8222329	1.2390569	1.1010259	H	-3.5583529	4.5375675	-0.9950829
C	3.0721488	2.4203207	1.1807676	H	0.1825243	2.3751243	3.8686710
C	1.8969180	2.4127345	1.9155693	H	-2.2293422	-1.8430279	3.3572326
H	1.3254856	3.3269687	2.0114377	C	-1.8330762	0.0584143	2.5062735
C	2.9381267	4.7420073	0.7641938	C	-1.3504647	-1.2535924	3.0829499
H	2.9405627	5.0128820	1.8259814	C	-2.8405887	2.4026871	1.3395077
H	1.9063986	4.7317101	0.3982185	C	0.1715393	1.3897521	3.3952098
H	3.5102939	5.4801483	0.2040611	C	-1.6560566	2.4079400	2.0505633
C	5.0537938	1.2776134	-0.9236736	H	-1.1214396	3.3495399	2.1140112
H	6.1107212	1.2841089	-1.1978272	C	4.7415496	-1.1977239	-1.2528917
H	4.5866047	2.2011535	-1.2719403	C	3.9604314	-2.2455990	-1.7092413
C	-2.4845975	-4.4403052	-0.7688669	H	4.2294021	-3.2733514	-1.4932299
H	-3.0583945	-4.6681610	0.1395923	C	2.8106801	-1.9628910	-2.4250413
H	-2.7149207	-5.2142723	-1.5054354	H	2.1360295	-2.7497609	-2.7381301
C	-0.5114969	-3.7123046	0.3221556	C	2.5032780	-0.6344744	-2.6904610
C	-1.1798802	-2.9067136	1.2313037	C	4.3356283	0.1026148	-1.5261504

C	1.2329256	-0.2794442	-3.4118133	5c.xyz		
H	1.1414121	-0.8948049	-4.3123887	97		
H	1.2940605	0.7713681	-3.7380985	Energy = -2408.548048874		
C	-0.9246750	4.2561939	-1.4847150	O	-4.2290133	-1.8393096 1.6403348
C	0.3814045	3.8902332	-1.7759661	O	3.1147341	4.1403054 -0.9110529
H	1.1188420	4.6428173	-2.0337158	O	0.5298476	4.9997596 -0.7238943
C	0.7426252	2.5561061	-1.7057788	O	2.0623399	-4.2062572 0.1908253
H	1.7634493	2.2330182	-1.8780934	O	4.0460006	-2.4632522 -0.4986460
C	-0.2375558	1.6125445	-1.3965709	C	-4.7912611	0.6105611 -0.2090369
C	-1.8331131	3.2532520	-1.1770146	H	-4.8752891	-0.4730856 -0.3292099
C	0.0638977	0.1374502	-1.3015863	C	-1.3003505	0.9377287 2.6953508
H	1.0239094	-0.0099158	-0.8032981	C	-3.2908831	-0.9056033 1.9841374
H	-0.7000206	-0.3193624	-0.6699708	C	-2.0844891	-1.3238684 2.5148692
C	-4.1249305	-2.5361182	-1.0000817	H	-1.9474505	-2.3901124 2.6586342
C	-2.8853437	-3.0860018	-1.3048302	C	-5.4306594	-1.7724736 2.3912592
C	-2.2566610	-1.2393444	-2.4923444	H	-5.9229944	-0.8035307 2.2760903
C	-3.4621088	-0.6033990	-2.2265615	H	-5.2312347	-1.9528271 3.4532202
H	-3.6234875	0.4134467	-2.5597734	H	-6.0802747	-2.5601313 2.0091704
C	-4.4179201	-1.2724066	-1.4815772	H	0.2851835	1.6722581 3.9387361
H	-5.3539078	-0.7888228	-1.2324503	C	0.6143874	2.4781214 1.9803303
C	-1.1663159	-0.5669008	-3.2846983	C	1.9130371	2.0006574 1.8138778
H	-1.0204369	-1.1348742	-4.2098948	C	2.7017349	2.5648999 0.8117223
H	-1.4999508	0.4435994	-3.5742370	H	3.7270087	2.2390902 0.6794046
N	0.0910976	-0.5722653	-2.5727072	C	2.2469533	3.5605076 -0.0270819
N	3.2514575	0.3747237	-2.2471491	C	0.9307565	4.0194949 0.1193741
N	-1.9876293	-2.4638110	-2.0515119	C	0.1449091	3.4755242 1.1231849
N	-1.5009637	1.9642374	-1.1732218	H	-0.8628812	3.8436836 1.2660934
H	-4.8287029	-3.0747018	-0.3743668	C	-0.7177667	5.6024504 -0.4793276
H	5.6335709	-1.3713183	-0.6622282	H	-0.7493466	6.0609211 0.5154320
H	-1.2326465	5.2955355	-1.4836360	H	-1.5390559	4.8841561 -0.5700393
				H	-0.8336419	6.3772817 -1.2357765

C	2.8872182	3.8510935	-2.2905494	H	-2.7098240	2.4020783	1.9852473
H	3.6477216	4.4270860	-2.8217883	C	4.1862181	1.6968613	-2.2521209
H	1.8970278	4.1888340	-2.6035859	C	4.2041311	0.3182577	-2.3770799
C	0.9130858	-5.0077248	0.3132445	H	5.0813138	-0.2560078	-2.1032553
H	0.7544986	-5.3146835	1.3553654	C	3.0638524	-0.3276601	-2.8205027
H	1.1419611	-5.9072380	-0.2638610	H	3.0125654	-1.4083435	-2.8641047
C	2.0872031	-3.0030822	0.8124986	C	1.9534513	0.4366697	-3.1551170
C	1.1786209	-2.5855743	1.7718264	C	3.0173883	2.3791511	-2.5658531
H	0.3608126	-3.2387931	2.0483880	C	0.6731980	-0.2313988	-3.5732612
C	3.1348332	-2.1393583	0.4656483	H	0.8833854	-0.9669446	-4.3562580
C	3.2216159	-0.9098160	1.0833485	H	0.0035712	0.5279261	-4.0083361
H	4.0438129	-0.2666882	0.7891063	C	-3.6208892	2.3600477	-1.6177134
C	2.3075901	-0.4800583	2.0454052	C	-2.4389707	2.8056972	-2.1915298
C	1.2651890	-1.3378465	2.3933810	H	-2.4009467	3.7639774	-2.6983330
C	4.9458384	-3.5016119	-0.1546100	C	-1.2990713	2.0280829	-2.0852941
H	4.4213618	-4.4406890	0.0355265	H	-0.3440169	2.3614590	-2.4764514
H	5.5343602	-3.2265995	0.7284241	C	-1.3908389	0.7897125	-1.4493139
H	5.6144344	-3.6271633	-1.0063505	C	-3.6203205	1.1196781	-0.9954182
H	0.6266505	-0.3158927	4.1712179	C	-0.2026055	-0.1254189	-1.2895801
C	2.5079522	0.8917064	2.6464945	H	0.6823960	0.4618020	-1.0372810
H	2.1188969	0.9232843	3.6640815	H	-0.4019991	-0.7863224	-0.4441549
H	3.5828417	1.0700094	2.7339274	C	-1.5799231	-4.6184631	0.3291787
O	-4.6403862	0.9351055	1.1837876	C	-0.3352794	-4.3539630	-0.2297683
H	-5.7229305	1.0918280	-0.5071683	C	-1.2167943	-2.8599349	-1.7145249
H	-0.8704111	2.8715133	3.4385719	C	-2.4971860	-3.0484155	-1.2111256
H	-0.0335919	-1.9131400	3.9700343	H	-3.3205506	-2.4569490	-1.5895947
C	-1.0704101	-0.4328383	2.8614218	C	-2.6819999	-3.9566884	-0.1830788
C	0.2135471	-0.9970542	3.4272178	H	-3.6637811	-4.1000653	0.2498446
C	-3.4949670	0.4562473	1.7638619	C	-0.9384751	-1.8747379	-2.8193460
C	-0.3046488	2.0054590	3.0850113	H	-0.5862933	-2.4342908	-3.6926671
C	-2.5131032	1.3482515	2.1499169	H	-1.8806748	-1.3805766	-3.1097560

N	0.1059513	-0.9473315	-2.4509901
N	1.9322417	1.7624884	-3.0263321
N	-0.1637150	-3.5176882	-1.2403370
N	-2.5403767	0.3428391	-0.9507462
H	-1.6755650	-5.3027349	1.1655881
H	5.0449181	2.2425860	-1.8784643
H	-4.5214108	2.9631043	-1.6399446

Ts56c.xyz

97

Energy = -2408.546345000

O	-4.6793348	1.2264463	0.4746970
O	5.0807681	1.2582323	0.6395585
O	3.6018520	3.5513241	0.7416952
O	-1.0185401	-4.4737510	-0.7168411
O	1.7070280	-4.3565827	-0.6560610
C	-3.1798414	3.6541135	-0.6192011
H	-3.8717101	2.9274200	-1.0520469
C	-1.1299204	1.2293358	2.6642468
C	-3.5231377	1.2203868	1.2065364
C	-3.0170688	0.0563604	1.7568738
H	-3.5728488	-0.8629050	1.6050283
C	-5.8504634	0.9664278	1.2206046
H	-5.9825345	1.7096578	2.0141385
H	-5.8331108	-0.0328891	1.6694269
H	-6.6879485	1.0298519	0.5252274
H	0.1657268	0.5921835	4.2514229
C	1.4264518	1.2442476	2.6450780
C	2.1617377	0.0677729	2.5134065
C	3.3628570	0.1143792	1.8062295
H	3.9741562	-0.7759963	1.7148762

C	3.8430286	1.2673181	1.2215492
C	3.0889753	2.4440966	1.3275348
C	1.9020102	2.4106816	2.0423958
H	1.3261487	3.3199292	2.1571439
C	2.9554436	4.7775643	0.9833322
H	2.9389054	5.0138609	2.0532226
H	1.9302424	4.7770532	0.5993165
H	3.5352994	5.5346237	0.4573828
C	5.1025563	1.3729101	-0.7834745
H	6.1632427	1.3836052	-1.0426653
H	4.6439892	2.3092692	-1.1082148
C	-2.3984246	-4.3504085	-0.9553648
H	-2.9796453	-4.6150426	-0.0621595
H	-2.6139517	-5.0997328	-1.7213585
C	-0.4432866	-3.6701737	0.2097737
C	-1.1340838	-2.8982570	1.1297619
H	-2.2165657	-2.8978842	1.1152254
C	0.9574579	-3.6526168	0.2426729
C	1.5955258	-2.8678704	1.1796561
H	2.6800089	-2.8765367	1.1746303
C	0.9071615	-2.0825150	2.1044615
C	-0.4864625	-2.0999266	2.0751273
C	1.6714337	-5.7638837	-0.4993318
H	0.6604391	-6.1567705	-0.6288635
H	2.0520160	-6.0528785	0.4872865
H	2.3213412	-6.1783008	-1.2700998
H	-0.8321579	-1.1513926	3.9712932
C	1.7203710	-1.2604972	3.0774259
H	1.1730668	-1.1199401	4.0093999
H	2.6135762	-1.8328709	3.3410931
O	-3.2408467	3.5858428	0.8144714

H	-3.5034887	4.6660599	-0.8638057
H	0.1498123	2.3068146	3.9600064
H	-2.2343326	-1.8987443	3.2623453
C	-1.8249293	0.0287189	2.4773903
C	-1.3515589	-1.2992447	3.0245220
C	-2.8109592	2.4077791	1.3579374
C	0.1525825	1.3367726	3.4557024
C	-1.6429036	2.3917915	2.0974813
H	-1.1182563	3.3338837	2.2135358
C	4.7714695	-1.0895706	-1.1771008
C	3.9880554	-2.1189279	-1.6701115
H	4.2285383	-3.1542236	-1.4591798
C	2.8600937	-1.8061348	-2.4076038
H	2.1821690	-2.5779524	-2.7498497
C	2.5753488	-0.4692138	-2.6538395
C	4.3874743	0.2209533	-1.4323475
C	1.3224441	-0.0859885	-3.3912170
H	1.2462111	-0.6732645	-4.3117863
H	1.3938110	0.9740320	-3.6833677
C	-0.8683814	4.3945974	-1.3495728
C	0.4419421	4.0381639	-1.6338327
H	1.1838424	4.7990931	-1.8512104
C	0.8019454	2.7020152	-1.6057872
H	1.8257385	2.3843664	-1.7708821
C	-0.1840447	1.7494712	-1.3476844
C	-1.7834746	3.3825957	-1.0953864
C	0.1156792	0.2721042	-1.2920271
H	1.0670500	0.1095026	-0.7820683
H	-0.6590568	-0.2021926	-0.6868219
C	-4.0620996	-2.4644766	-1.1633737
C	-2.8042513	-2.9822534	-1.4507767

C	-2.1770644	-1.0886254	-2.5629257
C	-3.3995940	-0.4813440	-2.3086848
H	-3.5706160	0.5428660	-2.6132156
C	-4.3636684	-1.1915125	-1.6141249
H	-5.3196201	-0.7358566	-1.3880077
C	-1.0813526	-0.3761977	-3.3121026
H	-0.9182506	-0.9068416	-4.2565142
H	-1.4207531	0.6414505	-3.5674736
N	0.1643281	-0.4001094	-2.5823726
N	3.3235746	0.5222005	-2.1720803
N	-1.8988485	-2.3223751	-2.1533460
N	-1.4515889	2.0937900	-1.1366588
H	-4.7748013	-3.0372700	-0.5793639
H	5.6458245	-1.2856586	-0.5673662
H	-1.1749730	5.4336843	-1.3125716

