

Supporting Information

DFT Study of Mechanisms of [8+2] cycloadditions of Dienylfurans/ Dienylisobenzofurans with DMAD

Qi Cui[†], Yuanyuan Chen[†], James W. Herndon[‡], and Zhi-Xiang Yu^{†,*}

[†]Beijing National Laboratory for Molecular Sciences (BNLMS), Key Laboratory of Bioorganic Chemistry and Molecular Engineering of the Ministry of Education, College of Chemistry, Peking University, Beijing 100871, P. R. China.

Email: yuzx@pku.edu.cn

[‡]New Mexico State University, Department of Chemistry and Biochemistry, MSC 3C, Las Cruces, New Mexico 88003, USA.

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1. Computed enthalpies and Gibbs free energies in the gas phase.

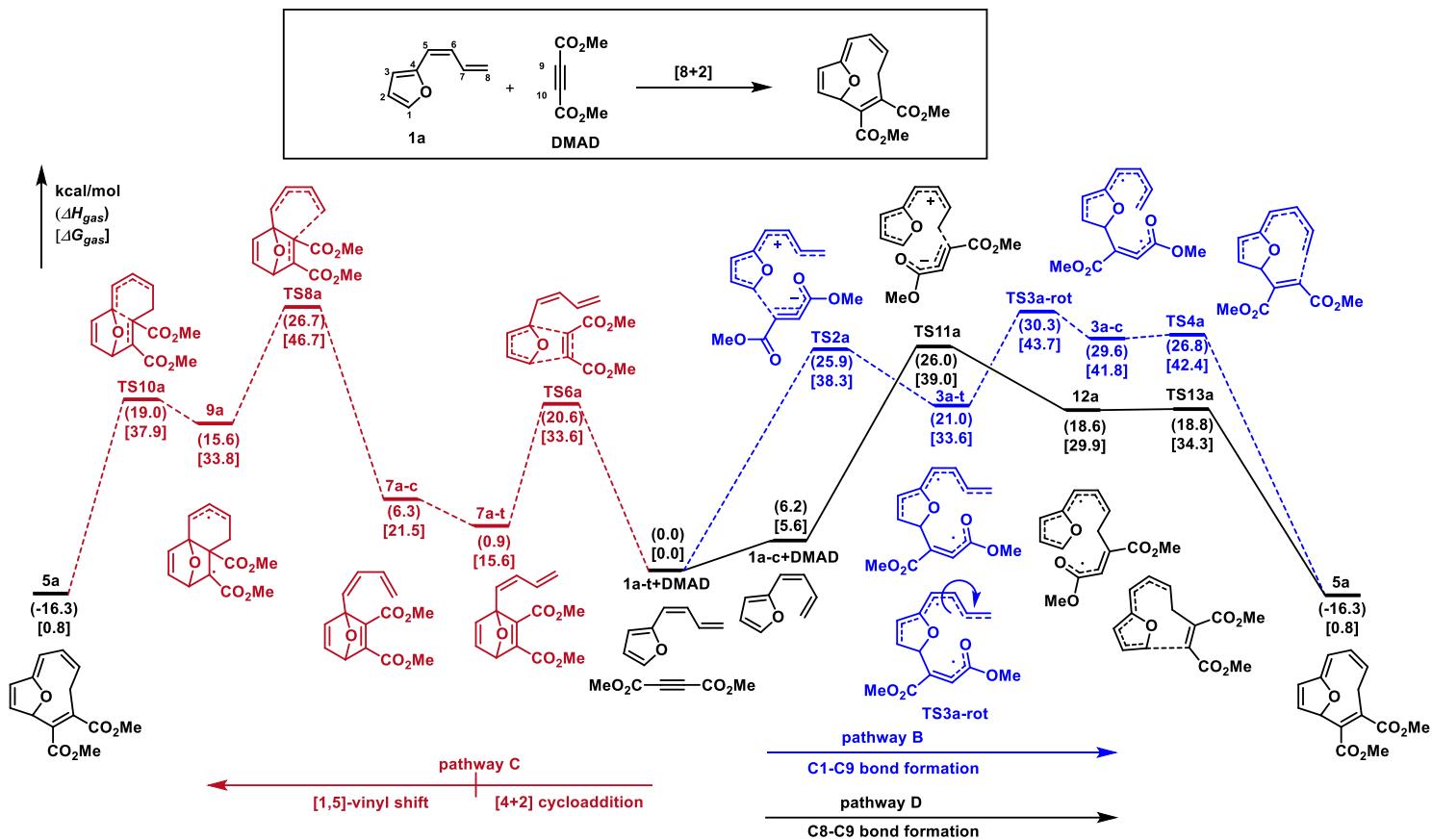


Figure S1. Computed potential energy surfaces in the gas phase of pathways B, C and D of [8+2] reaction between dienylfuran **1a** and DMAD at the (U)B3LYP/6-311+G(d,p)/(U)B3LYP/6-31+G(d) level.

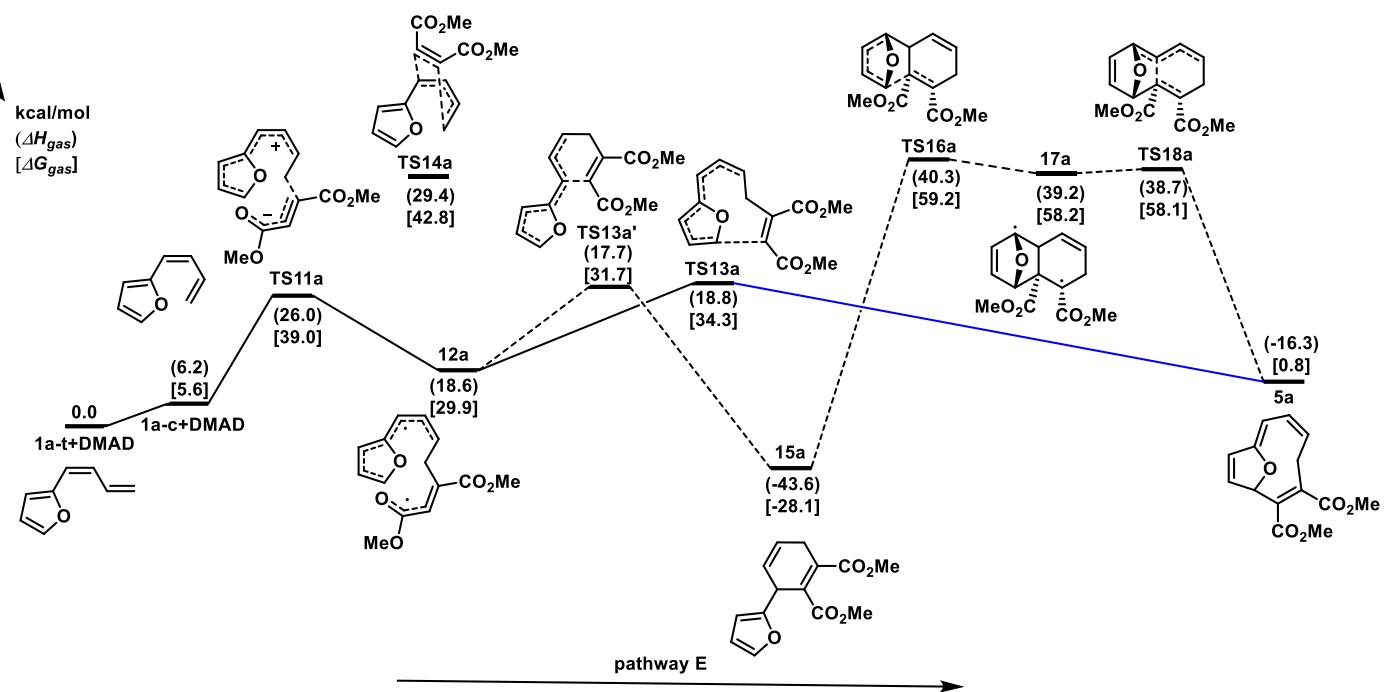


Figure S2. Computed Gibbs energy profiles of pathway E of [8+2] reaction of dienylfuran **1a** with DMAD at the (U)B3LYP/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

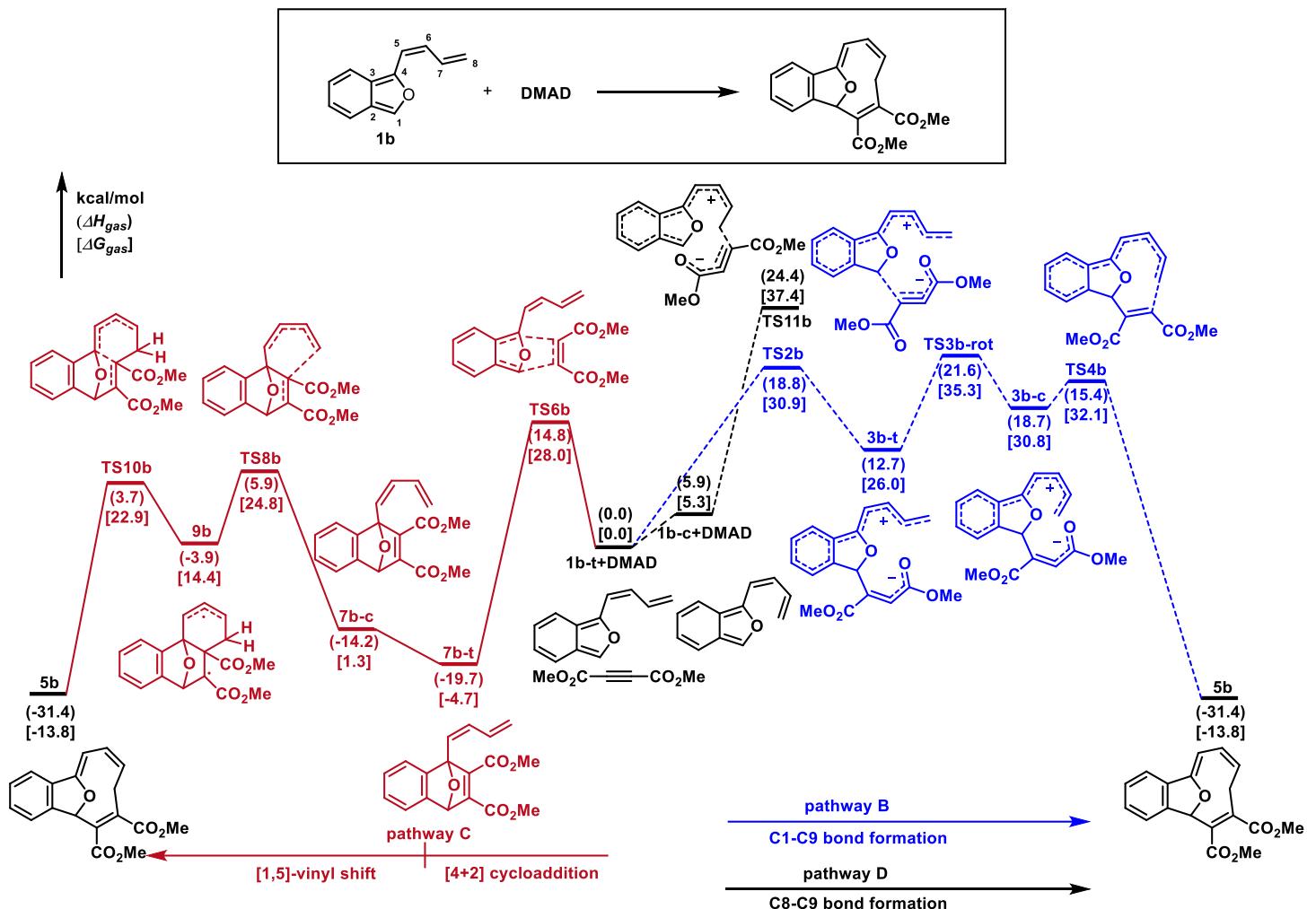


Figure S3. Computed potential energy surfaces in the gas phase of pathways B, C and D of [8+2] reaction between dienylisobenzofuran **1b** and DMAD at the (U)B3LYP/6-311+G(d,p)/(U)B3LYP/6-31+G(d) level.

2. Potential energy surfaces of the reaction of dienylisobenzofuran and dienophiles.

In reconsideration of the reactions of dienylisobenzofuran and C₂H₂/DMAD, the stepwise [1,5]-vinyl shift and the **TS3-rot** step have been added. As a result, the pathway D is not favored in these cases. For the comparison of pathways B and C, according to the potential energy surfaces, pathway C is more favored in these cases, which gives similar conclusion we discussed before (**Figures S4-S6**).

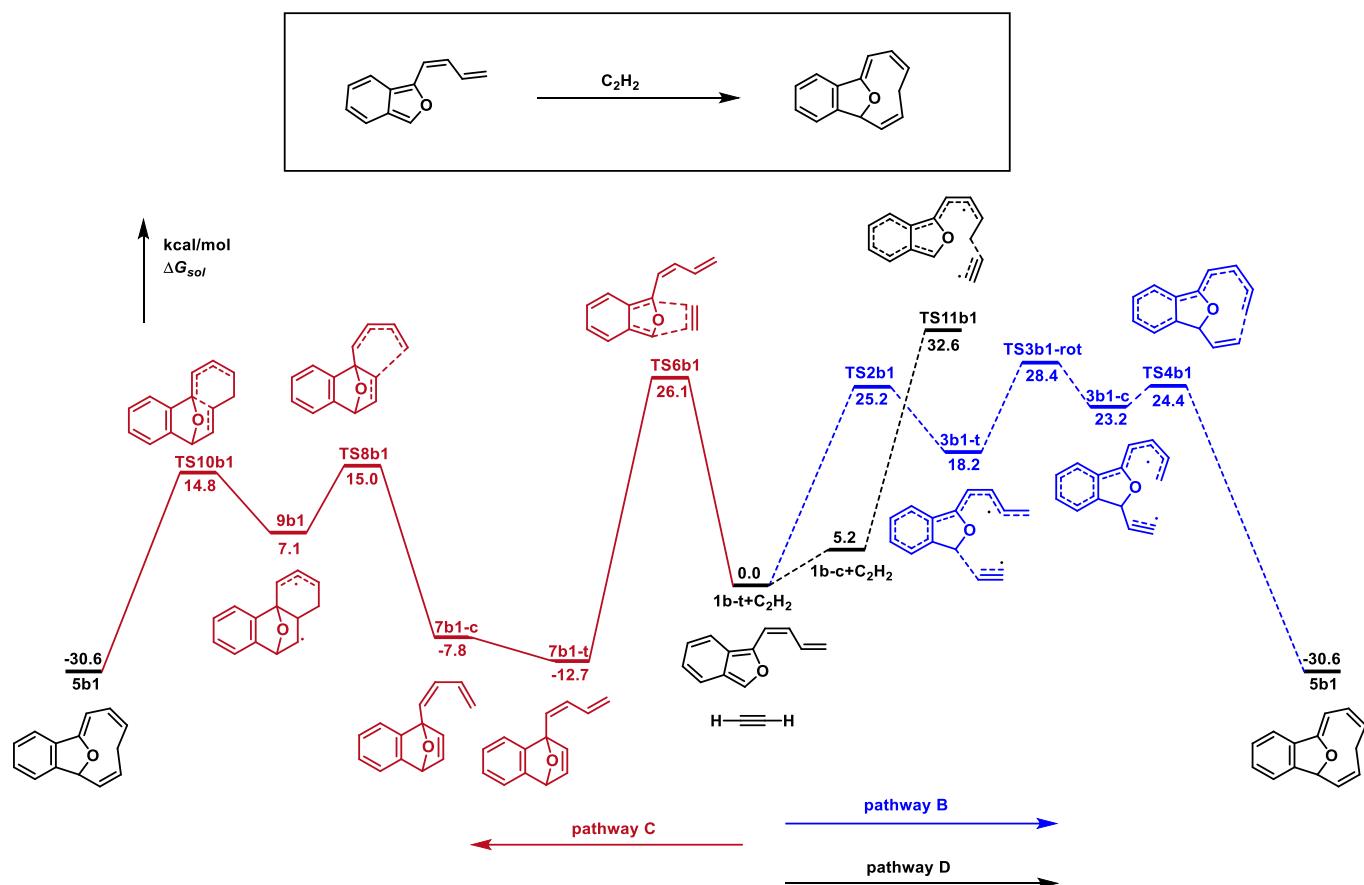


Figure S4. Computed Gibbs energy profiles of pathways B, C and D of [8+2] reaction between dienylisobenzofuran **1b** and C₂H₂ at the SMD/(U)B3LYP-D3/6-311+G(d,p)/(U)B3LYP/6-31+G(d) level.

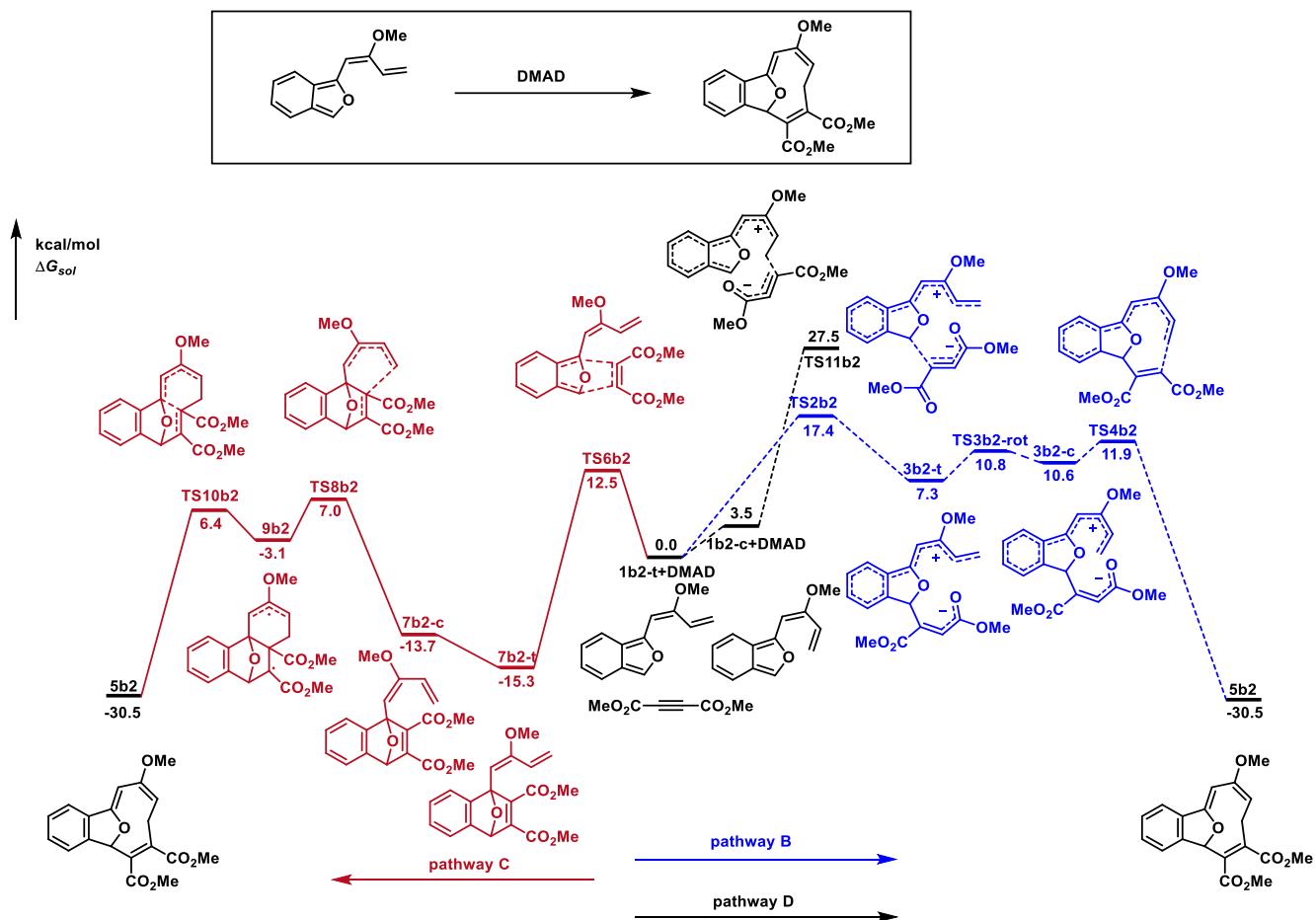


Figure S5. Computed Gibbs energy profiles of pathways B, C and D of [8+2] reaction between dienylisobenzofuran **1b2** and DMAD at the SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

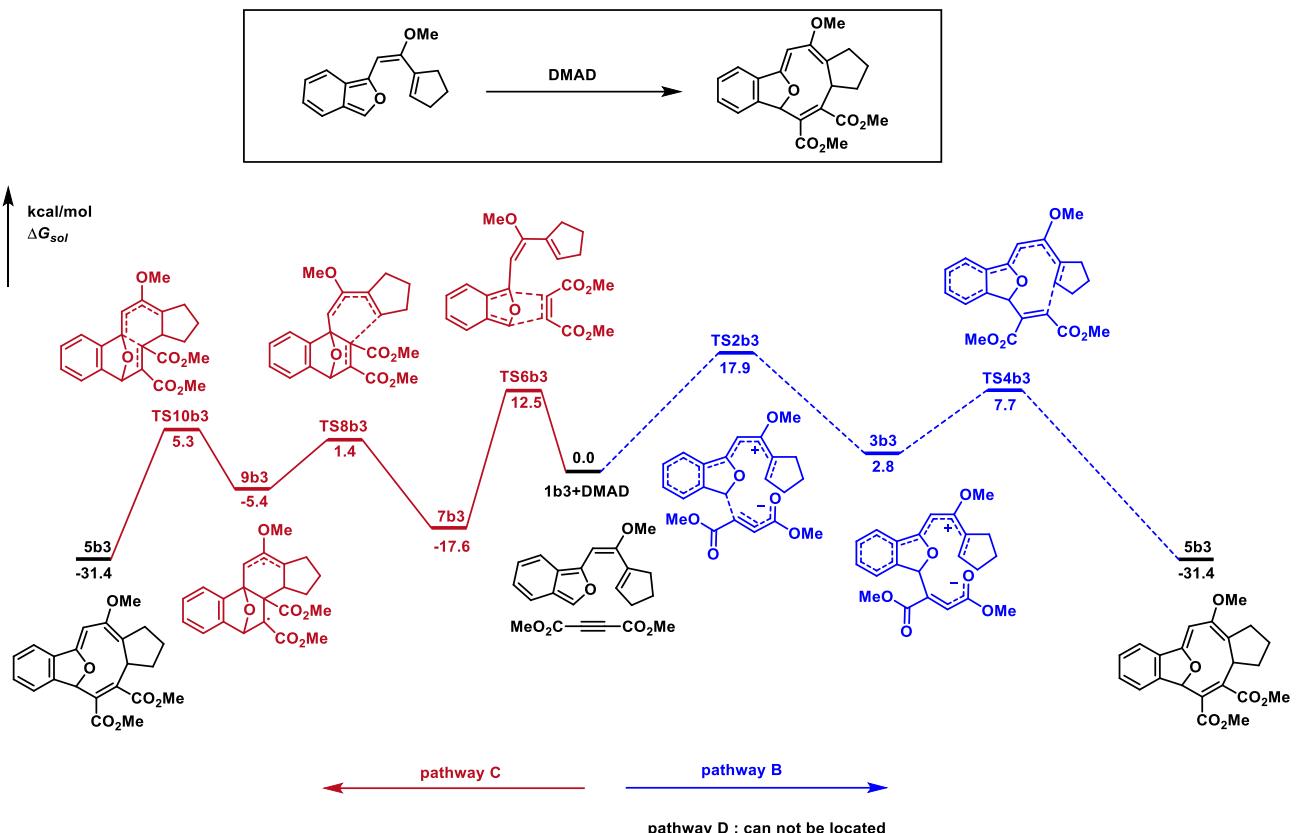


Figure S6. Computed Gibbs energy profiles of pathways B and C of [8+2] reaction between dienylisobenzofuran **1b3** and DMAD at the SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

3. Other reaction pathways and discussions of calculation methods

3.1 Other reaction pathways

We considered a possibility in pathway B: intermediate **3a-c** could be formed by the C1–C9 formation from **1a-c** and DMAD via the transition state **TS2a-c**. However, the activation Gibbs free energy was 34.7 kcal/mol and this process was not favored (**Figure S7**).