6c.xyz

97

Energy = -2408.550596753

O	-2.1063565	4.4474628	1.0413649
O	4.2320818	-3.1810605	0.6477260
O	5.0726074	-0.5967543	0.8749226
O	-4.3084067	-1.7880529	-0.5140415
O	-2.4138590	-3.8330767	-0.7666827
C	0.5975843	4.6123490	-0.4027705
H	-0.4323209	4.6217648	-0.7695222
C	0.2134971	1.5113150	2.8725440
C	-1.3940627	3.4534801	1.6269698
C	-1.9498468	2.3247483	2.2039482
H	-3.0245244	2.1933792	2.1875883
C	-3.4825809	4.5067355	1.3224231

H	-3.6647479	4.5337352	2.4024541	H	-2.4908845	-2.5103665	-2.3722464
H	-4.0243847	3.6593605	0.8905245	H	-3.9391703	-3.5197357	-2.1487366
H	-3.8475122	5.4291578	0.8719121	H	-2.4366992	-4.2678665	-2.7318063
H	0.6013956	0.0316176	4.3731804	H	-1.3724747	-0.2983974	4.1888453
C	1.8693763	-0.4445610	2.7166567	C	0.0972559	-2.2636027	3.0336470
C	1.4121730	-1.7450004	2.5029172	H	-0.1090595	-1.8370646	4.0156198
C	2.2184295	-2.6148251	1.7688276	H	0.1981404	-3.3400316	3.1939569
H	1.9127940	-3.6445470	1.6205756	O	0.6060753	4.6595787	1.0307884
C	3.4358689	-2.2385081	1.2396519	H	1.1095342	5.5226188	-0.7164285
C	3.8748130	-0.9202892	1.4174552	H	1.8980292	1.1558964	4.0992428
C	3.0875814	-0.0538022	2.1585714	H	-2.8770381	0.3662635	3.6161604
H	3.4345707	0.9553264	2.3393208	C	-1.1677132	1.3344744	2.8013360
C	5.5971327	0.6770697	1.1606393	C	-1.8667790	0.0926609	3.3001111
H	5.7509181	0.8125643	2.2370461	C	-0.0020066	3.5906696	1.6295218
H	4.9461068	1.4748860	0.7880251	C	1.1417659	0.5559702	3.5852190
H	6.5584396	0.7302941	0.6517740	C	0.7633700	2.6431733	2.2738154
C	4.3942339	-3.0617627	-0.7635943	H	1.8362054	2.8023516	2.2855007
H	5.1240779	-3.8302788	-1.0260050	C	2.4170903	-4.4937162	-1.3645132
H	4.7924774	-2.0812725	-1.0324232	C	1.1716452	-4.6167737	-1.9544456
C	-4.9567041	-0.5691031	-0.7554264	H	0.6108905	-5.5415635	-1.8803639
H	-5.4421387	-0.1829749	0.1505939	C	0.6440355	-3.5288414	-2.6271656
H	-5.7537676	-0.8130333	-1.4636697	H	-0.3369996	-3.5685273	-3.0794630
C	-3.2284867	-1.8022782	0.3152559	C	1.3835729	-2.3563613	-2.6947869
C	-3.0295472	-0.8844959	1.3310573	C	3.0896608	-3.2825742	-1.4752793
H	-3.7319792	-0.0670441	1.4419804	C	0.8114487	-1.1312548	-3.3512329
C	-2.3107299	-2.8504783	0.1617759	H	0.3463452	-1.4156161	-4.3006459
C	-1.2659069	-2.9424141	1.0641691	H	1.6357779	-0.4396743	-3.5873902
H	-0.5750662	-3.7677275	0.9286106	C	2.6719880	3.3647230	-1.1236692
C	-1.0772543	-2.0389356	2.1076691	C	3.2750161	2.1518391	-1.4168049
C	-1.9743229	-0.9785965	2.2373371	H	4.3402812	2.0993660	-1.6146981
C	-2.8510910	-3.4989114	-2.0772478	C	2.5058644	1.0010551	-1.4308341

H	2.9441483	0.0261647	-1.6126208	O	1.2480454	-4.3850929	0.6425067
C	1.1350453	1.1080389	-1.1986236	C	-2.9060998	3.1973240	-1.7914976
C	1.3035307	3.3801337	-0.8880510	H	-3.5600819	2.3486095	-2.0100391
C	0.2246323	-0.0968910	-1.2079090	C	-1.2901106	2.0001587	2.2432391
H	0.7236106	-0.9385564	-0.7246423	C	-3.6405381	1.6280026	0.7484234
H	-0.6560550	0.1401025	-0.6094199	C	-3.2338918	0.6968832	1.6886749
C	-4.3957421	1.8377604	-1.2161586	H	-3.8369885	-0.1863816	1.8579801
C	-4.0650155	0.4952174	-1.3517013	C	-5.7612715	0.6373310	0.4624085
C	-2.1706557	0.9902240	-2.5327039	H	-6.0309139	0.8380390	1.5052483
C	-2.4169334	2.3542842	-2.4376936	H	-5.4388903	-0.4046865	0.3717425
H	-1.7067722	3.0620606	-2.8451249	H	-6.6323200	0.7964464	-0.1724919
C	-3.5578141	2.7815362	-1.7839623	H	-0.0576186	1.7715985	3.9849269
H	-3.7716080	3.8398970	-1.6893427	C	1.2549478	2.0024330	2.3052142
C	-0.9550887	0.4811286	-3.2612606	C	1.9485511	0.7982444	2.4185028
H	-1.2916151	0.0260827	-4.2005279	C	3.1817123	0.6787887	1.7695951
H	-0.3254649	1.3442295	-3.5358462	H	3.7655332	-0.2232247	1.9094794
N	-0.2258507	-0.5322333	-2.5289989	C	3.7201466	1.6934551	0.9970151
N	2.5868583	-2.2428998	-2.1349916	C	2.9901425	2.8825613	0.8443667
N	-2.9929917	0.0838078	-2.0131528	C	1.7885281	3.0199252	1.5143776
N	0.5536984	2.2818256	-0.9580661	H	1.2418505	3.9505017	1.4370657
H	-5.2850128	2.1312918	-0.6684037	C	2.9273722	5.1011932	0.0467348
H	2.8619752	-5.3087290	-0.8057825	H	2.8932817	5.5439755	1.0488705
H	3.2473909	4.2813891	-1.0623551	H	1.9093458	5.0529283	-0.3557062

Ts67c.xyz

97

Energy = -2408.541513490

O	-4.7753348	1.5326011	0.0123779
O	4.9841432	1.7001197	0.5049373
O	3.5443099	3.8385571	0.0642155
O	-1.5631168	-4.3971087	0.6653750

C	5.5452654	0.6991630	-0.3381047
H	6.4679614	0.3657764	0.1449597
H	5.8076718	1.1997487	-1.2751878
C	-2.8568392	-4.1640017	0.1775352
H	-3.5687582	-3.9794696	0.9929052
H	-3.1515271	-5.1067499	-0.2926001
C	-0.8884750	-3.3664522	1.2487344

C	-1.5132650	-2.3365749	1.9283590	C	4.6977673	-0.4912624	-0.6701445
H	-2.5962198	-2.3170575	1.9599325	C	1.8011946	-1.0945410	-2.8244833
C	0.5110638	-3.3996077	1.2135207	H	1.8269425	-1.8545190	-3.6124893
C	1.2052352	-2.3996808	1.8739563	H	1.9327243	-0.1173432	-3.3136534
H	2.2879119	-2.4486757	1.8334075	C	-0.4916011	3.6988252	-2.3527944
C	0.5830452	-1.3667613	2.5713621	C	0.8321921	3.2878962	-2.3307089
C	-0.8131087	-1.3370150	2.6009084	H	1.6266835	3.9639348	-2.6267651
C	0.7914405	-4.9922938	-0.5582830	C	1.1348939	2.0103661	-1.8928596
H	0.2888008	-4.2655734	-1.2008015	H	2.1615514	1.6735492	-1.8055222
H	0.1101671	-5.8180727	-0.3500992	C	0.0893041	1.1582446	-1.5402012
H	1.6840304	-5.3841288	-1.0501878	C	-1.4706324	2.7930210	-1.9656007
H	-1.0807374	0.0939007	4.1845725	C	0.3340726	-0.2526868	-1.0664336
C	1.4656670	-0.3551354	3.2707881	H	1.2081611	-0.2735935	-0.4133732
H	0.9586707	0.0288433	4.1570156	H	-0.5214200	-0.5650150	-0.4665615
H	2.3453355	-0.8863046	3.6436294	C	-4.1623248	-2.4162156	-1.0683265
O	-3.1401069	3.6592524	-0.4528711	C	-2.9458941	-3.0463879	-0.8362440
H	-3.1704412	4.0415143	-2.4290835	C	-1.8686222	-1.7179576	-2.3544456
H	-0.0431734	3.3605878	3.2794964	C	-3.0377101	-1.0246640	-2.6409010
H	-2.5240923	-0.7644746	3.7233573	H	-3.0169426	-0.1905086	-3.3300948
C	-2.0513746	0.8466214	2.4166624	C	-4.2061636	-1.3949045	-2.0008782
C	-1.6274538	-0.2848378	3.3215789	H	-5.1317082	-0.8674049	-2.2005614
C	-2.8286083	2.7433422	0.5144158	C	-0.5773422	-1.3581357	-3.0416766
C	-0.0365520	2.2958315	3.0302453	H	-0.3343208	-2.1602656	-3.7489365
C	-1.7020403	2.9246176	1.2854928	H	-0.7433394	-0.4467604	-3.6401105
H	-1.1149899	3.8166244	1.0970589	N	0.5372519	-1.2363406	-2.1279034
C	4.9689165	-1.7318926	-0.1110520	N	3.7089622	-0.2961506	-1.5440449
C	4.1820780	-2.8145659	-0.4728926	N	-1.8358933	-2.7225297	-1.4832506
H	4.3553696	-3.7971185	-0.0496871	N	-1.1835786	1.5437919	-1.6048115
C	3.1574404	-2.6089906	-1.3725209	H	-5.0489147	-2.7153488	-0.5192684
H	2.5021957	-3.4122698	-1.6758498	H	5.7803339	-1.8409886	0.5993177
C	2.9493190	-1.3317608	-1.8829763	H	-0.7645327	4.7061346	-2.6462414

PATH AB**Ts12b.xyz**

97

Energy = -2408.525272940

O	-1.7411613	4.1891708	0.6486103
O	3.4790598	-3.2347576	-0.3517729
O	4.8920079	-0.9495488	0.0461493
O	-4.2563553	-1.7732613	0.0679940
O	-2.9300215	-4.0044652	0.1244707
C	2.3013611	4.3673238	-0.0033487
H	2.4562043	5.2889205	-0.5713427
C	0.7170077	1.5236416	2.6987968
C	-0.9052396	3.3589921	1.3373112
C	-1.4491947	2.3467831	2.0995350
H	-2.5315396	2.2965356	2.1460442
C	-1.7326589	5.5429667	1.0614523
H	-0.7489412	5.9989160	0.9270749
H	-2.0343496	5.6294125	2.1118095
H	-2.4603380	6.0607969	0.4366308
H	1.1985578	0.1810826	4.3076084
C	2.1814214	-0.5180423	2.5228341
C	1.5532580	-1.7564539	2.4020302
C	2.0113476	-2.6334670	1.4196014
H	1.5236349	-3.5899105	1.2699182
C	3.0768746	-2.3383583	0.5985541
C	3.7805944	-1.1447727	0.8000923
C	3.3094869	-0.2502889	1.7441915
H	3.8240749	0.6922513	1.8836857
C	5.8388461	-0.0295816	0.5311129
H	6.1136990	-0.2575983	1.5668119

H	5.4753630	1.0014099	0.4776393
H	6.7169258	-0.1284495	-0.1065859
C	3.1815581	-2.8252668	-1.6875791
H	3.7704029	-3.4899223	-2.3231708
H	3.5010286	-1.7939528	-1.8520480
C	-5.0883509	-0.6487812	0.0703790
H	-5.3378511	-0.3477402	1.0976834
H	-6.0197091	-0.9753577	-0.3986158
C	-3.2064516	-1.8169222	0.9242121
C	-2.8316840	-0.8033933	1.7806731
H	-3.3966650	0.1192038	1.7867933
C	-2.4733771	-3.0138213	0.9277143
C	-1.3542529	-3.1037706	1.7308176
H	-0.7699987	-4.0146753	1.7243181
C	-0.9356814	-2.0500295	2.5479551
C	-1.7077605	-0.8965172	2.6037141
C	-2.3320962	-5.2677054	0.2618632
H	-2.4206943	-5.6416843	1.2886574
H	-1.2742305	-5.2507613	-0.0213999
H	-2.8700208	-5.9342685	-0.4114304
H	-0.8091746	-0.0409610	4.3583848
C	0.3856864	-2.1966281	3.2573394
H	0.3838828	-1.6592612	4.2050634
H	0.5323164	-3.2503489	3.5111710
O	0.9689472	4.4367854	0.4272554
H	2.9992947	4.3914869	0.8438180
H	2.5232466	1.1751029	3.7657841
H	-2.3222182	0.6790269	3.8872512
C	-0.6710588	1.4031539	2.7684597
C	-1.3821388	0.2851580	3.4907660
C	0.4874421	3.4457999	1.2201955