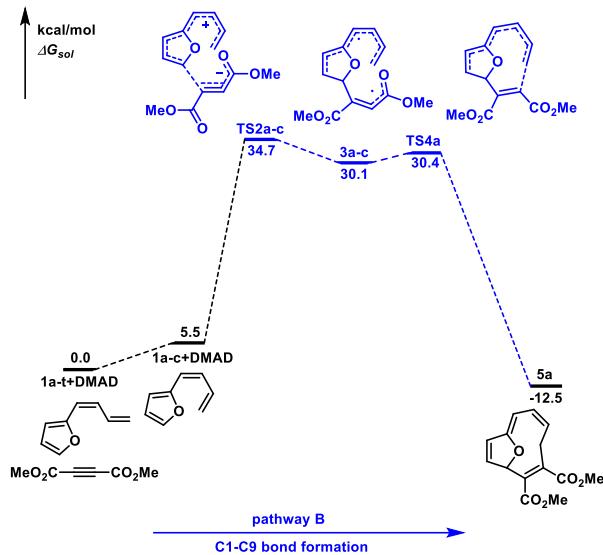


Figure S7. Computed Gibbs energy profile of [8+2] reaction between dienylfuran **1a** and DMAD via **TS3a-c** at the SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

We also considered a possibility in pathway D: intermediate **12a-t** could be formed by the C8–C9 formation from **1a-t** and DMAD via the transition state **TS11a-t**. However, the transformation from **12a-t** to **12a** was difficult (the activation Gibbs free energy of this pathway was 35.9 kcal/mol). So this process was not favored. (**Figure S8**)

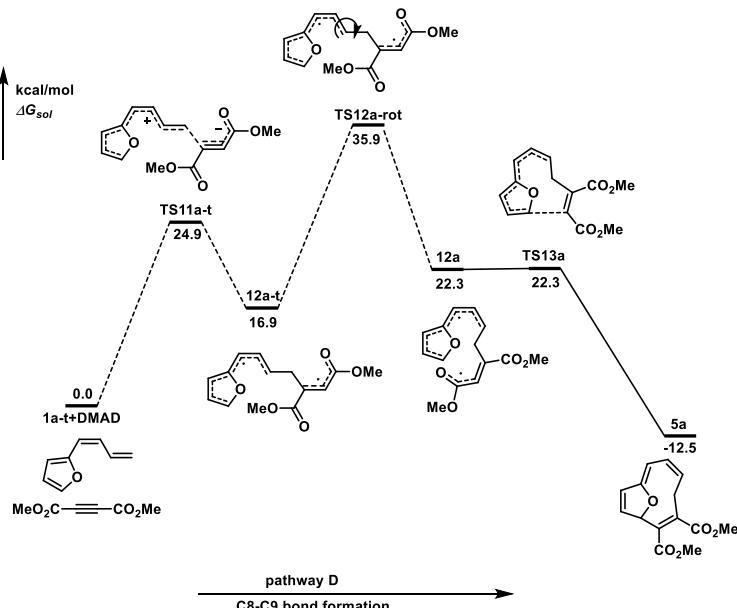


Figure S8. Computed Gibbs energy profile of [8+2] reaction between dienylfuran **1a** and DMAD via **TS11a-t** at the SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

t at the SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

Pathway E to give [4+2] product **15a** was studied (**Figure S9**). **15a** could be formed by a radical ring closure from **12a** via a singlet diradical transition state **TS13a'**. This step has a similar activation Gibbs free barrier compared with the C1–C10 bond formation. However, we couldn't identify any [4+2] products in crude H-NMR or isolated them (*Org. Lett.* **2005**, *7*, 1665–1667). We also tried different DFT functional (**Table S1, Entries 1–4**) or optimized the structures in solution phase (**Table S1 Entry 5**), finding that the Gibbs energies of **TS13a** and **TS13a'** are very close. Considering the calculation of singlet diradical species is not absolutely accurate for DFT calculations, the relative Gibbs free energy of **TS13a'** could be underestimated and we ruled out this based on the experimental results.

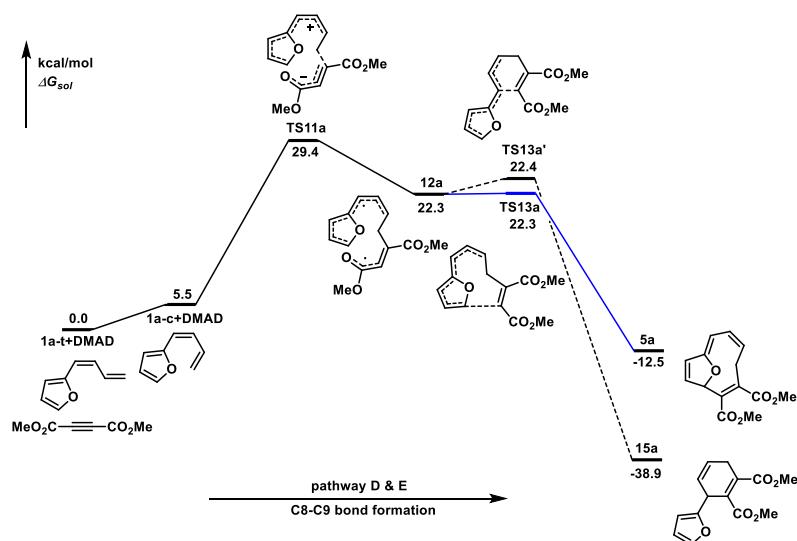


Figure S9. Computed Gibbs energy profile of [8+2] reaction between dienylfuran **1a** and DMAD via **TS11a-t** at the SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

Table S1 Calculations for the difference between ΔG (**TS13a'**) and ΔG (**TS13a**), See also **Figure S9**

	ΔG (TS13a') - ΔG (TS13a)
SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d)	0.16
SMD/(U)M06-2X/6-311+G(d,p)//(U)B3LYP/6-31+G(d)	0.05
SMD/(U)M06-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d)	0.92
SMD/(U)BMK-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d)	1.41
SMD/(U)B3LYP-D3/6-311+G(d,p)	-0.30

3.2 Discussions of calculation methods

We also performed the calculations by (U)M06-2X functional, which was suggested also a good way to compute diradicals (Ess, D. H., Cook, T. C. Unrestricted Prescriptions for Open-Shell Singlet Diradicals: Using Economical Ab Initio and Density Functional Theory to Calculate Singlet–Triplet Gaps and Bond Dissociation Curves *J. Phys. Chem. A* **2012**, *116*, 20, 4922–4929). However, the results were different. In the case of dienylfuran **1a** and DMAD, the pathway C was favored now (**TS6a** vs **TS11a**, **Figure S10**, for detailed data: see part 5 in SI), which gives opposite result with (U)B3LYP functional. In the case of dienylisobenzofuran **1d**, the energy barrier between [4+2] pathway and [8+2] pathway was 7.0 kcal/mol (**TS6d** vs **TS11d**), which was not in accord with our previous experiment because the [4+2] pathway and [8+2] pathway should be competitive considering the facts that two cycloadducts could be isolated and [4+2] product could not transform to [8+2] product (Chen, Y.; Ye, S.; Jiao, L.; Liang, Y.; Sinha-Mahapatra, D. K.; Herndon, J. W.; Yu, Z.-X. Mechanistic Twist of the [8+2] Cycloadditions of Dienylisobenzofurans and Dimethyl Acetylenedicarboxylate: Stepwise [8+2] versus [4+2]/[1,5]-Vinyl Shift Mechanisms Revealed through a Theoretical and Experimental Study. *J. Am. Chem. Soc.* **2007**, *129*, 10773–10784.) So, (U)M06-2X functional is not suitable for investigating the present reaction.

Houk *et al.* also gave a comparison between (U)B3LYP and (U)M06-2X, and they thought (U)B3LYP was a suitable functional for the calculations of singlet diradicals (James, N. C.; Um, J. M.; Padias, A. B.; Hall, H. K. Jr., Houk, K. N. Computational Investigation of the Competition between the Concerted Diels–Alder Reaction and Formation of Diradicals in Reactions of Acrylonitrile with Nonpolar Dienes. *J. Org. Chem.* **2013**, *78*, 6582–6592). Herein, we used (U)B3LYP functional to illustrate the potential energy surfaces which involve singlet diradicals and have comparison of the reaction selectivity.