C	1.6703628	0.5879956	3.4140692	H	-1.1020966	2.5469261	-2.5377948
C	1.2687526	2.5423793	1.9203995	H	-0.8647739	2.1316899	-0.8719463
H	2.3472092	2.6045322	1.8442280	N	-0.4373207	0.5906824	-2.2074649
C	1.1287908	-4.2040810	-2.1078367	N	1.0276483	-1.8186107	-2.1654981
C	-0.2272000	-4.2765605	-2.3830233	N	-3.2487521	0.5776888	-0.9483934
H	-0.7221438	-5.2368728	-2.4756951	N	1.5970740	2.6232144	-1.5341692
C	-0.9418194	-3.1046179	-2.5333224	H	-6.4821844	1.4758840	-0.8593636
H	-2.0097806	-3.1221897	-2.7179799	H	1.7281816	-5.0967275	-1.9715963
C	-0.2751818	-1.8848666	-2.4219075	H	4.7296805	3.2568235	-0.5133352
C	1.7144574	-2.9502841	-2.0047489				
C	-1.0826684	-0.6209365	-2.6248715	2b.xyz			
H	-1.9936148	-0.7426591	-2.0386794	97			
H	-1.3993821	-0.6005277	-3.6881934	Energy = -2408.543613005			
C	3.9261920	2.7650813	-1.0518325	O	-3.2085726	3.8304208	0.2464521
C	4.1781620	1.7095821	-1.9113141	O	3.8545724	-3.1681591	0.7792187
H	5.1886297	1.3470512	-2.0604603	O	4.3192378	-0.5666710	-0.0725066
C	3.1160832	1.1037752	-2.5565466	O	-3.4753943	-2.8968934	-0.1969959
H	3.2690973	0.2542032	-3.2098527	O	-2.0106732	-4.8341576	0.7509722
C	1.8316151	1.5912736	-2.3417150	C	0.6487693	5.1112022	-0.2833354
C	2.6108486	3.1836990	-0.8933681	H	0.5273154	6.1068668	-0.7199080
C	0.6571831	0.9885743	-3.0660412	C	-0.1760833	1.8008372	2.2579527
H	0.3180190	1.7217439	-3.8239237	C	-2.1960001	3.1922453	0.9037591
H	1.0133872	0.1124171	-3.6037436	C	-2.4875216	2.1123758	1.7108143
C	-5.4237992	1.5455405	-1.0856583	H	-3.5328204	1.8396572	1.8111709
C	-4.5488430	0.5396321	-0.6938017	C	-3.5138055	5.1240648	0.7355388
C	-2.7435065	1.6092465	-1.6244469	H	-2.6626028	5.8020916	0.6339837
C	-3.5543961	2.6537583	-2.0642500	H	-3.8203273	5.0789366	1.7868242
H	-3.1196142	3.4827495	-2.6085104	H	-4.3445544	5.4951579	0.1353703
C	-4.9080479	2.6228849	-1.7828964	H	0.5879178	0.8964283	4.0332340
H	-5.5566574	3.4258762	-2.1150125	C	1.6462994	-0.0298491	2.4182490
C	-1.2558590	1.7362131	-1.8138721	C	1.4398385	-1.3471869	2.8323980

C	2.2058566	-2.3521159	2.2454449	H	0.6413419	-2.6684042	4.3088894
H	2.0600041	-3.3865822	2.5357048	O	-0.6531956	4.6481398	-0.0711044
C	3.1453994	-2.1077929	1.2642733	H	1.1869398	5.2409460	0.6648144
C	3.3521145	-0.7872618	0.8470855	H	1.7108513	1.9315895	3.2057881
C	2.5946798	0.2189205	1.4266764	H	-2.9786961	0.4070531	3.5483166
H	2.7619160	1.2424884	1.1127241	C	-1.5065830	1.3957322	2.3923154
C	4.1489021	0.5473000	-0.9215588	C	-1.9359155	0.2407239	3.2621655
H	4.3138713	1.4934030	-0.3940672	C	-0.8620186	3.5796405	0.7397924
H	3.1526912	0.5351216	-1.3729402	C	0.9505186	1.1627837	3.0399505
H	4.9007873	0.4510606	-1.7047809	C	0.1224980	2.8817789	1.4243624
C	3.8723129	-3.3580106	-0.6402201	H	1.1590906	3.1799985	1.3197501
H	4.3362665	-4.3378198	-0.7688097	C	1.5865537	-4.3597002	-0.9440432
H	4.4792766	-2.5965236	-1.1280367	C	0.3017408	-4.2670388	-1.4426883
C	-4.2452116	-1.8848293	-0.7858393	H	-0.4421670	-5.0230298	-1.2273332
H	-5.0366822	-1.5527750	-0.0986318	C	-0.0394613	-3.1591562	-2.2006082
H	-4.7398640	-2.3678051	-1.6328101	H	-1.0518539	-3.0191982	-2.5561475
C	-2.7417819	-2.6078109	0.9042057	C	0.9290756	-2.2004660	-2.4576171
C	-2.7612284	-1.4114062	1.5905125	C	2.4897054	-3.3393918	-1.2293772
H	-3.4520165	-0.6350891	1.2859370	C	0.6136306	-0.9857613	-3.2895058
C	-1.8902234	-3.6287207	1.3591413	H	-0.4149025	-1.0727678	-3.6770937
C	-0.9792571	-3.3388922	2.3536232	H	1.2877073	-0.9816376	-4.1522454
H	-0.2663439	-4.0948486	2.6559289	C	2.8294154	4.5318115	-1.3782939
C	-0.8994931	-2.0747198	2.9463448	C	3.5484144	3.7835627	-2.2933611
C	-1.8486013	-1.1196512	2.6078718	H	4.6049933	3.9708882	-2.4488601
C	-1.2591523	-5.8969282	1.2784099	C	2.9010732	2.7795111	-2.9933349
H	-1.4814259	-6.0578040	2.3394425	H	3.4367804	2.1529998	-3.6961944
H	-0.1814636	-5.7303127	1.1642057	C	1.5479587	2.5632143	-2.7602604
H	-1.5447154	-6.7832558	0.7129813	C	1.4725247	4.2671740	-1.2298157
H	-1.3724480	0.2439743	4.1953537	C	0.8255594	1.4175887	-3.4148890
C	0.3292943	-1.7700862	3.7702095	H	-0.1857903	1.7390869	-3.7078427
H	0.1336238	-1.0113386	4.5270701	H	1.3550620	1.1489728	-4.3321966

C	-4.2007258	0.4692740	-1.6316956	H	-3.7045264	-1.8272626	1.3255805
C	-3.4837885	-0.6644274	-1.2646625	C	-6.0734082	-0.1734007	1.2213509
C	-1.4773786	0.4105776	-1.5303114	H	-6.2403293	0.3882892	2.1471238
C	-2.1151995	1.5956778	-1.8852086	H	-5.9618274	-1.2351398	1.4666398
H	-1.5337768	2.4978365	-2.0303345	H	-6.9354744	-0.0509313	0.5656945
C	-3.4975362	1.6123984	-1.9635805	H	-0.0906114	-0.4985074	4.1393147
H	-4.0182762	2.5272905	-2.2183973	C	1.2586028	0.2185740	2.6387317
C	0.0217141	0.3484045	-1.3467141	C	2.0643187	-0.9208178	2.5964514
H	0.3360708	1.2373635	-0.7999087	C	3.2969700	-0.8349710	1.9529160
H	0.2447152	-0.5137021	-0.7162307	H	3.9399429	-1.7057926	1.8910199
N	0.8327820	0.2454601	-2.5558827	C	3.7499521	0.3173956	1.3429447
N	2.1714698	-2.2924083	-1.9828749	C	2.9421964	1.4604084	1.3838733
N	-2.1599446	-0.7045217	-1.2577796	C	1.7141840	1.3835343	2.0226655
N	0.8487196	3.3192423	-1.9132948	H	1.0928674	2.2703725	2.0639718
H	-5.2856550	0.4618970	-1.6210785	C	2.4931761	3.5136686	0.3220406
H	1.8976108	-5.1967181	-0.3290202	H	1.9554665	4.0348732	1.1218451
H	3.3056650	5.3124563	-0.7950013	H	1.7857888	3.0093138	-0.3423807

Ts23b.xyz

97

Energy = -2408.541995141

O	-4.9562702	0.3288444	0.5194322	C	-1.6684413	-3.7136956	-2.2983485
O	4.9855533	0.2913441	0.7638574	H	-2.4370626	-4.2850300	-1.7581098
O	3.4336229	2.5931286	0.8316542	H	-1.7023375	-4.0404061	-3.3411493
O	-0.3881805	-4.0693610	-1.8537933	C	-0.0410662	-3.8055131	-0.5713266
O	2.0507250	-4.6891017	-1.1700657	C	-0.8822143	-3.3066956	0.4013443
C	-3.1917685	3.8603716	1.3654945	H	-1.9292047	-3.1548487	0.1706807
H	-3.9997949	4.5831103	1.2193361	C	1.2983488	-4.0620462	-0.2329587
C	-1.3271454	0.2352984	2.5622231	C	1.7651808	-3.6386440	0.9940497
C	-3.7734275	0.2856355	1.1985103	H	2.8136909	-3.7600311	1.2325786
C	-3.1859267	-0.9065035	1.5715063	C	0.9420668	-2.9952267	1.9237094

C	-0.4150624	-2.8902879	1.6507958	H	0.3174666	6.5938750	0.0030664
C	3.3528899	-5.0646582	-0.8015339	C	-0.0445041	4.8927595	-1.2595986
H	3.3485985	-5.7138683	0.0813814	H	0.7531911	5.1144269	-1.9582199
H	3.9858488	-4.1931214	-0.5965624	C	-0.8299820	3.7600432	-1.4375387
H	3.7641370	-5.6125843	-1.6485663	C	-2.0462849	4.2266418	0.4482472
H	-0.9969881	-2.2879917	3.6267435	C	-0.5421373	2.7890200	-2.5499278
C	1.6164767	-2.2857016	3.0739845	H	-1.4898385	2.4316700	-2.9813422
H	0.9652245	-2.2115081	3.9439564	H	-0.0074717	3.3162511	-3.3436677
H	2.4924547	-2.8560054	3.3932941	C	-3.3371409	-1.8526230	-2.4136887
O	-3.7711731	2.6153900	1.1101172	C	-2.0168412	-2.2406349	-2.2116664
H	-2.8707703	3.9473500	2.4123235	C	-1.3817811	-0.1080186	-1.6621996
H	-0.0669188	1.2271695	3.9413770	C	-2.6828833	0.3611236	-1.8179207
H	-2.2623625	-3.0171544	2.6826756	H	-2.9216546	1.3847470	-1.5567164
C	-1.9714333	-0.9648216	2.2501430	C	-3.6665122	-0.5225983	-2.2287478
C	-1.4220081	-2.3189766	2.6234771	H	-4.6893815	-0.1846574	-2.3421665
C	-3.1221376	1.4880330	1.4887887	C	-0.2799561	0.7856645	-1.1402590
C	-0.0581292	0.2863962	3.3831890	H	-0.6749182	1.3608047	-0.3027742
C	-1.9096910	1.4403284	2.1633359	H	0.5105524	0.1445608	-0.7471251
H	-1.3999507	2.3644032	2.4097542	N	0.3230676	1.7162398	-2.0891353
C	4.1796684	-1.3432806	-1.7273998	N	3.0877060	0.7662031	-1.9570175
C	3.1942003	-1.9549645	-2.4774468	N	-1.0595525	-1.3842179	-1.8892502
H	3.2155007	-3.0186976	-2.6756987	N	-1.8297424	3.4573937	-0.6086232
C	2.1422064	-1.1862774	-2.9472948	H	-4.0919875	-2.5859479	-2.6781353
H	1.3196410	-1.6392302	-3.4850348	H	5.0132729	-1.9043051	-1.3199762
C	2.1332304	0.1734264	-2.6747515	H	-1.4934631	5.9624517	1.5983104
C	4.0803081	0.0231164	-1.4798725				
C	1.0206636	1.0558800	-3.1750987	3b.xyz			
H	0.3477061	0.4591535	-3.8130481	97			
H	1.4627813	1.8337032	-3.8059729	Energy = -2408.546681657			
C	-1.2895957	5.3616669	0.7185913	O	-3.1396351	3.9539410	0.2833835
C	-0.2835348	5.7073726	-0.1656978	O	3.9229308	-3.0958317	0.7815554