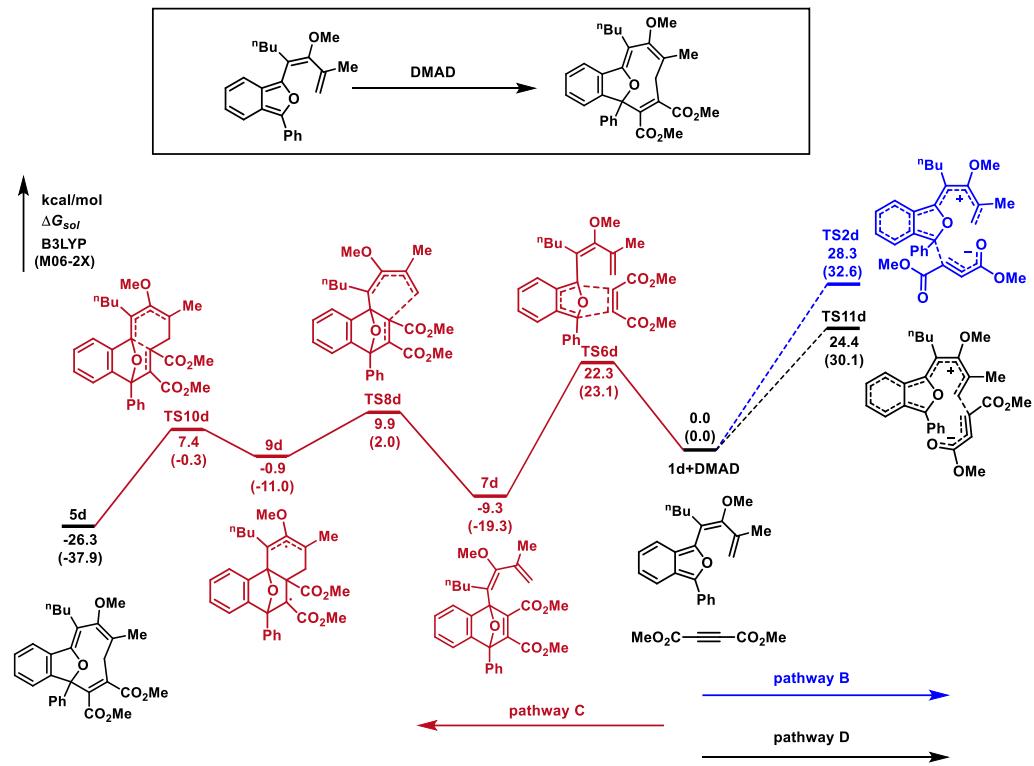


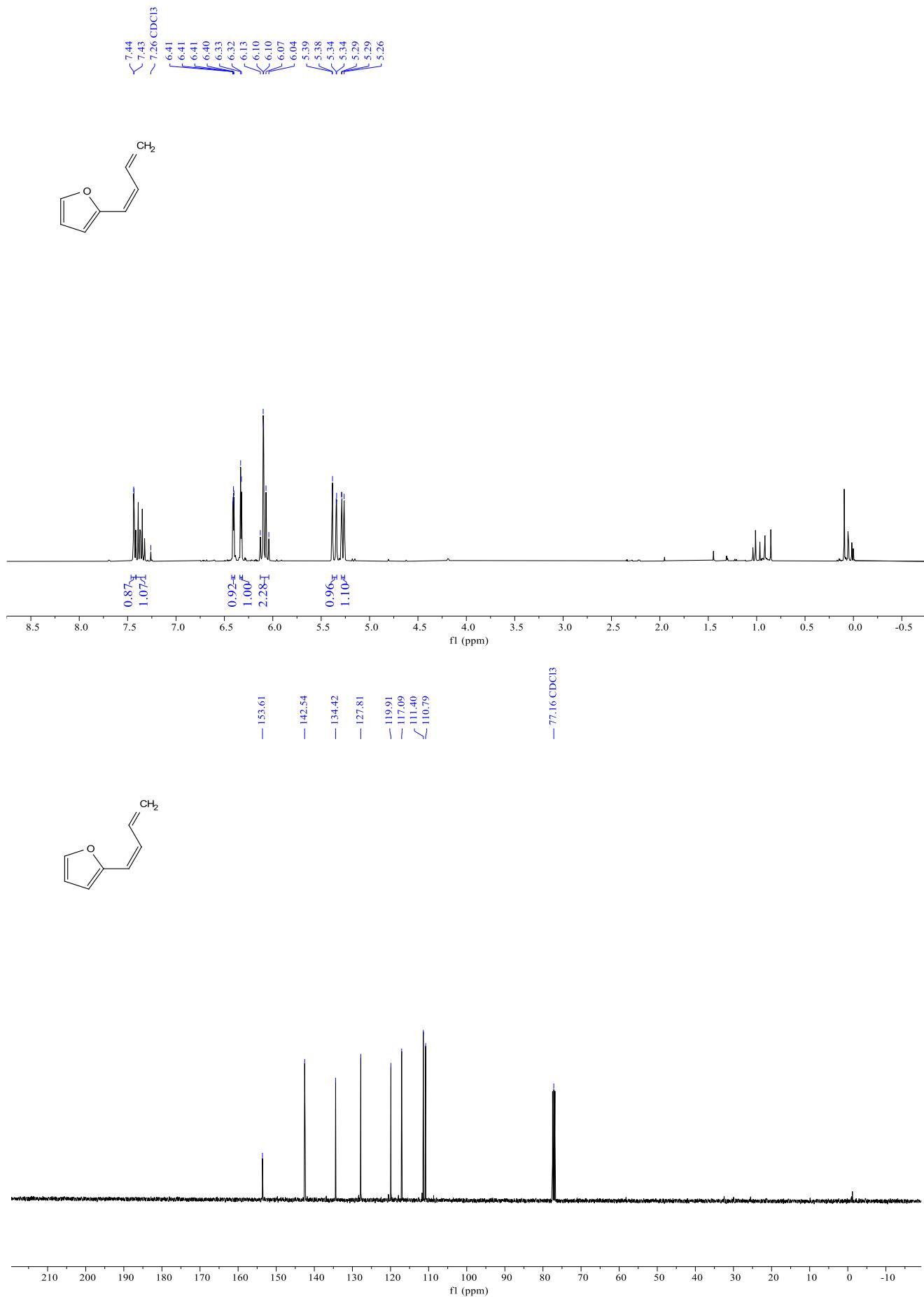
Figure S10. Computed Gibbs energy profiles of pathways B, C and D of [8+2] reaction between substituted dienylisobenzofuran **1d** and DMAD at SMD/(U)B3LYP-D3/6-311+G(d,p)//(U)B3LYP/6-31+G(d) or SMD/(U)M06-2X/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level.

4. Experimental part (NMR spectra of 1a and kinetic studies)

General Information for experiments:

Air- and moisture-sensitive reactions were carried out in oven-dried glassware sealed with rubber septa under a positive pressure of dry argon. Reactions were stirred using Teflon coated magnetic stir bars. Elevated temperatures were maintained using thermostat-controlled silicone oil baths. Organic solutions were concentrated using a rotary evaporator with a desktop vacuum pump. Tetrahydrofuran (THF) was distilled from sodium and benzophenone prior to use. Synthetic reagents were purchased and used without further purification unless otherwise indicated. Analytical TLC was performed with 0.25 mm silica gel G plates with a 254 nm fluorescent indicator. The TLC plates were visualized by ultraviolet light.

NMR spectra of **1a** (400 MHz for ^1H , 101 MHz for $^{13}\text{C}\{\text{H}\}$)



Kinetic studies:

Table S2: Original data of activation energy test.

(A=Z-dienylfuran **1a**)

NMR areas for $\delta=5.030-5.150$ ($\delta=0.760-0.835$ as the internal standard) at 70°C

Time(s)	Area [A]	Relative area [A]/[A ₀]	-ln([A]/[A ₀])
0	1.0092	1.0000	0.0000
1200	0.966	0.9572	0.0437
2400	0.9232	0.9148	0.0891
3600	0.9101	0.9018	0.1034
4200	0.8909	0.8828	0.1247
4800	0.8663	0.8584	0.1527

NMR areas for $\delta=5.030-5.150$ ($\delta=0.760-0.835$ as the internal standard) at 75°C

Time(s)	Area [A]	Relative area [A]/[A ₀]	-ln([A]/[A ₀])
0	1.0092	1.0000	0.0000
1200	0.9486	0.9400	0.0619
2400	0.8636	0.8557	0.1558
3600	0.8316	0.8240	0.1936
4800	0.7958	0.7885	0.2376

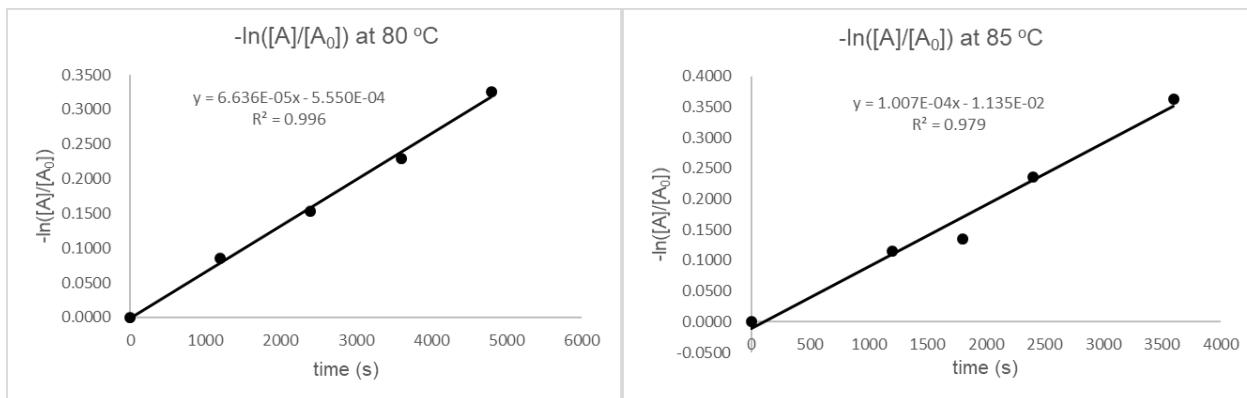
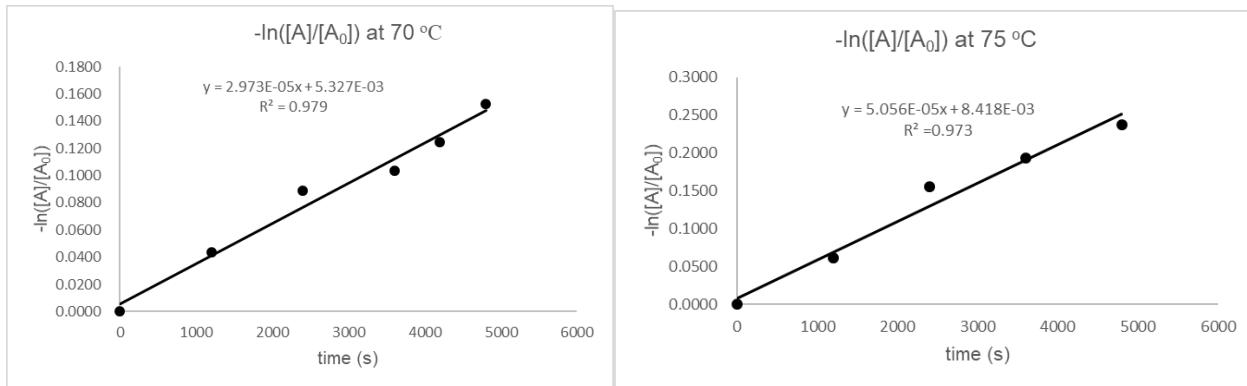
NMR areas for $\delta=5.030-5.150$ ($\delta=0.760-0.835$ as the internal standard) at 80°C

Time(s)	Area [A]	Relative area [A]/[A ₀]	-ln([A]/[A ₀])
0	1.0092	1.0000	0.0000
1200	0.9271	0.9186	0.0849
2400	0.8654	0.8575	0.1537
3600	0.8028	0.7955	0.2288
4800	0.7283	0.7217	0.3262

NMR areas for $\delta=5.030-5.150$ ($\delta=0.760-0.835$ as the internal standard) at 85°C

Time(s)	Area [A]	Relative area [A]/[A ₀]	-ln([A]/[A ₀])
0	1.0092	1.0000	0.0000
1200	0.8992	0.8910	0.1154
2400	0.8815	0.8735	0.1353
3600	0.7965	0.7892	0.2367
4800	0.7023	0.6959	0.3626

Linear fitting plot for k_{obs}

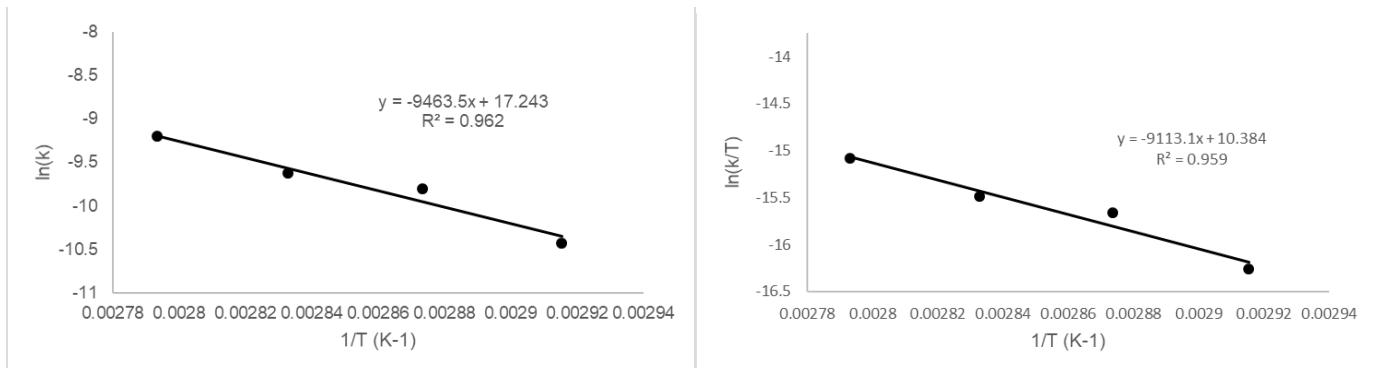


Calculation for Arrhenius plot

T	1/T	K_{obs}	$\ln(K_{\text{obs}})$	$\ln(K_{\text{obs}}/T)$
343	0.002915	2.9730E-05	-10.4234	-16.2611
348	0.002874	5.5060E-05	-9.8071	-15.6593
353	0.002833	6.6360E-05	-9.6204	-15.4869
358	0.002793	1.0075E-04	-9.2029	-15.0834

Arrhenius plot

Eyring plot



Analysis of the kinetic data:

The rate of the [8+2] reaction is

$$r = k[A]^a[DMAD]^b$$

Considering [8+2] cycloaddition is a bimolecular reaction, we assume that:

$$\begin{aligned}a &= b = 1 \\-\ln \frac{[A]}{[A]_0} &= k_{obs} t \\k_{obs} &= k[DMAD] \\[DMAD] &= 1.0 \text{ mol/L}\end{aligned}$$

Arrhenius equation:

$$\begin{aligned}\ln k &= -\frac{E_a}{RT} + \ln A \\E_a &= 18.8 \text{ kcal/mol}\end{aligned}$$

Eyring equation:

$$\begin{aligned}\ln \left(\frac{k}{T} \right) &= \frac{-\Delta H^\ddagger}{RT} + \ln \frac{k_B}{h} + \frac{\Delta S^\ddagger}{R} \\\Delta G^\ddagger &= \Delta H^\ddagger - T\Delta S^\ddagger \\\Delta H^\ddagger &= 18.6 \text{ kcal/mol} \\\Delta G^\ddagger &= 26.0 \text{ kcal/mol}\end{aligned}$$

5. Computed energies of all of the stationary points

Thermal correction to Enthalpy \mathbf{CH} , Thermal correction to Gibbs Free Energy \mathbf{CG} , Single point energy in gas phase energy E_{gas} , Single point energy in 1, 4-dioxane E_{sol} , gas phase energy for triplet species E_T , Total spin-squared operator of singlet diradical S^2 (S for singlet diradical, T for triplet diradical correlation), $\Delta G_{(without\ corr)}$, delta Gibbs free energy without YJH correction, ΔG , delta Gibbs free energy with YJH correction.