O	4.3794398	-0.4953884	-0.0746491	H	-4.7136064	-2.2685288	-1.5825183
O	-3.4230795	-2.8057983	-0.1731719	C	-2.6846598	-2.5266397	0.9287174
O	-1.9538405	-4.7519290	0.7548976	C	-2.7027231	-1.3366567	1.6251399
C	0.6001137	5.1795625	-0.2807690	H	-3.3924405	-0.5569044	1.3270729
H	0.4542998	6.1689733	-0.7242424	C	-1.8307964	-3.5508227	1.3713945
C	-0.1405651	1.8548432	2.2640651	C	-0.9137060	-3.2672303	2.3621387
C	-2.2026476	3.2258379	0.9322564	H	-0.1965626	-4.0238962	2.6524413
C	-2.4711617	2.1570026	1.7642453	C	-0.8331635	-2.0080506	2.9653784
H	-3.4987363	1.8568235	1.9249478	C	-1.7880008	-1.0534656	2.6429764
C	-4.4870096	3.6816609	0.5740455	C	-1.2066274	-5.8203328	1.2774744
H	-4.7019016	3.8152516	1.6405211	H	-1.4265626	-5.9821665	2.3388020
H	-4.7676242	2.6651899	0.2760871	H	-0.1283753	-5.6596382	1.1604483
H	-5.0722939	4.3970019	-0.0022245	H	-1.4989557	-6.7036642	0.7108106
H	0.6597598	0.9719662	4.0344843	H	-1.2897330	0.3024316	4.2304699
C	1.7041737	0.0393451	2.4153325	C	0.4020672	-1.7041185	3.7799244
C	1.5053331	-1.2779582	2.8345923	H	0.2122131	-0.9471067	4.5397742
C	2.2741291	-2.2814548	2.2490044	H	0.7197218	-2.6031689	4.3140319
H	2.1337062	-3.3155791	2.5432575	O	-0.6881495	4.6804971	-0.0785829
C	3.2111122	-2.0363148	1.2657629	H	1.1255467	5.3291476	0.6721589
C	3.4128428	-0.7161763	0.8453874	H	1.7596529	2.0090596	3.1803370
C	2.6507853	0.2884587	1.4219942	H	-2.9099511	0.4594587	3.6177778
H	2.8129966	1.3119629	1.1051220	C	-1.4636538	1.4559894	2.4311222
C	4.2158054	0.6255792	-0.9152425	C	-1.8721224	0.3008888	3.3093411
H	4.3839990	1.5669228	-0.3802422	C	-0.8672115	3.6136090	0.7385456
H	3.2200855	0.6215161	-1.3678107	C	1.0038047	1.2318705	3.0327147
H	4.9685686	0.5316582	-1.6979111	C	0.1312483	2.9284827	1.4071565
C	3.9374184	-3.2876266	-0.6374101	H	1.1625027	3.2357735	1.2778586
H	4.3986299	-4.2687365	-0.7661993	C	1.6485436	-4.2845753	-0.9371757
H	4.5449946	-2.5280438	-1.1275785	C	0.3629639	-4.1884679	-1.4329656
C	-4.1912415	-1.7879339	-0.7509848	H	-0.3819755	-4.9434379	-1.2178504
H	-4.9620338	-1.4381709	-0.0487797	C	0.0223896	-3.0787649	-2.1886395

H	-0.9903411	-2.9372760	-2.5428594
C	0.9925026	-2.1221476	-2.4466091
C	2.5534999	-3.2659905	-1.2234530
C	0.6801723	-0.9059937	-3.2771108
H	-0.3474095	-0.9908740	-3.6682358
H	1.3562513	-0.9017816	-4.1381912
C	2.8145774	4.6426696	-1.3339127
C	3.5655757	3.9067626	-2.2329608
H	4.6217574	4.1125108	-2.3662699
C	2.9513596	2.8901367	-2.9450402
H	3.5128853	2.2722309	-3.6352316
C	1.5978389	2.6511299	-2.7398793
C	1.4594008	4.3549982	-1.2127398
C	0.9063475	1.4934476	-3.4061120
H	-0.0989390	1.8035926	-3.7312701
H	1.4642153	1.2236521	-4.3061716
C	-4.1364624	0.5302591	-1.6945769
C	-3.4240233	-0.5829306	-1.2602094
C	-1.4146777	0.4893293	-1.5280386
C	-2.0489880	1.6604682	-1.9345870
H	-1.4678865	2.5597349	-2.0973627
C	-3.4283028	1.6633545	-2.0530379
H	-3.9457489	2.5601798	-2.3743253
C	0.0833581	0.4297227	-1.3362941
H	0.3934576	1.3197581	-0.7893072
H	0.3040140	-0.4309680	-0.7032205
N	0.8989603	0.3245536	-2.5423313
N	2.2357928	-2.2177132	-1.9751268
N	-2.1007879	-0.6158008	-1.2257159
N	0.8677765	3.3962397	-1.9098262
H	-5.2212215	0.5123788	-1.7250534

H	1.9591473	-5.1230924	-0.3239925
H	3.2648665	5.4313318	-0.7409483

Ts34b.xyz

97

Energy = -2408.541540524

O	-3.0349929	4.1488886	0.3773408
O	3.5374013	-3.4441280	1.1290046
O	4.2644630	-0.7682628	0.9854537
O	-3.6953406	-2.4922037	-1.5218808
O	-2.2534537	-4.5650304	-0.8374400
C	0.7815582	5.0993293	0.9793624
H	0.7989675	6.1641003	0.7291589
C	-0.7082856	1.4201618	2.4902740
C	-2.3184720	3.2218796	1.0543906
C	-2.8256069	2.0311387	1.5340667
H	-3.8688157	1.7949433	1.3684911
C	-4.4248696	3.9575676	0.2942317
H	-4.8808324	3.8978008	1.2890486
H	-4.6778647	3.0518216	-0.2684169
H	-4.8200262	4.8261583	-0.2308435
H	-0.4170580	0.1278822	4.1617382
C	1.0034507	-0.5244403	2.7024365
C	0.6627024	-1.8775475	2.7523048
C	1.5454760	-2.8049535	2.2047159
H	1.3063137	-3.8623382	2.2245826
C	2.7327348	-2.4464261	1.5991205
C	3.0718714	-1.0897561	1.5380474
C	2.1996855	-0.1603718	2.0854347
H	2.4712361	0.8883595	2.0553058
C	4.3544072	0.4932724	0.3595570

H	4.3775768	1.3116106	1.0876778	C	-0.9624452	3.5141531	1.2671137
H	3.5232431	0.6329327	-0.3374590	C	0.1833198	0.5640089	3.3624308
H	5.2942354	0.4935830	-0.1926813	C	-0.1908165	2.6179747	1.9836350
C	3.9444559	-3.3728525	-0.2415186	H	0.8507929	2.8492702	2.1734467
H	4.4238493	-4.3361202	-0.4256244	C	1.8432556	-4.1846577	-1.3623066
H	4.6632363	-2.5684060	-0.3929188	C	0.7448340	-3.9282798	-2.1601970
C	-3.7116960	-1.4496993	-2.4868185	H	-0.0143283	-4.6811896	-2.3302423
H	-4.7580799	-1.1782231	-2.6565835	C	0.6087864	-2.6696498	-2.7211233
H	-3.3361713	-1.9023609	-3.4123977	H	-0.2649135	-2.4100685	-3.3041789
C	-3.0537224	-2.4139670	-0.3304929	C	1.5943033	-1.7223288	-2.4869251
C	-3.1880981	-1.3769189	0.5710520	C	2.7758440	-3.1700668	-1.1641508
H	-3.8323587	-0.5455437	0.3065792	C	1.4995769	-0.3438949	-3.0841908
C	-2.2803932	-3.5275915	0.0340884	H	0.5980334	-0.2883951	-3.7163610
C	-1.5933839	-3.4994665	1.2311842	H	2.3649221	-0.1981375	-3.7392225
H	-0.9535131	-4.3309414	1.4959757	C	3.1648789	4.5989978	0.3805301
C	-1.6499669	-2.4043136	2.0949007	C	4.0897515	3.9814776	-0.4421912
C	-2.4942400	-1.3439391	1.7835093	H	5.1521379	4.1338890	-0.2882503
C	-1.6836040	-5.7669691	-0.3857792	C	3.6369608	3.1533741	-1.4553320
H	-2.1681099	-6.1187668	0.5320599	H	4.3304406	2.6314750	-2.1035769
H	-0.6075660	-5.6680569	-0.2007345	C	2.2678663	2.9770745	-1.6161953
H	-1.8421311	-6.4971388	-1.1788177	C	1.8130011	4.3888451	0.1313123
H	-2.3842663	-0.4072144	3.7113235	C	1.7303283	2.0162523	-2.6415203
C	-0.6722777	-2.3856750	3.2465292	H	0.8158064	2.4348304	-3.0897456
H	-1.0416198	-1.7903884	4.0804129	H	2.4642903	1.9172210	-3.4450191
H	-0.5451305	-3.4015503	3.6286958	C	-3.5244468	1.0415667	-2.4222625
O	-0.5374523	4.6974591	0.7600122	C	-2.9224231	-0.1958047	-2.2271494
H	1.0535239	5.0148770	2.0403038	C	-0.9384283	0.7746289	-1.6094450
H	0.8859277	1.2354450	3.8648718	C	-1.4630226	2.0544489	-1.7916442
H	-3.7812902	0.0242183	2.7697241	H	-0.8583948	2.9207851	-1.5515320
C	-2.0437148	1.1146912	2.2401066	C	-2.7664482	2.1848145	-2.2298988
C	-2.7052283	-0.1595339	2.6994923	H	-3.1962181	3.1689270	-2.3764586

C	0.4655310	0.5840767	-1.0870764
H	0.6451240	1.3191199	-0.3026715
H	0.5269312	-0.4026977	-0.6261013
N	1.5394582	0.6928704	-2.0714210
N	2.6603318	-1.9722752	-1.7275244
N	-1.6492949	-0.3238163	-1.8638539
N	1.3797975	3.6089413	-0.8484511
H	-4.5659680	1.1020502	-2.7178171
H	1.9836512	-5.1469847	-0.8830077
H	3.4805094	5.2401482	1.1964171

4b.xyz

97

Energy = -2408.550945630

O	-3.0322861	4.1476913	0.2790830
O	3.4606046	-3.4328985	1.2308452
O	4.2445211	-0.7633201	1.0803586
O	-4.1529831	-2.1193247	-1.2588736
O	-2.5625549	-4.2868963	-0.8213859
C	0.7739822	5.1186583	0.8766194
H	0.7878115	6.1762112	0.5968077
C	-0.7342986	1.5096638	2.5342803
C	-2.3314225	3.2588927	1.0193103
C	-2.8583737	2.1189269	1.5901937
H	-3.9100247	1.8995045	1.4606000
C	-4.4132128	3.9270740	0.1393463
H	-4.9221792	3.9366121	1.1100671
H	-4.6222168	2.9761821	-0.3638959
H	-4.7910271	4.7462529	-0.4708134
H	-0.4196963	0.2366708	4.2198408
C	0.9580656	-0.4502255	2.7358800

C	0.5818321	-1.7955353	2.7700603
C	1.4513978	-2.7413750	2.2338247
H	1.1905988	-3.7938511	2.2536082
C	2.6626315	-2.4114787	1.6582369
C	3.0326382	-1.0629255	1.6033933
C	2.1715146	-0.1152119	2.1372513
H	2.4718855	0.9259131	2.1186714
C	4.3645402	0.4852591	0.4318281
H	4.3768749	1.3177987	1.1437523
H	3.5544648	0.6189171	-0.2907241
H	5.3191010	0.4650220	-0.0941531
C	3.9483529	-3.3861738	-0.1129514
H	4.4412744	-4.3504414	-0.2486422
H	4.6715473	-2.5812262	-0.2370397
C	-3.4181715	-1.8176679	-2.4512928
H	-4.1652683	-1.8181087	-3.2460643
H	-2.6774897	-2.5986877	-2.6419463
C	-3.3834779	-2.1982022	-0.1302501
C	-3.4429440	-1.1913163	0.8057094
H	-4.1095154	-0.3622520	0.5961182
C	-2.5496096	-3.2992708	0.1061515
C	-1.7663163	-3.3039156	1.2458947
H	-1.0915325	-4.1305416	1.4264646
C	-1.7816619	-2.2490688	2.1618694
C	-2.6568707	-1.1872237	1.9581146
C	-1.8910888	-5.4801886	-0.5023281
H	-2.2837666	-5.9222187	0.4202546
H	-0.8129215	-5.3234504	-0.3911417
H	-2.0704007	-6.1626130	-1.3323472
H	-2.3816247	-0.2457877	3.8735078
C	-0.7580570	-2.2797316	3.2732672

H	-1.0902904	-1.6975674	4.1319535
H	-0.6473238	-3.3076427	3.6275420
O	-0.5382653	4.7000822	0.6504171
H	1.0314780	5.0646106	1.9431269
H	0.8882249	1.3254818	3.8780890
H	-3.8255137	0.2298157	3.0251151
C	-2.0840710	1.2324577	2.3424216
C	-2.7654706	0.0008845	2.8842779
C	-0.9697492	3.5439706	1.2109055
C	0.1656677	0.6568084	3.4010628
C	-0.2019317	2.6698255	1.9574521
H	0.8485814	2.8867475	2.1121812
C	1.9673984	-4.2578180	-1.3959566
C	0.9243640	-4.0287223	-2.2739317
H	0.2255998	-4.8175761	-2.5268417
C	0.7746121	-2.7640123	-2.8154860
H	-0.0550448	-2.5288455	-3.4691389
C	1.6937226	-1.7788649	-2.4818614
C	2.8363721	-3.2099440	-1.1070780
C	1.5896035	-0.3986136	-3.0738395
H	0.6924335	-0.3538009	-3.7127522
H	2.4565770	-0.2481654	-3.7266202
C	3.1669784	4.6060759	0.3265742
C	4.1038713	3.9711458	-0.4691155
H	5.1639780	4.1254529	-0.3018168
C	3.6651815	3.1240849	-1.4724994
H	4.3670970	2.5883431	-2.1000971
C	2.2981538	2.9469665	-1.6503177
C	1.8189448	4.3916963	0.0612611
C	1.7740819	1.9652578	-2.6610247
H	0.8452850	2.3582427	-3.1028346