SMD/(U)B3LYP-D3/6-311+G(d,p)/(U)B3LYP/6-31+G(d) level:

For the case of dienylfuran **1a**

	\mathbf{CH}	\mathbf{CG}	$E(gas)$	E_{sol}	E_T	S^2 (S)	S^2 (T)	$\Delta G_{(without\ corr)}$	ΔG
1a-t	0.145928	0.103847	-384.9383709	-384.9524318					
DMAD	0.127062	0.076477	-533.2385426	-533.2548165					
TS2a	0.273176	0.200289	-918.1358134	-918.1777469				29.2	29.2
3a-t	0.273886	0.201321	-918.1399128	-918.1827982	-918.125112	0.4718	2.0545	26.6	23.9
TS3a-rot	0.27235	0.201092	-918.1238549	-918.1682873	-918.105338	0.3719	2.0425	35.6	33.0
3a-c	0.274069	0.20077	-918.1274144	-918.1733869	-918.1167834	0.4912	2.0552	32.2	30.1
TS4a	0.273893	0.206161	-918.1351781	-918.1815999				30.4	30.4
5a	0.277683	0.212298	-918.2076264	-918.2561585				-12.5	-12.5
TS6a	0.273145	0.201324	-918.1443078	-918.187774				23.5	23.5
7a-t	0.275652	0.206481	-918.1782107	-918.2206186				6.1	6.1
7a-c	0.27559	0.207064	-918.1694396	-918.2145783				10.3	10.3
TS8a	0.271908	0.211079	-918.1272458	-918.1761989	-918.108468	0.492	2.0261	36.9	33.1
9a	0.274545	0.210814	-918.1536469	-918.203678	-918.1536877	1.0302	2.0334	19.5	19.5
TS10a	0.273315	0.210765	-918.1409482	-918.1912732	-918.129103	0.686	2.0301	27.2	23.4
TS11a	0.273857	0.202018	-918.1363949	-918.1790463				29.4	29.4
12a	0.274533	0.199881	-918.1462076	-918.1856066	-918.1430224	0.929	2.0493	24.0	22.3
TS13a	0.273813	0.205867	-918.1424664	-918.1888959	-918.1299844	0.6175	2.0497	25.7	22.3
TS14a	0.273544	0.202256	-918.1306318	-918.1757483				31.6	31.6
15a	0.277814	0.209859	-918.2512406	-918.295737				-38.9	-38.9
TS16a	0.273386	0.210833	-918.1057516	-918.1552819	-918.089868	0.6369	2.013	49.9	45.3
17au	0.275192	0.212709	-918.1113583	-918.1608749	-918.1045032	0.8713	2.0119	47.5	44.2
TS18a	0.273664	0.21192	-918.1086925	-918.1586858	-918.0864804	0.4936	2.0138	48.4	43.9
1a-c	0.146198	0.103037	-384.9287136	-384.9429199				5.5	5.5
1a-E	0.14496	0.10272	-384.9415696	-384.955556				-2.7	-2.7
1a-E-c	0.145636	0.102751	-384.9356967	-384.9497599				1.0	1.0
TS14a-E	0.273676	0.201949	-918.148867	-918.1917798				21.4	21.4
TS13a'	0.273447	0.203136	-918.1450489	-918.1871431	-918.1386318	0.8057	2.0501	25.0	22.4
TS2a-c	0.273403	0.199795	-918.1262389	-918.1684415				34.7	34.7
TS11a-t	0.273616	0.200394	-918.1449962	-918.1846208				24.9	24.9
12a-t	0.274404	0.201268	-918.1553827	-918.1942374	-918.1498856	0.8686	2.0476	19.4	16.9
TS12a-rot	0.272357	0.20021	-918.1212895	-918.1607591	-918.1113519	0.7709	2.0181	39.8	35.9

For the case of dienylisobenzofuran **1b**

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1b-t	0.195258	0.146757	-538.6036081	-538.6261186					
TS2b	0.322712	0.242977	-1071.812614	-1071.863131				21.7	21.7
3b-t	0.324575	0.246672	-1071.824157	-1071.881081				12.7	12.7
TS3b-rot	0.322793	0.24547	-1071.808182	-1071.866118				21.4	21.4
3b-c	0.324771	0.245032	-1071.814853	-1071.871858				17.5	17.5
TS4b	0.323807	0.251354	-1071.819088	-1071.876826				18.3	18.3
5b	0.327598	0.256669	-1071.897511	-1071.957355				-28.9	-28.9
TS6b	0.322772	0.244667	-1071.818993	-1071.872869				16.6	16.6
7b-t	0.32602	0.250909	-1071.877299	-1071.928869				-14.6	-14.6
7b-c	0.325955	0.251486	-1071.868396	-1071.922933				-10.5	-10.5
TS8b	0.32361	0.254639	-1071.83132	-1071.890711	-1071.802563	0.1782	2.0261	11.7	9.9
9b	0.324714	0.254717	-1071.850885	-1071.910734	-1071.851002	1.032	2.0321	-0.8	-0.8
TS10b	0.32348	0.254955	-1071.831243	-1071.89114	-1071.816124	0.5842	2.0287	11.6	7.8
TS11b	0.323212	0.244901	-1071.804153	-1071.85559				27.6	27.6
1b-c	0.195522	0.146128	-538.5944628	-538.6172356				5.2	5.2

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1e-t	0.348176	0.282416	-886.4863281	-886.5354347					
1e-c	0.347883	0.281901	-886.4768579	-886.5271466				4.9	4.9
TS2c	0.474827	0.379337	-1419.682187	-1419.766105				26.1	26.1
5c	0.479331	0.39131	-1419.768394	-1419.857716				-23.9	-23.9
TS6c	0.475389	0.381832	-1419.692981	-1419.778457				19.9	19.9
7e-t	0.477939	0.387114	-1419.743707	-1419.828101				-7.9	-7.9
7e-c	0.477645	0.386593	-1419.736296	-1419.821793				-4.3	-4.3
TS8c	0.475596	0.389708	-1419.701492	-1419.788927	-1419.672173	0.143	2.0258	18.3	16.9
9c	0.476673	0.389747	-1419.719141	-1419.807365	-1419.719192	1.0308	2.0328	6.7	6.8
TS10c	0.475509	0.39002	-1419.702643	-1419.791997	-1419.685533	0.4902	2.0295	16.5	13.1
TS11c	0.475549	0.380771	-1419.689124	-1419.769557				24.8	24.8

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1d	0.464697	0.381435	-1080.886583	-1080.952099					
TS2d	0.591663	0.480181	-1614.076109	-1614.180436				28.7	28.7
5d	0.596344	0.491688	-1614.173327	-1614.279593				-26.3	-26.3
TS6d	0.59221	0.48281	-1614.090349	-1614.193307				22.3	22.3
7d	0.594932	0.486828	-1614.144397	-1614.247679				-9.3	-9.3
TS8d	0.59288	0.489133	-1614.113637	-1614.217623	-1614.084183	0.1078	2.024	11.0	9.9
9d	0.594057	0.4895	-1614.131482	-1614.236364	-1614.130947	1.0092	2.0323	-0.5	-0.9
TS10d	0.592692	0.488877	-1614.111963	-1614.217692	-1614.096167	0.5142	2.0278	10.8	7.4
TS11d	0.592225	0.481266	-1614.090355	-1614.18833				24.4	24.4

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
C₂H₂	0.029515	0.009748	-77.35648978	-77.35593659					
TS2b1	0.225262	0.169902	-615.919156	-615.948017	-615.896243	0.3199	2.0441	27.9	25.2
3b1-t	0.22735	0.172413	-615.9362291	-615.9646653	-615.934839	1.013	2.0498	19.0	18.2
TS3b1-rot	0.225869	0.171607	-615.9181813	-615.9470307	-615.9162529	0.9854	2.0377	29.6	28.4
3b1-c	0.227593	0.172044	-615.9274681	-615.9562673	-615.9260728	1.0129	2.0495	24.0	23.2
TS4b1	0.226305	0.175242	-615.9207562	-615.9529205	-615.9115419	0.8079	2.0483	28.2	24.4
5b1	0.232734	0.184271	-616.0206668	-616.0555435				-30.6	-30.6
TS6b1	0.226048	0.172426	-615.9232369	-615.9533552				26.1	26.1
7b1-t	0.230474	0.178728	-615.9894272	-616.0215327				-12.7	-12.7
7b1-c	0.2306	0.180046	-615.9815753	-616.0149691				-7.8	-7.8
TS8b1	0.228185	0.181164	-615.9398977	-615.9744163	-615.9137671	0.3428	2.027	18.4	15.0
9b1	0.229393	0.181319	-615.9581851	-615.992602	-615.958278	1.0301	2.0307	7.1	7.1
TS10b1	0.228483	0.181642	-615.9388527	-615.9737099	-615.918122	0.5035	2.0268	19.1	14.8
TS11b1	0.225584	0.169957	-615.9067849	-615.9355444	-615.882556	0.3527	2.0452	35.7	32.6

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1b2-t	0.23032	0.175119	-653.1542423	-653.1822975					
1b2-c	0.230084	0.174337	-653.1478162	-653.1759284				3.5	3.5
TS2b2-t	0.358283	0.272318	-1186.37146	-1186.427135				17.4	17.4
3b2-t	0.360058	0.276206	-1186.380981	-1186.447131				7.3	7.3
TS3b2-rot	0.358706	0.276154	-1186.375443	-1186.441448				10.8	10.8
3b2-c	0.359822	0.276248	-1186.373317	-1186.441861				10.6	10.6
TS4b2c	0.359216	0.280899	-1186.380742	-1186.444446				11.9	11.9
5b2	0.362569	0.285078	-1186.451696	-1186.516152				-30.5	-30.5
TS6b2	0.358345	0.274365	-1186.377643	-1186.437011				12.5	12.5
7b2-t	0.360956	0.279299	-1186.426306	-1186.486109				-15.3	-15.3
7b2-c	0.360804	0.279455	-1186.423429	-1186.48387				-13.7	-13.7
TS8b2	0.35874	0.283431	-1186.387358	-1186.45177	-1186.359131	0.1958	2.0268	8.9	7.0
9b2	0.359916	0.283584	-1186.405971	-1186.471186	-1186.40606	1.0314	2.0324	-3.2	-3.1
TS10b2	0.358555	0.283269	-1186.384823	-1186.449786	-1186.3688	0.5434	2.0271	10.0	6.4
TS11b2	0.357753	0.272199	-1186.354046	-1186.410802				27.5	27.5