H	2.5021591	1.8724314	-3.4707755
C	-3.4030985	0.7012313	-2.6073218
C	-2.7309002	-0.4859532	-2.3412699
C	-0.8569007	0.6389416	-1.6297417
C	-1.4652390	1.8728431	-1.8517814
H	-0.9386134	2.7859386	-1.5996347
C	-2.7498376	1.8986194	-2.3671086
H	-3.2403781	2.8466803	-2.5575365
C	0.5447384	0.5379372	-1.0812493
H	0.6913117	1.3154720	-0.3319856
H	0.6454159	-0.4243095	-0.5772396
N	1.6167741	0.6462618	-2.0702511
N	2.7090212	-2.0035136	-1.6507010
N	-1.4798666	-0.5112543	-1.8873517
N	1.3984956	3.5923689	-0.9085922
H	-4.4211345	0.6784299	-2.9794816
H	2.1142885	-5.2259340	-0.9307055
H	3.4705718	5.2633102	1.1341988

PATH AD

Ts12d.xyz

97

Energy = -2408.525942458

O	-4.8073239	0.8223021	-0.6401904
O	4.7909844	1.2468364	0.6290414
O	3.4092899	3.5632028	-0.1926674
O	-0.6287961	-4.4179602	0.6387237
O	1.8729582	-4.3822566	1.6832512
C	-2.7799778	3.7446761	-2.2037540
H	-3.2583055	3.4108888	-3.1288489
C	-1.5277232	1.9118775	1.6881755

C	-3.7155101	1.1913863	0.0945507	H	2.4568388	-2.2761367	3.0082742
C	-3.2768246	0.3733250	1.1172681	C	0.5814913	-1.2116513	2.9916821
H	-3.8309638	-0.5422920	1.2935783	C	-0.7582563	-1.2968186	2.6194420
C	-5.9737036	1.5822918	-0.3792733	C	1.5688130	-5.6188033	2.3031870
H	-5.8225301	2.6389677	-0.6128849	H	0.6029650	-6.0068565	1.9704142
H	-6.2760949	1.4799380	0.6695178	H	1.5645086	-5.5140380	3.3939720
H	-6.7585866	1.1785745	-1.0195878	H	2.3560159	-6.3143593	2.0120780
H	-0.5787061	2.0819163	3.6021069	H	-1.4636863	0.2784376	3.8932150
C	0.9898146	2.0834271	2.1356653	C	1.1835080	0.0087232	3.6414653
C	1.7129265	0.9862607	2.6145447	H	0.4694074	0.4965017	4.3043881
C	2.9809949	0.7433017	2.0927741	H	2.0175996	-0.3048901	4.2742120
H	3.5472050	-0.1215330	2.4185462	O	-3.5484816	3.1740018	-1.1434889
C	3.5549095	1.5550892	1.1344130	H	-2.8911092	4.8301149	-2.1288587
C	2.8693760	2.6972601	0.7192256	H	-0.4973074	3.5129768	2.6169495
C	1.6002647	2.9316012	1.2136749	H	-2.6955777	-0.8046046	3.3163278
H	1.0781788	3.8129395	0.8588781	C	-2.1828232	0.6968806	1.9148352
C	4.5485249	4.2717234	0.2698384	C	-1.7945846	-0.2663997	3.0092561
H	5.3550824	3.5912352	0.5529191	C	-3.0285592	2.3773254	-0.1749223
H	4.2864228	4.9020498	1.1266209	C	-0.4144161	2.4235863	2.5796688
H	4.8768080	4.9039636	-0.5552065	C	-1.9638162	2.7268455	0.6442143
C	4.7484820	0.7766385	-0.7227606	H	-1.4759969	3.6795040	0.4779125
H	5.7959547	0.6677565	-1.0121140	C	4.4558667	-1.6304623	-0.0968235
H	4.2713743	1.5137408	-1.3725607	C	3.7149015	-2.7943285	-0.1515187
C	-1.9562688	-4.5615578	0.2032447	H	3.9884013	-3.6616943	0.4356160
H	-2.6246936	-4.7018992	1.0630017	C	2.5779099	-2.8247039	-0.9407603
H	-1.9574684	-5.4916990	-0.3716134	H	1.9484103	-3.7056600	-0.9627905
C	-0.3175463	-3.3919711	1.4674884	C	2.2308739	-1.6980312	-1.6763810
C	-1.1836265	-2.3845951	1.8574560	C	4.0183526	-0.5344920	-0.8307386
H	-2.2152699	-2.4079198	1.5321703	C	1.0405414	-1.7753617	-2.6002625
C	0.9936623	-3.3723700	1.9593660	H	0.4698633	-2.6572739	-2.3155269
C	1.4216426	-2.2817258	2.6849009	H	1.4126985	-1.9478979	-3.6301824

C	-0.3697247	4.3599581	-1.9615817	O	-4.6889947	1.0337606	-0.6001844
C	0.9683041	4.0225165	-2.0535677	O	4.6950444	1.3925122	0.6052200
H	1.7461100	4.7280257	-1.7908577	O	3.2177123	3.6737483	-0.1610315
C	1.2977633	2.7429890	-2.4537672	O	-0.6263242	-4.3706634	0.6834267
H	2.3314924	2.4274077	-2.5033210	O	1.8899805	-4.3238195	1.6929843
C	0.2842015	1.8468603	-2.7831095	C	-2.9998600	3.0747956	-2.2415222
C	-1.3218416	3.3983955	-2.2744910	H	-3.4722708	2.1178255	-2.4750385
C	0.6630384	0.4904571	-3.3153647	C	-1.5333930	2.0408812	1.9351783
H	0.3572355	0.4328934	-4.3764521	C	-3.6413741	1.3828201	0.2071705
H	1.7475969	0.4274453	-3.2879981	C	-3.2177611	0.5031854	1.1875913
C	-3.8605369	-3.1904476	-0.6410482	H	-3.7538152	-0.4348917	1.2800035
C	-2.4945634	-3.4437521	-0.6613559	C	-5.8508220	1.8314317	-0.4348001
C	-2.1074663	-1.7628065	-2.1628375	H	-5.6507585	2.8825911	-0.6564181
C	-3.4586218	-1.4295828	-2.1859440	H	-6.2352404	1.7429035	0.5872097
H	-3.7982992	-0.5788664	-2.7620241	H	-6.5936914	1.4459308	-1.1332350
C	-4.3486377	-2.1621682	-1.4258092	H	-0.5428861	2.0788549	3.8411414
H	-5.4003044	-1.9034731	-1.4139361	C	0.9663164	2.1681400	2.3106472
C	-1.1835222	-0.9902051	-3.0691365	C	1.7079100	1.0556239	2.7158805
H	-1.0979466	-1.5547654	-4.0209543	C	2.9519652	0.8341736	2.1296336
H	-1.6900185	-0.0557396	-3.3082741	H	3.5382992	-0.0330003	2.4098622
N	0.1316506	-0.6406533	-2.5626181	C	3.4730127	1.6693765	1.1605327
N	2.9450528	-0.5719590	-1.6125971	C	2.7507844	2.8046675	0.7865812
N	-1.6416548	-2.7637210	-1.4159186	C	1.5155392	3.0297315	1.3628482
N	-1.0037193	2.1765390	-2.6962160	H	0.9710309	3.9131398	1.0485352
H	-4.5175577	-3.7714580	-0.0029448	C	4.3641747	4.4137945	0.2290674
H	5.3425475	-1.5486286	0.5210953	H	5.2016316	3.7551599	0.4715147
H	-0.6798670	5.3489144	-1.6433059	H	4.1365178	5.0462597	1.0941053
				H	4.6288767	5.0454631	-0.6187710
				C	4.6178115	0.9238407	-0.7433859
				H	5.6542271	0.8887016	-1.0874873
				H	4.0594759	1.6259692	-1.3663201

2d.xyz

97

Energy = -2408.536069800

C	-1.9515851	-4.4977915	0.2293771	H	4.0646544	-3.5069946	0.5643904
H	-2.6374397	-4.6024338	1.0799612	C	2.6958871	-2.8186156	-0.9312721
H	-1.9607592	-5.4399890	-0.3246564	H	2.1251856	-3.7386301	-0.9530354
C	-0.3050746	-3.3371155	1.4980752	C	2.3280930	-1.7461228	-1.7343294
C	-1.1662795	-2.3266265	1.8944211	C	3.9767905	-0.4352322	-0.8278824
H	-2.2005818	-2.3512970	1.5784663	C	1.2094985	-1.9330683	-2.7287260
C	1.0105661	-3.3173217	1.9782041	H	0.6619535	-2.8263896	-2.4307618
C	1.4413224	-2.2314309	2.7094978	H	1.6613496	-2.1478514	-3.7182322
H	2.4781466	-2.2284943	3.0277046	C	-0.6711388	3.9947883	-2.0688268
C	0.6031187	-1.1658038	3.0361937	C	0.6932053	3.8084949	-2.1756057
C	-0.7386846	-1.2449211	2.6653750	H	1.3907581	4.5777043	-1.8674951
C	1.5944158	-5.5647604	2.3090938	C	1.1632948	2.5952960	-2.6496140
H	0.6352641	-5.9623397	1.9687764	H	2.2256742	2.3969884	-2.7091797
H	1.5813220	-5.4615112	3.3999372	C	0.2540009	1.6145489	-3.0226160
H	2.3916926	-6.2506417	2.0227565	C	-1.5124059	2.9478616	-2.4302203
H	-1.4581638	0.2685170	4.0022583	C	0.7478082	0.2980945	-3.5615733
C	1.2117726	0.0355560	3.7177231	H	0.4849183	0.2252722	-4.6321543
H	0.5094654	0.4892608	4.4165348	H	1.8327051	0.3001778	-3.4920740
H	2.0620413	-0.2974737	4.3181294	C	-3.7591615	-2.9673062	-0.5741381
O	-3.3297561	3.4965296	-0.9147772	C	-2.4376982	-3.3864557	-0.6715996
H	-3.4157142	3.8485171	-2.8910594	C	-1.9840090	-1.8759878	-2.3269875
H	-0.4856291	3.5761682	2.9542416	C	-3.2801391	-1.3731100	-2.2702560
H	-2.6842382	-0.7826378	3.3578696	H	-3.5605484	-0.5328556	-2.8923597
C	-2.1617836	0.7958979	2.0474055	C	-4.1860501	-1.9391692	-1.3940226
C	-1.7801055	-0.2299406	3.0878969	H	-5.1949158	-1.5527635	-1.3233128
C	-2.9715988	2.5969977	0.0549461	C	-1.0284716	-1.3076719	-3.3428716
C	-0.4109627	2.4915603	2.8413162	H	-0.8818083	-2.0604831	-4.1407723
C	-1.9532287	2.9124663	0.9352019	H	-1.5222355	-0.4517986	-3.7984923
H	-1.4750534	3.8778049	0.8176755	N	0.2479017	-0.8504355	-2.8177474
C	4.4366886	-1.4715749	-0.0243392	N	2.9618651	-0.5735347	-1.6728039
C	3.7751991	-2.6826509	-0.0750887	N	-1.5777692	-2.8731152	-1.5410869

N	-1.0636616	1.7948407	-2.9106313
H	-4.4264593	-3.4218329	0.1502521
H	5.2752776	-1.3072385	0.6420573
H	-1.0918447	4.9171685	-1.6860771

Ts2d_D.xyz

97

Energy = -2408.528847693

O	-4.7489159	1.2416497	0.1849882
O	4.7981809	1.1971585	0.3965416
O	3.3337818	3.6099286	0.3528208
O	-1.0206677	-4.7680721	0.0900951
O	1.6868487	-4.6479625	0.2941230
C	-3.1177167	3.5912183	-1.1223040
H	-3.6417697	2.7263062	-1.5359267
C	-1.2835275	1.5477849	2.4866347
C	-3.6063387	1.3678135	0.9275327
C	-3.1255870	0.2750279	1.6266801
H	-3.6943201	-0.6459058	1.5691189
C	-5.8496536	2.0007342	0.6613470
H	-5.6207847	3.0689372	0.6797298
H	-6.1351934	1.6727161	1.6667498
H	-6.6749034	1.8153444	-0.0260949
H	-0.0677469	1.1141783	4.2035324
C	1.2504516	1.5573070	2.5654859
C	1.9713783	0.3611159	2.5857620
C	3.1531635	0.2805100	1.8546180
H	3.7297070	-0.6368343	1.8518474
C	3.6274145	1.3335343	1.0965864
C	2.9174582	2.5354622	1.0901413
C	1.7482810	2.6256887	1.8225554

H	1.2179613	3.5713268	1.8035615
C	4.5249473	4.2225435	0.8220605
H	5.3592412	3.5170291	0.8320877
H	4.3775617	4.6265299	1.8296772
H	4.7451296	5.0397795	0.1353745
C	4.6119892	1.0440050	-1.0122288
H	5.6201715	1.0676831	-1.4323639
H	4.0357249	1.8781678	-1.4193340
C	-1.9995730	-4.6240705	-0.9418430
H	-2.8404113	-5.2638586	-0.6599316
H	-1.5414063	-5.0297427	-1.8476407
C	-0.4891898	-3.7478129	0.8099038
C	-1.2281998	-2.8145143	1.5230243
H	-2.3079492	-2.8493523	1.4561694
C	0.9016404	-3.7455755	0.9561685
C	1.4949049	-2.8056250	1.7746781
H	2.5749935	-2.8369089	1.8662961
C	0.7607749	-1.8500727	2.4716094
C	-0.6312607	-1.8596603	2.3465641
C	1.6410341	-5.9647379	0.8157084
H	0.6301539	-6.3765348	0.7684456
H	1.9945546	-5.9821043	1.8531743
H	2.3081047	-6.5674568	0.1990954
H	-1.0699189	-0.6630142	4.0718267
C	1.5211616	-0.8705352	3.3348401
H	0.9343021	-0.5950271	4.2105929
H	2.4096069	-1.3775346	3.7194599
O	-3.3137726	3.6771887	0.2917865
H	-3.5646499	4.5045084	-1.5216958
H	-0.0602262	2.7803364	3.6994656
H	-2.4405983	-1.4816692	3.3824222

C	-1.9647133	0.3291489	2.3942269
C	-1.5365182	-0.9251817	3.1218121
C	-2.8945335	2.5663094	0.9763742
C	-0.0421677	1.7546804	3.3222621
C	-1.7668210	2.6392229	1.7716442
H	-1.2523370	3.5916582	1.8199196
C	4.4056779	-1.4526460	-0.8520211
C	3.6870514	-2.6046591	-1.1056025
H	4.0009385	-3.5616757	-0.7067489
C	2.5245503	-2.5158570	-1.8524056
H	1.9153115	-3.3942468	-2.0232873
C	2.1294721	-1.2789925	-2.3457072
C	3.9163928	-0.2482148	-1.3453158
C	0.9059379	-1.1947160	-3.2212068
H	0.3668436	-2.1353730	-3.1162904
H	1.2361867	-1.1303678	-4.2769732
C	-0.7558169	4.4269275	-0.9666439
C	0.5872901	4.2553338	-1.2389930
H	1.3338058	4.9256110	-0.8305171
C	0.9757118	3.1795521	-2.0197065
H	2.0224390	2.9896827	-2.2195139
C	0.0065180	2.3230086	-2.5246290
C	-1.6581089	3.4995804	-1.4768497
C	0.4094993	1.1699827	-3.4053801
H	0.0250557	1.3459010	-4.4264813
H	1.4952639	1.1630124	-3.4618806
C	-3.7470843	-2.8367330	-0.7824617
C	-2.5060482	-3.2466685	-1.2543246
C	-2.1816340	-1.2709674	-2.3688678
C	-3.3913691	-0.7693603	-1.8972714
H	-3.6924450	0.2396985	-2.1471707

C	-4.1935438	-1.5687574	-1.1064498
H	-5.1387366	-1.1923998	-0.7357625
C	-1.3741637	-0.4414192	-3.3315136
H	-1.3668933	-0.9558515	-4.3108149
H	-1.9031358	0.4997602	-3.4655325
N	-0.0220245	-0.1257979	-2.8981884
N	2.8186330	-0.1663137	-2.0866458
N	-1.7505998	-2.4898817	-2.0462540
N	-1.2896609	2.4857887	-2.2500029
H	-4.3407896	-3.5021594	-0.1655525
H	5.3119884	-1.4651089	-0.2579095
H	-1.1117652	5.2415584	-0.3468822

D.xyz

97

Energy = -2408.539011941

O	-4.7512697	0.9155783	-0.3974134
O	4.5963258	1.3624887	0.6347381
O	3.1487434	3.6923788	-0.0764971
O	-1.3530402	-4.4632961	1.2786888
O	1.4575663	-4.3358323	1.6202514
C	-3.0369476	2.8758946	-2.1309237
H	-3.4379545	1.8732041	-2.2951221
C	-1.6154264	2.0495419	2.1097121
C	-3.7230983	1.3161337	0.4105083
C	-3.3330043	0.5051282	1.4604839
H	-3.8858288	-0.4155936	1.6103350
C	-5.9197141	1.7169169	-0.3095107
H	-5.7134376	2.7558241	-0.5780586
H	-6.3354236	1.6790811	0.7032502
H	-6.6392506	1.2935957	-1.0100559

H	-0.5521725	2.1411295	3.9777574	H	-1.5167551	0.3970210	4.2723104
C	0.8945982	2.1774532	2.3873708	C	1.1217746	0.0179670	3.7536054
C	1.6151695	1.0365451	2.7517685	H	0.4830464	0.4917859	4.4984216
C	2.8465656	0.8036073	2.1463936	H	1.9872010	-0.3631697	4.3016766
H	3.4227644	-0.0744529	2.4115456	O	-3.3800472	3.3575016	-0.8318575
C	3.3770084	1.6486686	1.1902289	H	-3.5223982	3.5660703	-2.8258184
C	2.6737774	2.8064214	0.8507647	H	-0.5257920	3.6111404	3.0446990
C	1.4509037	3.0456744	1.4504865	H	-2.8431896	-0.6084942	3.7606006
H	0.9275095	3.9528306	1.1695296	C	-2.2812809	0.8372837	2.3117380
C	4.3113155	4.4017281	0.3240209	C	-1.9219458	-0.1347890	3.4119732
H	5.1387978	3.7225067	0.5429547	C	-3.0346442	2.5107060	0.1884241
H	4.1012566	5.0149178	1.2071137	C	-0.4602279	2.5233209	2.9614744
H	4.5808390	5.0506234	-0.5090244	C	-2.0152904	2.8623205	1.0528800
C	4.5353046	0.9677690	-0.7355518	H	-1.5135963	3.8058390	0.8757820
H	5.5757629	0.9451676	-1.0698772	C	4.1760025	-1.4238847	-0.0411485
H	3.9914736	1.7043754	-1.3311988	C	3.5108636	-2.6230165	-0.2090380
C	-1.1266055	-4.5557030	-0.1275434	H	3.6677468	-3.4506936	0.4718769
H	-1.5185961	-5.5352666	-0.4133066	C	2.6028321	-2.7412143	-1.2476310
H	-0.0586818	-4.5254260	-0.3548496	H	2.0338708	-3.6516152	-1.3880468
C	-0.7491521	-3.3869787	1.8738662	C	2.4067778	-1.6628688	-2.1001430
C	-1.5236686	-2.3470957	2.3520219	C	3.8887909	-0.3805756	-0.9140736
H	-2.5963067	-2.4224835	2.2211564	C	1.4499473	-1.7782414	-3.2581148
C	0.6343586	-3.3346665	2.0565698	H	0.9750215	-2.7558686	-3.1967897
C	1.1860022	-2.2251658	2.6705553	H	2.0272526	-1.7512688	-4.1999086
H	2.2623548	-2.2120510	2.8011475	C	-0.7485167	3.9000089	-1.9169336
C	0.4127158	-1.1570829	3.1201846	C	0.6182509	3.8027444	-2.0930640
C	-0.9749561	-1.2258883	2.9677794	H	1.2862833	4.5732019	-1.7277888
C	1.3157218	-5.5646988	2.3166842	C	1.1311051	2.6772911	-2.7155271
H	0.2984866	-5.9553778	2.2356763	H	2.1991026	2.5468731	-2.8368691
H	1.5733068	-5.4383262	3.3738672	C	0.2575138	1.6953614	-3.1636085
H	2.0141119	-6.2637435	1.8570356	C	-1.5482408	2.8514277	-2.3572461

C	0.7883736	0.4782491	-3.8753120	H	-3.2162153	4.7250458	-1.4750917
H	0.4656307	0.5155779	-4.9314841	C	-1.1554606	1.4917743	2.1456016
H	1.8751647	0.5391376	-3.8659208	C	-3.5474730	1.0574616	0.7429546
C	-3.1134624	-3.0722691	-0.5551038	C	-3.0931315	0.1536033	1.6820812
C	-1.8215806	-3.4601198	-0.8921213	H	-3.6946532	-0.7191190	1.9057668
C	-1.6887316	-1.8906576	-2.5552613	C	-5.7588364	0.2602673	0.7822852
C	-2.9573863	-1.4128829	-2.2545203	H	-6.6767728	0.4336164	0.2208411
H	-3.3558882	-0.5617217	-2.7921740	H	-5.8806459	0.6307390	1.8063011
C	-3.6854631	-2.0217006	-1.2463027	H	-5.5658641	-0.8168922	0.8194100
H	-4.6723719	-1.6549530	-0.9917224	H	-0.0684940	1.4508228	3.9854255
C	-0.8906965	-1.2677046	-3.6709119	C	1.4014969	1.5680420	2.4291584
H	-0.7941576	-2.0016421	-4.4912753	C	2.1198732	0.4205970	2.7585034
H	-1.4632511	-0.4253251	-4.0549479	C	3.3471799	0.2098317	2.1309878
N	0.4050360	-0.7719014	-3.2470293	H	3.9153422	-0.6921286	2.3289507
N	3.0410460	-0.5020000	-1.9279068	C	3.8656477	1.0767012	1.1961868
N	-1.1340453	-2.8969325	-1.8776813	C	3.1777299	2.2639925	0.9168206
N	-1.0607491	1.7860058	-2.9805755	C	1.9607679	2.4852946	1.5361493
H	-3.6346300	-3.5765358	0.2494265	H	1.4080691	3.3893605	1.3149505
H	4.8885411	-1.2745255	0.7608407	C	3.0341859	4.2587785	-0.3314643
H	-1.2010424	4.7536812	-1.4273852	H	2.8875057	4.9259960	0.5261610

PATH AE

TsA1e.xyz

97

Energy = -2408.535280372

O	-4.7439707	0.9629687	0.1087459	C	-1.9941817	-4.5373279	-0.1588011
O	5.0291878	0.7455642	0.5611701	H	-2.5581792	-4.7441323	0.7607734
O	3.7531697	3.1064431	0.0294279	H	-2.0882376	-5.4148113	-0.8050436
O	-0.6255043	-4.4407427	0.1143656	C	-0.2077700	-3.5666920	1.0621343
O	1.8757957	-4.6007562	0.7700012	C	-1.0034743	-2.6533738	1.7237481
C	-2.5091336	4.1100886	-0.9110626	H	-2.0633226	-2.6122324	1.5041683

C	1.1611628	-3.6293935	1.3805558	H	0.2440401	0.6880638	-0.6768957
C	1.6776696	-2.7111083	2.2694187	H	-0.4748264	-0.9172497	-0.6560750
H	2.7370213	-2.7255746	2.4877542	C	-0.5209540	4.9353511	-2.1803618
C	0.8858425	-1.7335842	2.8817557	C	0.5632879	4.6950839	-3.0064883
C	-0.4812779	-1.7337007	2.6425952	H	1.1930973	5.5124707	-3.3405540
C	3.2273810	-4.7313017	1.1333062	C	0.8418503	3.3928440	-3.3792206
H	3.3357170	-4.9341654	2.2050640	H	1.6993232	3.1593953	-4.0005778
H	3.8028057	-3.8351707	0.8763166	C	0.0106882	2.3717929	-2.9286597
H	3.6131162	-5.5783017	0.5674559	C	-1.2977112	3.8532198	-1.7813087
H	-1.0030131	-0.3572054	4.2077981	C	0.2996154	0.9354687	-3.3334230
C	1.5990503	-0.6644505	3.6745116	H	0.0019415	0.8138176	-4.3820291
H	0.9562848	-0.2468510	4.4484781	H	1.3910643	0.8108949	-3.3211818
H	2.4477134	-1.1151479	4.1959188	C	-3.9826197	-3.1373614	-0.7357200
O	-3.2291476	2.9713690	-0.5474984	C	-2.6126999	-3.3482270	-0.8610638
H	-2.2143186	4.6951401	-0.0288249	C	-2.3682252	-1.5126577	-2.2086673
H	-0.0166226	2.9695441	3.1421901	C	-3.7198514	-1.2070850	-2.1043606
H	-2.3238593	-1.3302481	3.6237469	H	-4.1139411	-0.3154109	-2.5738964
C	-1.8937795	0.3330968	2.3739574	C	-4.5433161	-2.0547772	-1.3849522
C	-1.4433978	-0.7676293	3.2996008	H	-5.6066065	-1.8576157	-1.3166451
C	-2.7419964	2.1587945	0.4190057	C	-1.4982556	-0.6878359	-3.1155384
C	0.0377393	1.8871549	2.9920550	H	-1.2112096	-1.3588519	-3.9466480
C	-1.5810301	2.3671727	1.1419339	H	-2.1410150	0.0870117	-3.5514828
H	-0.9803633	3.2449131	0.9365337	N	-0.3315740	-0.0667390	-2.5482885
C	4.1078281	-1.8415967	-1.3996303	N	2.5875819	-0.0281938	-1.1189624
C	3.0419098	-2.7082665	-1.6130058	N	-1.8331733	-2.5777810	-1.6054570
H	3.2162697	-3.7599333	-1.8105056	N	-1.0432839	2.6058531	-2.1521829
C	1.7525517	-2.2206022	-1.5384711	H	-4.5874868	-3.8079519	-0.1347948
H	0.8891310	-2.8635752	-1.6666455	H	5.1327196	-2.1951006	-1.4208816
C	1.5668455	-0.8641281	-1.2733829	H	-0.7647704	5.9399634	-1.8517455
C	3.8344286	-0.5049352	-1.1552048				
C	0.1853260	-0.2624367	-1.2203409				