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1b3	0.297226	0.235404	-769.9146462	-769.9536008					
TS2b3	0.425206	0.3336	-1303.131385	-1303.198526				17.9	17.9
3b3	0.42729	0.337783	-1303.14994	-1303.226918				2.8	2.8
TS4b3	0.426433	0.343486	-1303.149727	-1303.224766				7.7	7.7
5b3	0.429293	0.346997	-1303.212475	-1303.290594				-31.4	-31.4
TS6b3	0.425282	0.335676	-1303.138581	-1303.20926				12.5	12.5
7b3	0.428123	0.342185	-1303.191473	-1303.263762				-17.6	-17.6
TS8b3	0.425896	0.345912	-1303.156469	-1303.233762	-1303.131215	0.2449	2.0203	3.6	1.4
9b3	0.427179	0.346593	-1303.170215	-1303.248357	-1303.169863	1.0098	2.0261	-5.2	-5.4
TS10b3	0.425657	0.345519	-1303.147156	-1303.225075	-1303.132124	0.5471	2.0239	8.8	5.3

SMD/(U)M062X/6-311+G(d,p)//(U)B3LYP/6-31+G(d) level:

For the case of dienylfuran **1a**

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1a-t	0.145928	0.103847	-384.7633545	-384.7677505					
DMAD	0.127062	0.076477	-533.0206172	-533.0280037					
TS2a	0.273176	0.200289	-917.7459687	-917.7589336				33.7	33.7
3a-t	0.273886	0.201321	-917.7471198	-917.7622156	-917.7399351	0.5881	2.0701	32.3	30.5
TS3a-rot	0.27235	0.201092	-917.7345548	-917.7510802	-917.7233418	0.4106	2.0549	39.2	37.4
3a-c	0.274069	0.20077	-917.7372721	-917.7512509	-917.7311799	0.6533	2.0705	38.9	37.1
TS4a	0.273893	0.206161	-917.7524004	-917.7668773				32.4	32.4
5a	0.277683	0.212298	-917.8469911	-917.8595291				-21.8	-21.8
TS6a	0.273145	0.201324	-917.7591025	-917.7723305				26.0	26.0
7a-t	0.275652	0.206481	-917.8107579	-917.8221209				-2.0	-2.0
7a-c	0.27559	0.207064	-917.8049141	-917.8172395				1.4	1.4
TS8a	0.271908	0.211079	-917.7638868	-917.7759175	-917.745426	0.5821	2.0293	29.9	25.2
9a	0.274545	0.210814	-917.7958453	-917.8085035	-917.7959264	1.0393	2.0407	9.2	9.3
TS10a	0.273315	0.210765	-917.7785144	-917.7910898	-917.7680809	0.8103	2.0358	20.1	15.8
TS11a	0.273857	0.202018	-917.7473957	-917.7598432				34.3	34.3
12a	0.274533	0.199881	-917.7585953	-917.7702772	-917.7566882	1.023	2.0642	26.4	25.2
TS13a	0.273813	0.205867	-917.7612099	-917.7735421	-917.7536816	0.8916	2.0637	28.1	24.5
TS14a	0.273544	0.202256	-917.750933	-917.7635304				32.1	32.1
15a	0.277814	0.209859	-917.8897085	-917.9023563				-50.3	-50.3
TS16a	0.273386	0.210833	-917.7476347	-917.7592824	-917.7349591	0.7997	2.017	40.1	34.9
17au	0.275192	0.212709	-917.7596079	-917.7711142	-917.7544091	0.9452	2.0148	33.9	31.0
TS18a	0.273664	0.21192	-917.7521285	-917.763898	-917.7331133	0.6679	2.0156	37.9	32.0
1a-c	0.146198	0.103037	-384.7532592	-384.7575319				5.9	5.9
1a-E	0.14496	0.10272	-384.7667254	-384.7667254				-0.1	-0.1
1a-E-c	0.145636	0.102751	-384.7613261	-384.766087				0.4	0.4
TS14a-E	0.273676	0.201949	-917.7671622	-917.7781852				22.7	22.7

For the case of dienylisobenzofuran **1b**

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1b-t	0.195258	0.146757	-538.3649976	-538.3719526					
TS2b	0.322712	0.242977	-1071.361027	-1071.375204				26.0	26.0
3b-t	0.324575	0.246672	-1071.374413	-1071.396998				14.7	14.7
TS3b-rot	0.322793	0.24547	-1071.362189	-1071.384451				21.8	21.8
3b-c	0.324771	0.245032	-1071.364703	-1071.386736				20.1	20.1
TS4b	0.323807	0.251354	-1071.3795	-1071.395457				18.6	18.6
5b	0.327598	0.256669	-1071.478105	-1071.494098				-40.0	-40.0
TS6b	0.322772	0.244667	-1071.375033	-1071.389337				18.2	18.2
7b-t	0.32602	0.250909	-1071.449893	-1071.463336				-24.3	-24.3
7b-c	0.325955	0.251486	-1071.444069	-1071.458075				-20.6	-20.6
TS8b	0.32361	0.254639	-1071.409821	-1071.423851	-1071.38169	0.2401	2.0304	2.8	0.5
9b	0.324714	0.254717	-1071.434123	-1071.448788	-1071.43426	1.0398	2.0397	-12.8	-12.7
TS10b	0.32348	0.254955	-1071.408713	-1071.423432	-1071.39476	0.7037	2.0344	3.3	-1.3
TS11b	0.323212	0.244901	-1071.351595	-1071.366456				32.7	32.7
1b-c	0.195522	0.146128	-538.3554505	-538.3623217				5.6	5.6

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG_(without corr)</i>	<i>ΔG</i>
1e-t	0.348176	0.282416	-886.1049958	-886.0280037					
1e-c	0.347883	0.281901	-886.0974531	-886.1175872				4.3	4.3
TS2c	0.474827	0.379337	-1419.095443	-886.1102284				29.7	29.7
5c	0.479331	0.39131	-1419.213539	-1419.115766				-36.1	-36.1
TS6c	0.475389	0.381832	-1419.115288	-1419.232501				19.7	19.7
7e-t	0.477939	0.387114	-1419.182489	-1419.134108				-19.0	-19.0
7e-c	0.477645	0.386593	-1419.176675	-1419.201013				-15.5	-15.5
TS8c	0.475596	0.389708	-1419.141474	-1419.19491	-1419.112777	0.1962	2.0287	9.1	7.2
9c	0.476673	0.389747	-1419.164269	-1419.158833	-1419.164368	1.0384	2.039	-5.4	-5.3
TS10c	0.475509	0.39002	-1419.142241	-1419.182052	-1419.126576	0.6204	2.0342	7.9	3.6
TS11c	0.475549	0.380771	-1419.098956	-1419.161104				29.3	29.3

	<i>CH</i>	<i>CG</i>	<i>E(gas)</i>	<i>E_{sol}</i>	<i>E_T</i>	<i>S² (S)</i>	<i>S² (T)</i>	<i>ΔG</i>	
1d	0.464697	0.381435	-1080.415401	-1080.427849					
TS2d	0.591663	0.480181	-1613.402425	-1613.423205				32.6	32.6
5d	0.596344	0.491688	-1613.528015	-1613.54703				-37.9	-37.9
TS6d	0.59221	0.48281	-1613.423341	-1613.440987				23.1	23.1
7d	0.594932	0.486828	-1613.49491	-1613.512487				-19.3	-19.3
TS8d	0.59288	0.489133	-1613.462186	-1613.478492	-1613.433322	0.1558	2.0264	3.5	2.0
9d	0.594057	0.4895	-1613.48501	-1613.501667	-1613.484778	1.0309	2.0383	-10.8	-11.0
TS10d	0.592692	0.488877	-1613.459849	-1613.47794	-1613.445809	0.6324	2.0315	3.7	-0.3
TS11d	0.592225	0.481266	-1613.409937	-1613.428216				30.1	30.1

6. Cartesian coordinates of all computed structures

1a-t				C	-0.06290000	1.61370900	-0.54768400
C	-0.77090500	0.53569900	-0.00000400	O	0.86244800	1.39153400	-1.30726900
C	-2.08684700	0.94414400	0.00001400	O	-0.33262700	2.83167300	-0.03817800
C	-2.89230500	-0.23555600	0.00000700	C	0.53741900	3.89270300	-0.47434600
C	-2.02201900	-1.28627300	0.00000200	H	1.57117000	3.68255600	-0.18653100
O	-0.73328400	-0.83933800	-0.00002100	H	0.16953100	4.78597000	0.03116000
H	-2.14539900	-2.35882900	-0.00000300	H	0.48044500	4.01125000	-1.55984800
C	0.44551000	1.30829200	-0.00000900	C	-0.27654200	-1.61163100	-1.42742800
C	1.74538400	0.91243800	-0.00000400	C	1.02154400	-1.73155600	-1.90820900
C	2.27860500	-0.43891400	0.00000500	C	1.87962700	-1.36865700	-0.86414400
C	3.59942600	-0.70506400	0.00001000	O	1.15485700	-1.06692200	0.23703000
H	3.97396000	-1.72467800	0.00001700	C	3.30761100	-1.27763600	-0.86745500
H	4.34323900	0.08993400	0.00000500	C	4.15332600	-0.87615500	0.12426300
H	1.57067700	-1.26251800	0.00000900	C	3.82675100	-0.41665500	1.45843200
H	2.49067200	1.70776600	-0.00000800	C	4.77399500	-0.04742700	2.34454400
H	0.25317600	2.37948700	-0.00001500	H	-0.78617000	-1.50929000	0.74123600
H	-3.97213700	-0.29553100	0.00001400	H	3.75097200	-1.57975500	-1.81322700
H	-2.42901100	1.97048500	0.00002600	H	5.21638400	-0.89663300	-0.11524100
DMAD				H	2.78033200	-0.37267900	1.74294100
C	4.12449300	-0.62065400	-0.38973600	H	4.51552900	0.29566800	3.34200500
O	2.68649100	-0.60522200	-0.52831700	H	5.83319300	-0.07880000	2.09561600
C	2.03450100	0.24779900	0.27928300	H	-1.19874000	-1.79080300	-1.96465500
O	2.55724500	0.98132200	1.09315000	H	1.33428300	-2.00316900	-2.90738700
C	0.60265000	0.18827100	0.06118400	3a-t			
C	-0.60262300	0.18796200	-0.06139300	C	-0.24942900	-0.85945700	-0.48809600
C	-2.03452100	0.24810400	-0.27900900	C	-0.94307200	0.51124000	-0.07728100
O	-2.55739400	0.98317500	-1.09139600	C	-2.16296400	0.51775300	0.41133700
O	-2.68639700	-0.60630100	0.52721300	C	-3.11018200	-0.49770600	0.76989300
C	-4.12444600	-0.62118400	0.38908400	O	-2.95596800	-1.27699500	1.70769100
H	-4.53426600	0.36561500	0.61814800	O	-4.22334200	-0.48332700	-0.01072100
H	-4.46919700	-1.36266300	1.10915600	C	-5.23870800	-1.44079000	0.33519800
H	-4.40165200	-0.90636300	-0.62875000	H	-4.85618100	-2.46213500	0.24840200
H	4.40130000	-0.90766700	0.62768700	H	-6.04614700	-1.27233000	-0.37849400
H	4.53460500	0.36645500	-0.61693900	H	-5.58816200	-1.27481200	1.35816100
H	4.46932700	-1.36094800	-1.11098700	C	-0.14670700	1.74155200	-0.34974000
TS2a				O	0.82947900	1.77698800	-1.08021600
C	-0.20660400	-1.12614100	-0.09098100	O	-0.62411100	2.82204400	0.29630100
C	-1.03290000	0.60460300	-0.07574300	C	0.07970300	4.05290800	0.05699000
C	-2.25091900	0.63750900	0.29091000	H	1.12171800	3.96782700	0.37788200
C	-3.31714100	-0.18446400	0.76912200	H	-0.44626700	4.80101400	0.65095300
O	-3.32871100	-0.71298800	1.87675800	H	0.04920900	4.31172500	-1.00515200
O	-4.33372200	-0.30064600	-0.12597500	C	-0.14217500	-1.07259700	-1.94883100
C	-5.45739500	-1.08536900	0.30957400	C	1.17477100	-1.18652200	-2.28626000
H	-5.15430600	-2.11584100	0.51723400	C	1.93936700	-1.06908600	-1.09452700
H	-6.16619200	-1.05378000	-0.51882000	O	1.12273100	-0.92240500	-0.03314500
H	-5.89963200	-0.65290500	1.21145200	C	3.34757500	-1.08156700	-0.96133400