1e.xyz

97

Energy = -2408.548554988

O 0.3578734 -2.1643055 4.1046501
 O 1.7926646 2.0698962 -4.2229980
 O 3.9997596 1.6735898 -2.6618173
 O -4.4671330 -0.6349169 -0.2235356
 O -4.1066585 0.2515482 -2.6298000
 C 3.7309302 -0.2967455 3.1404707
 H 4.1497116 0.0010201 4.1059342
 C 1.6762637 -2.5279347 0.1738180
 C 0.7314076 -2.2909905 2.8110232
 C -0.0222707 -2.9026562 1.8293692
 H -0.9914367 -3.3101090 2.0857992
 C -0.8627044 -2.7477816 4.4872574
 H -0.9728642 -2.5477243 5.5519316
 H -0.8587245 -3.8313925 4.3212780
 H -1.7103182 -2.3032463 3.9541333
 H 1.8869586 -3.5794393 -1.6826204
 C 2.1706525 -1.4914405 -2.1008402
 C 1.1212619 -1.3180456 -3.0015723
 C 1.0492214 -0.1162925 -3.7036763
 H 0.2253577 0.0727581 -4.3825810
 C 1.9698987 0.8950415 -3.5474390
 C 3.0763107 0.6826958 -2.7169995
 C 3.1505294 -0.5003192 -2.0033823
 H 3.9864413 -0.6660699 -1.3354283
 C 5.2353356 1.3724447 -2.0638061
 H 5.7057235 0.5056489 -2.5417419
 H 5.1316559 1.1782323 -0.9917075
 H 5.8661113 2.2491258 -2.2075485
 C 1.4812922 3.1971140 -3.3931615

H 1.3665820 4.0300049 -4.0875559
 H 2.3149836 3.3981240 -2.7148345
 C -4.8469669 -1.1799868 1.0084332
 H -4.7399544 -2.2735823 1.0023419
 H -5.9141054 -0.9665014 1.1078648
 C -3.4041853 -1.1507220 -0.8873402
 C -2.5396123 -2.1097970 -0.4020979
 H -2.6821564 -2.4883314 0.6018086
 C -3.2004910 -0.6484605 -2.1842768
 C -2.1099799 -1.0917778 -2.9041840
 H -1.9353200 -0.6950130 -3.8953196
 C -1.2060353 -2.0286385 -2.3939251
 C -1.4407504 -2.5691234 -1.1360875
 C -3.9650526 0.7094973 -3.9508302
 H -4.0250677 -0.1159367 -4.6697905
 H -3.0193045 1.2435115 -4.0941286
 H -4.7927741 1.3959982 -4.1241301
 H -0.0102665 -4.1688839 -1.2589364
 C 0.0207969 -2.3319946 -3.2190235
 H 0.3837694 -3.3406321 -3.0247854
 H -0.2562612 -2.3117252 -4.2766476
 O 2.6477777 -1.1219023 3.4631532
 H 4.5166593 -0.8496632 2.6083007
 H 3.3626318 -2.9036403 -1.0561849
 H -1.1778021 -4.3326942 0.0222042
 C 0.4159120 -3.0130009 0.5066007
 C -0.5445129 -3.6057992 -0.4944541
 C 1.9729738 -1.7344972 2.4601287
 C 2.2983388 -2.6943381 -1.1976162
 C 2.4241067 -1.8794013 1.1629127
 H 3.3908283 -1.4724702 0.8925644

C	-1.0068811	3.4568927	-3.0030936
C	-2.1243820	3.1497882	-2.2364364
H	-3.1047466	3.5170749	-2.5192934
C	-1.9741507	2.3493993	-1.1210246
H	-2.8193334	2.0594577	-0.5085339
C	-0.6979878	1.8959414	-0.7908886
C	0.2275967	2.9724503	-2.5969829
C	-0.4863483	1.0161398	0.4062256
H	0.5143522	0.5673755	0.3385101
H	-1.2196511	0.2103804	0.3871099
C	4.3425948	1.6429734	1.6634356
C	3.9747554	2.7914132	0.9832046
H	4.7075626	3.3547727	0.4164337
C	2.6505355	3.1895363	1.0063481
H	2.3162272	4.0530047	0.4444854
C	1.7391921	2.4399280	1.7407268
C	3.3624157	0.9473128	2.3612894
C	0.2774103	2.8326167	1.8038533
H	0.0870385	3.3227957	2.7644215
H	0.0943214	3.5851791	1.0306242
C	-4.7203485	-0.6612219	3.4566221
C	-4.1212590	-0.6029610	2.2022960
C	-2.2442874	0.4144585	3.0417885
C	-2.7740824	0.4045163	4.3290933
H	-2.2046615	0.8199254	5.1522121
C	-4.0283293	-0.1434326	4.5367138
H	-4.4663702	-0.1566758	5.5286778
C	-0.8426784	0.9160130	2.8115205
H	-0.5317653	1.4773713	3.6935154
H	-0.1731265	0.0475187	2.7767265
N	-0.6847092	1.7628788	1.6429025

N	0.3748500	2.2265719	-1.5003945
N	-2.9196148	-0.0808016	2.0051088
N	2.1009633	1.3475142	2.4102805
H	-5.7097569	-1.0885915	3.5762654
H	-1.0897591	4.0599643	-3.9002297
H	5.3664012	1.2841908	1.6473129

Ts12e.xyz

97

Energy = -2408.539085765

O	-4.5158127	1.1047746	0.3203337
O	4.7899497	1.2840195	-0.0489421
O	3.5935607	3.6165398	0.2483661
O	-0.8032266	-4.4016169	-0.2374900
O	1.7629092	-4.6136329	0.0907804
C	-2.3149762	4.3571815	-0.3116975
H	-2.9673210	4.9958554	-0.9137731
C	-0.9838212	1.4646595	2.4909139
C	-3.3640974	1.1634332	1.0272329
C	-2.8727583	0.1440605	1.8183123
H	-3.4251652	-0.7841085	1.8860488
C	-5.3045402	-0.0503453	0.4614268
H	-6.1832629	0.1053143	-0.1625261
H	-5.6198093	-0.1957177	1.5012431
H	-4.7790229	-0.9468115	0.1142373
H	0.2619251	1.1110918	4.2018387
C	1.5470606	1.5584022	2.5335737
C	2.2534134	0.3584184	2.4675978
C	3.3500542	0.2833364	1.6084418
H	3.8983774	-0.6484281	1.5192805
C	3.7471558	1.3419999	0.8176690

C	3.1057631	2.5774635	0.9688690	H	0.2145720	2.7655509	3.6645788
C	2.0170105	2.6597694	1.8159681	H	-2.0464902	-1.5415496	3.5971745
H	1.4914857	3.6016738	1.9123730	C	-1.6774626	0.2607569	2.5338637
C	3.2443484	4.9080132	0.6757057	C	-1.1809584	-0.9601760	3.2663070
H	3.4752237	5.0506842	1.7376076	C	-2.6197158	2.3504538	0.9154139
H	2.1831450	5.1240955	0.5126090	C	0.2635610	1.7330279	3.3069914
H	3.8406293	5.5997819	0.0809201	C	-1.4658983	2.4841819	1.6625426
C	4.8419475	0.3588011	-1.1246285	H	-0.9015578	3.4065003	1.5998687
H	5.7163417	-0.2831907	-0.9741575	C	3.8459699	-1.8082050	-1.8649467
H	5.0347532	0.9628863	-2.0197372	C	2.7367319	-2.5725928	-2.2007819
C	-2.1954562	-4.5177023	-0.3246611	H	2.8550123	-3.5832746	-2.5742671
H	-2.6492530	-4.5287817	0.6761343	C	1.4781753	-2.0456124	-1.9981573
H	-2.3802201	-5.4999395	-0.7666002	H	0.5783884	-2.6168517	-2.1902244
C	-0.2556783	-3.5848284	0.6953355	C	1.3704503	-0.7530780	-1.4895329
C	-0.9512383	-2.7123878	1.5064646	C	3.6462762	-0.5146027	-1.4012942
H	-2.0274993	-2.6491222	1.4116605	C	0.0162227	-0.1897734	-1.1707793
C	1.1397515	-3.6705727	0.8343309	H	0.1446770	0.7431409	-0.6056797
C	1.7748497	-2.8001000	1.6973675	H	-0.5013035	-0.9005659	-0.5264552
H	2.8535068	-2.8308476	1.7794764	C	-0.0060830	4.7822245	-1.2158009
C	1.0757969	-1.8670839	2.4692277	C	1.0682672	4.3787387	-1.9894815
C	-0.3132047	-1.8593959	2.4121452	H	1.9625828	4.9873979	-2.0537016
C	3.1312593	-4.8236293	0.3311014	C	1.0032585	3.1618195	-2.6442181
H	3.3168555	-5.0865095	1.3789697	H	1.8476025	2.7867276	-3.2092029
H	3.7284599	-3.9429440	0.0705681	C	-0.1545721	2.4029254	-2.5305374
H	3.4274650	-5.6557834	-0.3064033	C	-1.1172954	3.9502456	-1.1427008
H	-0.6488684	-0.6791095	4.1744084	C	-0.2780785	1.0539212	-3.2084998
C	1.8846728	-0.8738992	3.2660954	H	-0.9309708	1.1514531	-4.0818612
H	1.3637621	-0.5907215	4.1804394	H	0.7095933	0.7689335	-3.5854356
H	2.8109121	-1.3581772	3.5881160	C	-4.1188164	-3.7517129	-1.7280630
O	-3.1335543	3.2927196	0.0878972	C	-2.8737163	-3.4676485	-1.1760795
H	-1.9837052	4.9552318	0.5477668	C	-2.8632717	-1.3490031	-2.0563229

C	-4.1061042	-1.5536492	-2.6493525	H	-4.4594733	2.4635611	2.7962778
H	-4.5644716	-0.7625896	-3.2310442	H	-4.3915044	1.4447254	1.3296953
C	-4.7404584	-2.7721200	-2.4812536	H	1.8081620	0.6546740	4.0267427
H	-5.7048715	-2.9595331	-2.9404088	C	2.7098270	0.5579324	2.0729712
C	-2.2106845	0.0066788	-2.1477767	C	2.6605069	-0.8160963	1.8562146
H	-2.6830180	0.5572783	-2.9624332	C	3.2791696	-1.3327472	0.7187420
H	-2.4697757	0.5671110	-1.2408158	H	3.1727601	-2.3899607	0.5113717
N	-0.7794981	-0.0203897	-2.3778112	C	3.9340413	-0.5358808	-0.1963527
N	2.4327161	0.0087500	-1.2481232	C	4.1299049	0.8165744	0.1122912
N	-2.2651939	-2.3012559	-1.3398920	C	3.4966599	1.3400738	1.2233943
N	-1.1938288	2.8036177	-1.8000766	H	3.5892197	2.3986144	1.4332372
H	-4.5787418	-4.7225660	-1.5803360	C	5.3934780	2.7653308	-0.2755488
H	4.8501118	-2.2050223	-1.9684519	H	5.8940011	2.6604249	0.6937445
H	0.0188141	5.7155170	-0.6631791	H	4.5953222	3.5098820	-0.1797893

2e.xyz

97

Energy = -2408.544298610

O	-3.1583066	3.1177818	1.3181492	H	6.1120727	3.1121007	-1.0177674
O	4.4194337	-0.9555793	-1.3926155	C	3.9736897	-2.1775227	-1.9160814
O	4.9114693	1.5304303	-0.7375738	H	4.1961055	-3.0071640	-1.2288895
O	-2.9826263	-3.4090576	0.4927380	H	4.5799606	-2.3425312	-2.8094196
O	-0.8083057	-4.6724157	-0.0982881	C	-4.2147678	-2.7968907	0.7522555
C	0.1098605	4.8783753	-0.0930233	H	-4.3285593	-2.5679424	1.8206029
H	-0.2793996	5.7525460	-0.6220591	H	-4.9712152	-3.5461785	0.5078126
C	0.5097389	1.6586918	2.6401191	C	-1.8627030	-2.9727642	1.1196375
C	-1.9915777	2.5944582	1.7583284	C	-1.7999215	-1.9536158	2.0468194
C	-1.8787120	1.4439090	2.5118792	H	-2.7025559	-1.4115882	2.2962891
H	-2.7740162	0.8949576	2.7723514	C	-0.6814566	-3.6550763	0.7832493
C	-4.3455888	2.4727632	1.7059127	C	0.5062070	-3.2523548	1.3614914
H	-5.1593694	3.0457017	1.2641723	H	1.4200340	-3.7708518	1.1025359
				C	0.5763102	-2.1940360	2.2729659
				C	-0.5996393	-1.5508248	2.6407037
				C	0.3504761	-5.3964486	-0.4223074
				H	0.7853811	-5.8766063	0.4624268

H	1.1043597	-4.7593242	-0.8972492	C	0.3825672	2.1732671	-2.5423806
H	0.0404085	-6.1642062	-1.1299579	C	0.7100583	3.9165556	-1.0941005
H	0.1728998	-0.4778679	4.3369600	C	-0.5926126	1.1764589	-3.1302273
C	1.9410196	-1.7842802	2.7698311	H	-1.3147080	1.7111460	-3.7545919
H	1.8765499	-1.3724918	3.7764772	H	-0.0412115	0.4999891	-3.7906942
H	2.5586633	-2.6830960	2.8569600	C	-5.7704165	-1.1995096	-0.4055280
O	-0.9944956	4.3686756	0.6056477	C	-4.4677835	-1.5558102	-0.0718008
H	0.8898321	5.2346331	0.5927706	C	-3.5928652	0.2721891	-1.1503217
H	2.4162358	2.1721651	3.4268989	C	-4.8615842	0.6938134	-1.5370470
H	-1.5644592	-0.4901913	4.2125030	H	-4.9765409	1.5960133	-2.1258483
C	-0.6444059	0.9425154	2.9367410	C	-5.9637354	-0.0514658	-1.1532722
C	-0.6469398	-0.4009799	3.6239413	H	-6.9630023	0.2538391	-1.4436114
C	-0.8189735	3.2741618	1.3855643	C	-2.3800242	1.1025626	-1.4727303
C	1.8904648	1.2615003	3.1252059	H	-2.6891055	1.9448348	-2.0913390
C	0.3954253	2.8094479	1.8510499	H	-2.0107401	1.5475342	-0.5405319
H	1.3005591	3.3412887	1.5844904	N	-1.3298945	0.3725386	-2.1708805
C	2.0238153	-3.2373080	-3.1043197	N	1.7118933	-1.2959846	-1.7665250
C	0.6592207	-3.2893406	-3.3519441	N	-3.4157430	-0.8349970	-0.4303257
H	0.2480433	-4.0686222	-3.9842918	N	-0.1110426	3.0506994	-1.6694178
C	-0.1719428	-2.3515783	-2.7668403	H	-6.6073569	-1.8165271	-0.0980220
H	-1.2455241	-2.3692794	-2.9062683	H	2.6992975	-3.9673408	-3.5377911
C	0.3999943	-1.3618547	-1.9723202	H	2.6991100	4.7130703	-0.9124202
C	2.5041702	-2.2227156	-2.2855145				
C	-0.4441251	-0.3422148	-1.2632329				
H	0.2250506	0.3269244	-0.7033809	Ts2e_E.xyz			
H	-1.0685050	-0.8618311	-0.5338828	97			
C	2.0640325	3.9810721	-1.3996151	Energy = -2408.533074267			
C	2.5788742	3.0805785	-2.3153259	O	-4.4051225	1.0154263	0.4496340
H	3.6345200	3.0745037	-2.5561251	O	4.6398999	1.5787075	0.2320136
C	1.7294575	2.1472231	-2.8823325	O	3.0810513	3.6684186	0.2030584
H	2.1071218	1.3902414	-3.5584396	O	-0.7782138	-4.5993211	0.4427066
				O	1.8040875	-4.2982344	0.2582000

C	-2.6101381	4.3796286	0.0059631	H	-2.0051928	-2.8257400	2.0693289
H	-3.2360325	5.2673005	-0.0983794	C	1.1663497	-3.4734560	1.1207284
C	-1.1097963	1.5695559	2.9288357	C	1.7933628	-2.5392823	1.9266006
C	-3.3535361	1.1510361	1.2895739	H	2.8712614	-2.4525962	1.8897678
C	-2.8178449	0.1273201	2.0528335	C	1.0876185	-1.6880296	2.7809953
H	-3.2613356	-0.8578174	1.9992753	C	-0.3000224	-1.7901541	2.8173720
C	-4.9648833	-0.2684646	0.3155040	C	3.1941632	-4.1435352	0.1214484
H	-5.7491963	-0.1788623	-0.4348381	H	3.7200558	-4.3724287	1.0559876
H	-5.4089446	-0.6132306	1.2570540	H	3.4568720	-3.1308242	-0.2036816
H	-4.2210231	-0.9998174	-0.0201635	H	3.5040819	-4.8530466	-0.6444273
H	0.2234034	1.2304684	4.5859704	H	-0.6707868	-0.5605764	4.5421579
C	1.3996356	1.7104741	2.8478035	C	1.8781239	-0.6881647	3.5998298
C	2.2038164	0.5746353	2.8364596	H	1.3509659	-0.4570841	4.5251679
C	3.3236587	0.5563258	2.0027118	H	2.8160126	-1.1627708	3.9019456
H	3.9369492	-0.3362649	1.9863112	O	-3.4027020	3.4390050	0.7081608
C	3.6123156	1.5792228	1.1255702	H	-1.7132436	4.6534169	0.5685519
C	2.7860606	2.7112656	1.1134967	H	0.1134393	2.8877771	4.0636802
C	1.7206767	2.7660147	1.9920343	H	-2.0474399	-1.4657122	3.9808458
H	1.0833169	3.6402867	1.9925066	C	-1.7014081	0.3103096	2.8700371
C	2.1368561	4.6933416	0.0183379	C	-1.1859729	-0.8850300	3.6389158
H	2.0528019	5.3346430	0.9041849	C	-2.7825377	2.4274658	1.3823436
H	1.1486207	4.2855346	-0.2274865	C	0.1570123	1.8578838	3.6978365
H	2.4991240	5.2926642	-0.8160388	C	-1.6874788	2.6098017	2.2004910
C	5.1366862	0.3584209	-0.2532363	H	-1.2563361	3.6007926	2.2794978
H	5.4522797	-0.3038563	0.5653235	C	4.5875854	-1.2111106	-2.1718368
H	6.0370464	0.6152621	-0.8146038	C	3.6215428	-1.8767243	-2.9160529
C	-2.1363961	-4.5349283	0.0432498	H	3.9163526	-2.5332493	-3.7273882
H	-2.7801238	-4.1532772	0.8400613	C	2.2836519	-1.7000515	-2.6102307
H	-2.4225255	-5.5683324	-0.1577020	H	1.5010419	-2.2088947	-3.1603065
C	-0.2310640	-3.5999418	1.1881543	C	1.9524770	-0.8447295	-1.5624529
C	-0.9267067	-2.7564382	2.0277581	C	4.1629879	-0.3751917	-1.1475949

C	0.5356324	-0.6237856	-1.1184466	E.xyz			
H	0.5608645	-0.0377387	-0.1882247	97			
H	0.0966950	-1.5917509	-0.8697681	Energy = -2408.536928941			
C	-2.8502928	4.2740123	-2.5042187	C	2.1371449	-1.4903858	2.9683152
C	-2.4394983	3.7442935	-3.7156409	H	2.4520910	-1.0569979	3.9217637
H	-2.9057364	4.0597142	-4.6423616	H	2.5758451	-2.4873463	2.9412387
C	-1.4265938	2.8008120	-3.7219258	C	2.7228335	-0.6402759	1.8628197
H	-1.0797767	2.3562969	-4.6475294	C	3.2124030	-1.1681343	0.6693249
C	-0.8538204	2.4186717	-2.5117477	C	3.8096030	-0.3046476	-0.2481700
C	-2.2085115	3.8550203	-1.3444152	H	4.2111137	-0.7216203	-1.1634886
C	0.2110206	1.3662643	-2.4444117	C	3.8828527	1.0590413	-0.0501740
H	0.7628246	1.3417920	-3.3907064	C	3.3360155	1.5984715	1.1218594
H	0.9146533	1.6774367	-1.6648450	C	2.7963866	0.7381534	2.0647728
C	-2.4573086	-4.2721806	-2.4463560	H	2.4006094	1.1454804	2.9856868
C	-2.2761340	-3.6984278	-1.1972188	C	2.7799958	3.5083889	2.3889107
C	-2.0626793	-1.5975773	-2.0969415	H	2.8629345	4.5881060	2.2727909
C	-2.2371944	-2.0921424	-3.3880725	H	1.7223673	3.2315572	2.4700925
H	-2.1838760	-1.4173387	-4.2341691	H	3.2989958	3.2072134	3.3066954
C	-2.4595306	-3.4445585	-3.5607597	C	4.3692047	1.7538401	-2.2998184
H	-2.6102650	-3.8574209	-4.5520289	H	5.1256072	2.4041892	-2.7405692
C	-1.6997827	-0.1567126	-1.8654910	H	4.5859383	0.7236133	-2.5994310
H	-2.2705840	0.4711723	-2.5509600	C	2.7326334	3.3092011	-3.4605393
H	-1.9731948	0.1276095	-0.8404391	C	1.4116757	3.6223546	-3.7524961
N	-0.2783948	0.0088971	-2.1412511	H	1.1727944	4.5172295	-4.3164781
N	2.8794778	-0.1963259	-0.8729341	C	0.4047683	2.7934569	-3.2924657
N	-2.1202968	-2.3851157	-1.0286684	H	-0.6408877	3.0207040	-3.4623681
N	-1.2284028	2.9564250	-1.3523881	C	0.7567209	1.6544182	-2.5715055
H	-2.5792846	-5.3444445	-2.5442920	C	2.9913220	2.1440892	-2.7536689
H	5.6428629	-1.3312743	-2.3908733	C	-0.2681947	0.7537253	-1.9510700
H	-3.6501139	5.0031402	-2.4527715	H	0.2642290	-0.1000059	-1.5070930
				H	-0.9368571	0.3621011	-2.7225678

C	3.0876872	-2.6255663	0.2978898	C	-0.0793574	-2.6416714	2.3987186
H	3.9260685	-2.8882463	-0.3532519	C	0.6286189	-1.5869180	2.9808427
H	3.1887416	-3.2581084	1.1793256	C	-0.0741446	-0.5658399	3.6160739
C	0.6863924	-3.5182291	0.1674384	H	0.4904700	0.2496575	4.0469087
C	-0.4239287	-3.8136474	-0.6247851	C	-1.4562467	-0.5451529	3.6840268
H	-1.2867113	-4.2671590	-0.1528352	C	-2.1648831	-1.6021659	3.1043831
C	-0.4790832	-3.5183685	-1.9705200	C	-1.4689286	-2.6217880	2.4842424
C	0.6243153	-2.8918938	-2.5680333	H	-2.0555539	-3.4261176	2.0539084
C	1.7487519	-2.6463939	-1.7989028	C	-4.2088327	-0.7918897	2.3174125
H	2.6095691	-2.1762016	-2.2556240	H	-3.9303530	0.2499097	2.5046322
C	1.8049453	-2.9501343	-0.4375132	H	-3.9991090	-1.0434658	1.2715650
C	1.5725397	-1.8745974	-4.4718551	H	-5.2737130	-0.9185822	2.5128972
H	1.7937309	-0.9395658	-3.9442589	C	-1.6646661	1.6899290	4.5682177
H	2.4800841	-2.4892783	-4.5060494	H	-2.2987248	2.1173675	5.3460758
H	1.2577777	-1.6504421	-5.4901453	H	-0.6435050	1.6350822	4.9579380
C	-2.8506340	-3.7038470	-2.3158979	C	-2.5697982	3.6165473	3.1885231
H	-3.4644086	-4.2579774	-3.0270970	C	-1.7123829	2.5339171	3.3237287
H	-2.9760781	-4.1576841	-1.3281196	C	-1.0059860	2.7115668	1.1458550
C	-4.1510562	-1.7003120	-3.1713392	C	-1.8247405	3.8172178	0.9259755
C	-4.4016676	-0.3370481	-3.0943854	H	-1.8525971	4.2807956	-0.0528853
H	-5.1058684	0.1299665	-3.7740436	C	-2.6055741	4.2804109	1.9691323
C	-3.7258040	0.4196992	-2.1546571	H	-3.2543649	5.1383663	1.8319131
H	-3.8650293	1.4917672	-2.0813784	C	-0.2070699	2.0796440	0.0454819
C	-2.8296474	-0.2220160	-1.3027201	H	0.4658431	1.3408097	0.5042018
C	-3.2550253	-2.2574806	-2.2703346	H	0.4117562	2.8331323	-0.4491608
C	-1.9982587	0.5310892	-0.3084628	N	-1.0777382	1.4638092	-0.9594408
H	-1.4643424	-0.2090701	0.3059014	O	3.3774019	2.9455700	1.2475527
H	-2.6498181	1.1048033	0.3558781	O	4.5020978	1.9302705	-0.8986229
C	0.5777782	-3.7810430	1.6519281	O	0.5025425	-2.5655116	-3.8755357
H	1.5553380	-4.0053734	2.0784129	O	-1.5213856	-3.8380437	-2.7906126
H	-0.0265002	-4.6796249	1.8015468	O	-3.5266407	-1.6731550	3.1898189

O	-2.1998956	0.4012559	4.3246140	H	-3.2013264	3.9258633	4.0131398
N	2.0222967	1.3278600	-2.3476433	H	3.5436973	3.9600600	-3.7652726
N	-0.9331156	2.1168754	2.3296079	H	-4.6334655	-2.3173008	-3.9202645
N	-2.6306298	-1.5322523	-1.3464274				