C	4.11297700	-0.92806400	0.17242000	C	-0.88336700	0.51827100	-0.11172600
C	3.67439300	-0.70333100	1.52633100	C	-2.11766300	0.49704600	0.33855700
C	4.54408500	-0.56720300	2.55377500	C	-3.07110400	-0.53096500	0.64095400
H	-0.79077700	-1.63625500	0.05843700	O	-2.94360000	-1.33092500	1.56498200
H	3.87181100	-1.23525100	-1.90125600	O	-4.15679900	-0.50307400	-0.17628000
H	5.19228000	-0.97833700	0.02948900	C	-5.17838900	-1.47314700	0.11240700
H	2.60759800	-0.64320300	1.71662400	H	-4.78710400	-2.49019200	0.01552600
H	4.19952100	-0.39819600	3.56957400	H	-5.96154600	-1.29206100	-0.62479100
H	5.62057900	-0.62097200	2.40224400	H	-5.56361600	-1.33220300	1.12622400
H	-1.00011500	-1.08622900	-2.60946700	C	-0.09226300	1.76722800	-0.31074600
H	1.59681400	-1.30606900	-3.27592500	O	0.90735800	1.83966200	-1.00523700
TS3a-rot				O	-0.60426800	2.81675800	0.35875000
C	-0.23473800	-0.96979200	-0.26952100	C	0.09376400	4.06322100	0.19255100
C	-0.84606200	0.50334900	-0.11452800	H	1.12467500	3.97539300	0.54666700
C	-2.08943300	0.65688800	0.28009700	H	-0.46107300	4.78207400	0.79622300
C	-3.10599500	-0.26108400	0.70410200	H	0.09740700	4.36316200	-0.85912800
O	-3.04499600	-0.92042800	1.74028000	C	0.05675500	-0.97229300	-2.00340200
O	-4.17268100	-0.30075300	-0.13928500	C	1.39281400	-1.07277800	-2.24562200
C	-5.25293200	-1.15954100	0.26295200	C	2.07244000	-1.00931300	-0.99493200
H	-4.92003400	-2.19969200	0.33018600	O	1.17695700	-0.90754800	0.00574600
H	-6.01067300	-1.04992100	-0.51402700	C	3.46792300	-1.03934800	-0.79595200
H	-5.64915000	-0.84726700	1.23336100	C	4.27604700	-0.96455900	0.32406500
C	0.05678100	1.61505400	-0.51908600	C	4.05317700	-0.81400800	1.74578800
O	1.07495900	1.46822400	-1.17615900	C	2.90700400	-0.69553800	2.45786100
O	-0.37489000	2.81613700	-0.08937700	H	-0.73249600	-1.63267700	-0.07980900
C	0.42714100	3.94333900	-0.47795400	H	4.00264100	-1.14930100	-1.73704100
H	1.43844000	3.85500900	-0.07081500	H	5.33475100	-1.03232400	0.07716300
H	-0.08105800	4.81210400	-0.05815800	H	4.98299400	-0.79690900	2.31456400
H	0.48286100	4.01795500	-1.56767400	H	2.95805400	-0.59099200	3.53833700
C	-0.12982600	-1.41450700	-1.67180600	H	1.92524600	-0.70041300	2.00493000
C	1.18559800	-1.66276700	-1.96057700	H	-0.74988600	-0.95723700	-2.72579000
C	1.93105300	-1.41083000	-0.78495700	H	1.88708600	-1.15099300	-3.20555500
O	1.12139800	-1.05525900	0.22029900	TS4a			
C	3.34705400	-1.50634400	-0.60811700	C	-2.12951700	1.08591800	-1.99845500
C	4.07993200	-1.20377000	0.49549400	C	0.23442200	0.42961600	0.09135900
C	3.60321100	-0.65999400	1.78829700	C	0.66559600	-0.77455600	-0.18066500
C	3.50000800	0.64167000	2.07106900	C	-0.37960100	-2.00477000	-0.18771500
H	-0.83986400	-1.59731900	0.39021200	O	-1.65353300	-1.46267200	-0.53624000
H	3.87236800	-1.88501100	-1.48211000	C	-2.25635200	-1.10973100	0.60831700
H	5.15150500	-1.39957000	0.42927700	C	-1.65920800	-1.82247500	1.69948200
H	3.36916200	-1.39637600	2.56079700	C	-0.54805300	-2.43951800	1.21233200
H	3.17105500	0.97759500	3.05089700	C	-3.41939500	-0.29399000	0.65431700
H	3.72076500	1.40764000	1.33163500	C	-3.85428700	0.70733400	-0.18135900
H	-0.97886300	-1.47231600	-2.34143300	C	-3.23954000	1.40030000	-1.28713100
H	1.61241500	-1.95622100	-2.91098600	H	-0.07209600	-2.74287100	-0.92617700
3a-c				H	-4.01048600	-0.45298800	1.55438100
C	-0.15952200	-0.82620000	-0.54500500	H	-4.79350100	1.15739100	0.13868500

H	-3.73067200	2.34330200	-1.52693400		H	-3.91251400	-2.14589000	0.57618300
H	-1.73675300	1.79328600	-2.72274100		C	-3.63616300	-1.62646700	-0.34471400
H	-1.61955500	0.14000100	-1.90420300		H	-4.39181600	-0.88796900	-0.61263000
C	0.76841300	1.75929300	0.12201000		H	-3.50216800	-2.35495000	-1.14851100
O	0.78019600	2.54149600	-0.82110900		H	0.87050800	-3.38542900	-0.70822400
O	1.20071700	2.10027900	1.37252300		H	2.71751400	-2.13902000	-2.18815000
C	1.69950700	3.43959300	1.50763200	TS6a				
H	1.98313000	3.53625500	2.55703900		C	1.26251600	-1.41220400	-0.86965100
H	2.56729100	3.59787500	0.86056200		C	0.42616700	-1.79988700	-1.93875500
H	0.92491900	4.16839300	1.25050700		C	-0.78276900	-2.18089700	-1.38988000
C	2.04534400	-1.27853400	-0.38426500		C	-0.71764900	-1.85560600	0.00647800
O	2.33219200	-2.46791400	-0.42555500		O	0.63369200	-1.64649900	0.30448600
O	2.95256700	-0.29377400	-0.50957000		C	2.62950800	-0.98354800	-0.92157100
C	4.31527000	-0.71235800	-0.70115300		C	3.48342900	-0.68972600	0.09947900
H	4.65925400	-1.29794600	0.15597400		C	3.22949000	-0.71392600	1.52557000
H	4.40619300	-1.31329400	-1.61007500		C	4.18909900	-0.43325800	2.42999700
H	4.88687500	0.21162200	-0.79181400		H	0.70076700	-1.76317600	-2.98462100
H	0.19686000	-3.00760800	1.75464200		H	-1.67982900	-2.50017400	-1.90332600
H	-2.01417200	-1.78946800	2.72152300		H	-1.24371600	-2.40058000	0.78182800
5a					H	3.00929400	-0.89432200	-1.93651700
C	1.12697800	-1.62374500	0.75350900		H	4.49303600	-0.39811400	-0.19002900
O	2.25195300	-0.73625000	0.77604800		H	2.22815700	-0.96114800	1.86298100
C	2.68104400	-0.60765400	-0.52718900		H	3.98602700	-0.44841000	3.49675900
C	2.34762600	-1.85356000	-1.21047300		H	5.20379900	-0.18057400	2.12752900
C	1.41601600	-2.48269000	-0.47156500		C	-0.70679200	0.78589800	-0.27088400
C	3.08048800	0.59384900	-0.99973600		C	-1.43163200	-0.19335200	0.07916600
C	2.85287500	1.87570100	-0.34718000		C	-2.84924900	-0.34835700	0.47714300
C	1.94360800	2.24507800	0.58950000		C	0.10433800	1.83539000	-0.75029300
C	0.93499800	1.44223900	1.39738600		O	-3.42888200	-1.42106900	0.54056100
C	-0.13906400	0.58658700	0.69798500		O	0.06310000	2.28450600	-1.89298000
C	-0.13841700	-0.75937800	0.55397500		O	0.93867900	2.31890100	0.21680700
H	1.10147900	-2.17963100	1.69561500		O	-3.43283000	0.83086400	0.75273800
H	3.52209500	0.61676800	-1.99340500		C	-4.82275500	0.76845000	1.12576500
H	3.45284600	2.69190600	-0.75035000		C	1.76468700	3.42403900	-0.18269300
H	1.95327600	3.30290300	0.84814500		H	-4.94905600	0.16470500	2.02848700
H	0.36225600	2.15861100	1.99832300		H	-5.11331400	1.80315500	1.30865800
H	1.47505900	0.80531400	2.09994900		H	-5.41564200	0.33725700	0.31471300
C	-1.33375900	1.43580900	0.33499000		H	2.40010200	3.14831700	-1.02903200
O	-2.10092700	1.91246100	1.14660300		H	1.14845700	4.28358800	-0.46279800
O	-1.35493100	1.70746600	-0.98127500		H	2.37152100	3.65775200	0.69325600
C	-2.41230600	2.57837200	-1.42640400	7a-t				
H	-2.35307300	3.54287500	-0.91518700		O	-1.35081500	-1.41062200	-0.32809300
H	-2.25383000	2.69785800	-2.49836500		C	-1.22546300	-0.39336400	0.68131800
H	-3.38525600	2.12133100	-1.22666300		C	0.20224900	0.15619600	0.27355600
C	-1.34569300	-1.57486300	0.24151900		C	0.87635300	-0.92245200	-0.15567200
O	-1.36207200	-2.78874800	0.37777800		C	-0.12284800	-2.09756500	-0.01443500
O	-2.42474400	-0.87247100	-0.14744800		C	-0.31760400	-2.35016300	1.49587300

C	-0.98303500	-1.28353700	1.93868000	H	4.76332000	-1.35676200	-0.83899200
H	0.04305900	-2.95235100	-0.66577500	H	5.03752900	0.03369900	0.26549600
C	0.61202100	1.54988400	0.55653900	H	4.60950500	-1.58192400	0.92419200
O	0.48989500	2.04633400	1.66277200	C	-2.13821300	1.20464200	-0.41317700
C	1.47451100	3.56735500	-0.30694300	C	-3.47679600	1.34471200	-0.35025100
H	1.79220200	3.92725900	-1.28542500	C	-4.52164900	0.38561400	0.02723700
H	0.63603500	4.15814200	0.07088200	C	-4.53855200	-0.93072100	-0.23672900
H	2.29963800	3.60638000	0.40900400	H	-1.57509200	2.06826100	-0.76031800
C	2.28096300	-1.15051600	-0.53009400	H	-3.85565300	2.33583500	-0.60507800
O	2.70084900	-2.24185900	-0.87985600	H	-5.38769600	0.82906300	0.52123700
O	3.05405400	-0.05183400	-0.42536200	H	-5.37960800	-1.54594100	0.07359100
C	4.43788900	-0.22307800	-0.78597400	H	-3.73191800	-1.41882400	-0.77418900
H	4.91076400	-0.96572400	-0.13789600	H	-2.10794000	-0.40009700	2.10358800
H	4.52149800	-0.54476100	-1.82739000	H	-0.97533800	-2.84646300	1.71189000
C	-2.33231400	0.60327200	0.77186500	TS8a			
H	4.89381600	0.75730200	-0.64639500	C	3.03332600	-0.26136300	0.15089600
H	-2.17872600	1.32043400	1.57624100	C	3.21489300	0.71827900	1.07687800
C	-3.44968900	0.72160600	0.02717600	C	2.11771800	1.30399000	1.78217200
C	-3.89750900	-0.09374600	-1.09715300	H	2.16874700	2.36400300	2.02400100
C	-5.04633200	0.15366400	-1.75083300	C	0.90510200	0.59380300	1.93400700
H	-4.12054800	1.53853700	0.29765700	C	1.69581400	-0.79993200	-0.23911000
H	-3.26850600	-0.92388000	-1.40134600	C	1.52100000	-1.30645000	-1.68125100
H	-5.36811300	-0.46084200	-2.58694400	C	0.52501100	-2.19946000	-1.64584700
H	-5.70027100	0.97782800	-1.46993400	H	2.07021500	-0.92191700	-2.53314100
O	1.06715700	2.20083600	-0.52211200	C	0.09720700	-2.25294100	-0.17090200
H	-1.28352400	-1.00958400	2.94214300	H	0.03741000	-2.72211100	-2.46020500
H	0.07841600	-3.19691800	2.04296900	H	-0.38731300	-3.15693600	0.19226600
7a-c							
C	-1.60621900	-0.80521000	1.23476200	C	0.39588600	0.07239200	0.11087900
C	-1.30622300	0.01207000	-0.05509200	C	-0.62160600	-0.92106500	0.09864800
O	-1.33735300	-1.05731600	-1.03961000	C	0.22847700	1.38099200	-0.61510200
C	-0.40302800	-1.91910300	-0.36052900	C	-2.06680700	-0.88178800	0.23678100
C	-1.05188100	-2.00144000	1.03853400	O	-1.05566500	1.68672800	-0.88413300
H	-0.22931400	-2.84324100	-0.90706200	O	-2.52280000	0.14338000	0.99722900
C	0.80118300	-0.95382100	-0.24003500	O	1.15830200	2.08855400	-0.95498700
C	0.25155300	0.25428600	-0.04444200	O	-2.80321400	-1.74272900	-0.23442300
C	0.84896000	1.55477700	0.34375500	C	-1.27146600	2.92739300	-1.58133200
O	0.65128000	2.06301300	1.43139000	H	-0.77551600	2.90813100	-2.55537600
O	1.56652100	2.11877100	-0.64030100	H	-0.88583200	3.766679800	-0.99631000
C	2.18369600	3.38322200	-0.32251200	H	-2.35258700	3.00392400	-1.70024900
H	1.42440600	4.11751900	-0.04105900	C	-3.94942500	0.21360900	1.15263000
H	2.69806300	3.68676600	-1.23423300	H	-4.43413300	0.34185900	0.18041000
H	2.89209300	3.25932000	0.50070600	H	-4.12815900	1.08125600	1.78906000
C	2.18740100	-1.43821100	-0.18326400	H	-4.33066800	-0.69614200	1.62516000
O	2.48390500	-2.61590600	-0.30340500	H	0.04789300	1.11808500	2.35254200
O	3.09052500	-0.45905000	0.03176900	H	0.98367800	-0.44398900	2.24230800
C	4.46620300	-0.87970100	0.09865700	H	4.20724000	1.14991400	1.19624500

H	3.88472700	-0.65340100	-0.39985300	H	0.19009800	-3.11014000	-0.63034900
9a				O	-1.51070700	-1.93587800	-0.33396100
C	-3.00558100	-0.22025500	-0.00475700	C	-0.39802200	0.17911800	-0.49596800
C	-3.20876700	0.55561300	-1.13966700	C	0.56974400	-0.88543400	-0.46952300
C	-2.18165900	0.87394900	-2.01740900	C	-0.04260100	1.50450500	0.10610800
H	-2.38007900	1.50422200	-2.87998600	C	2.01969800	-0.83234900	-0.43048900
C	-0.78773900	0.34940900	-1.83066200	O	0.64133000	1.37154600	1.26696600
C	-1.65657400	-0.73257800	0.34073000	O	2.52493500	0.35543400	-0.85254500
C	-1.32494200	-0.99803900	1.80929800	O	-0.37936800	2.58506400	-0.34384100
C	-0.34050600	-1.90445100	1.82226300	O	2.72816800	-1.78472300	-0.11391600
H	-1.76569300	-0.46500800	2.64361100	C	1.01277900	2.59935000	1.91509800
C	-0.05699400	-2.20287200	0.35091500	H	0.12371600	3.18256800	2.17101900
H	0.23919800	-2.27537200	2.65927300	H	1.65627300	3.19451800	1.26111800
H	0.39480600	-3.15765100	0.08987200	H	1.54991000	2.29992900	2.81595000
O	-1.36031700	-2.04008700	-0.24078900	C	3.95828100	0.45356700	-0.86728700
C	-0.43320900	0.09347800	-0.33477400	H	4.36346200	0.31020600	0.13861800
C	0.63917200	-0.95473600	-0.16633800	H	4.17461500	1.45879500	-1.23085900
C	-0.13713400	1.43808900	0.33799000	H	4.38629800	-0.29854300	-1.53618900
C	2.05791600	-0.86491800	-0.40186500	H	-0.69318200	1.00268200	-2.47593900
O	0.49276500	1.29740300	1.52297400	H	-1.29743000	-0.64403400	-2.27447000
O	2.43302600	0.33878400	-0.91877800	H	-4.35901600	1.10502400	-0.38735500
O	-0.43757100	2.51861700	-0.12570200	H	-3.39442600	-0.00206400	1.58098700
O	2.85271400	-1.77273600	-0.17050000	TS11a			
C	0.80584900	2.52088100	2.21523000	C	2.51332900	1.36125400	0.34300300
H	-0.10847200	3.07612600	2.44120400	C	3.77712900	0.97532400	0.75782800
H	1.46392400	3.14324200	1.60318500	C	4.30522300	0.11589700	-0.24367100
H	1.30804100	2.21165200	3.13235400	C	3.34103800	0.02799800	-1.20963800
C	3.83828900	0.49619500	-1.17699500	O	2.25447200	0.77261700	-0.87235700
H	4.41090800	0.39241700	-0.25090600	H	3.27622500	-0.49359400	-2.15296800
H	3.94589600	1.50121000	-1.58645000	C	1.59679700	2.24668200	0.98300600
H	4.18128900	-0.25271100	-1.89648900	C	0.32024300	2.69233900	0.71808700
H	-0.05359900	1.03626500	-2.26103400	C	-0.67017000	2.36534100	-0.25664500
H	-0.69000900	-0.60438100	-2.36787300	C	-0.72934900	1.31490800	-1.17705800
H	-3.83122600	-0.48010800	0.65151600	H	-1.46531500	1.42093200	-1.97097200
H	-4.20866100	0.93565700	-1.33966600	H	0.17464100	0.79122700	-1.45136400
TS10a				H	-1.57637000	2.96241800	-0.17925900
C	-2.91123300	-0.12040100	0.61312800	H	-0.01631200	3.44869300	1.42571500
C	-3.39475700	0.61117600	-0.48648800	H	2.04448500	2.67020700	1.88063000
C	-2.62965400	0.86846400	-1.60003500	H	5.26864400	-0.37507800	-0.25116900
H	-3.01305100	1.55863200	-2.34750800	H	4.25524000	1.28024100	1.67893900
C	-1.24501600	0.33955800	-1.79960000	C	1.59504500	-3.59231300	-0.21308300
C	-1.68531300	-0.86596700	0.58107100	O	0.47936300	-2.73461800	-0.50080200
C	-0.98686200	-1.32580200	1.80977500	C	0.13615400	-1.87126400	0.49863800
C	-0.02829500	-2.18289400	1.41597000	O	0.71878700	-1.82016500	1.57562500
H	-1.17740800	-0.93519300	2.80228200	C	-0.99309000	-1.08372500	0.15038500
C	-0.12402400	-2.21214900	-0.10184100	C	-1.66706000	-0.09351900	-0.24392300
H	0.76694200	-2.63838400	1.99156200	C	-3.09858800	0.28615200	-0.22938200

O	-3.55453300	1.33880000	-0.63825300	C	-2.79278100	-1.44119200	1.18496600	
O	-3.85632800	-0.69394400	0.29993600	C	-2.29739000	-2.41751900	0.30356600	
C	-5.26933600	-0.42292700	0.36066900	C	-2.91710500	1.09497300	0.94197900	
H	-5.46306200	0.45665100	0.98057500	C	-2.39895000	2.29984900	0.39993200	
H	-5.70890400	-1.31493500	0.80768400	C	-1.44020000	2.56440000	-0.55832200	
H	-5.66960500	-0.25449600	-0.64276100	C	-0.62172800	1.65025400	-1.41959200	
H	1.40079000	-4.19051500	0.68150500	C	0.47715100	0.85456700	-0.65270600	
H	2.50448200	-3.00241500	-0.05934400	C	0.49540800	-0.45075200	-0.50384900	
H	1.69678300	-4.23372700	-1.08971200	H	-1.77681800	-2.12774300	-1.87604000	
12a				H	-3.41665900	1.18650500	1.90433400	
C	3.54519000	1.04905400	-1.24604200	H	-2.75362000	3.18615800	0.92543000	
O	2.79907500	-0.01428000	-0.83058200	H	-1.17141100	3.61448400	-0.64055800	
C	3.31316100	-0.44535500	0.37351500	H	-0.09784400	2.26429100	-2.15950600	
C	4.40367200	0.36421400	0.69399000	H	-1.24134900	0.93174200	-1.94845700	
C	4.54081600	1.31913900	-0.34585600	C	1.56530300	1.74028300	-0.11263200	
C	2.78367800	-1.54340300	1.08628900	O	1.52091800	2.95710100	-0.14893200	
C	1.68287500	-2.41963900	0.91649900	O	2.59717400	1.05245500	0.41089300	
C	0.58963500	-2.47525600	0.07477300	C	3.65882200	1.84109100	0.97717900	
C	0.11563900	-1.51188300	-0.96369500	H	3.27553700	2.47088900	1.78444900	
C	-1.07438200	-0.67103500	-0.43731300	H	4.37820400	1.11767500	1.36159900	
C	-0.95298000	0.58323700	-0.09125700	H	4.11601800	2.47220400	0.21011400	
H	3.24895400	1.49079700	-2.18563200	C	1.22130100	-1.53909500	0.08519000	
H	3.39148400	-1.76534900	1.96131100	O	1.14285200	-1.87681400	1.25935400	
H	1.70333000	-3.23022900	1.64524100	O	1.96241600	-2.21246000	-0.83892800	
H	-0.08254100	-3.31397100	0.24384900	H	2.02488100	-4.08027500	0.09881400	
H	-0.25757300	-2.07059400	-1.83095800	C	2.70057700	-3.33810000	-0.33680700	
H	0.89878900	-0.83469900	-1.28987900	H	3.21839600	-3.75175600	-1.20327900	
C	-2.38943700	-1.39626900	-0.35588300	H	3.41927000	-3.01910100	0.42357300	
O	-2.53348300	-2.56372300	-0.66691800	H	-2.10324600	-3.45948200	0.51740500	
O	-3.38723600	-0.61206500	0.09145700	H	-3.03635100	-1.56364500	2.23172200	
C	-4.67856900	-1.23802500	0.21082800	TS14a				
H	-4.63005800	-2.07764300	0.90920400	C	-3.15995200	-1.51487600	-1.57573400	
H	-5.33899700	-0.45840400	0.59067700	C	-2.61240800	-2.71611000	-1.22144300	
H	-5.01999400	-1.59504500	-0.76450500	C	-1.86228000	-2.47387800	-0.03304800	
C	-1.36300000	1.83982100	0.44506100	O	-2.81002200	-0.55341800	-0.68668300	
O	-1.46695300	2.07183800	1.64281400	C	-1.99665100	-1.13455900	0.26309300	
O	-1.58002800	2.76283200	-0.52789500	H	-3.78727400	-1.19361300	-2.39357200	
H	-1.18668300	4.48928900	0.58217700	C	-1.61316900	-0.25546400	1.34115600	
C	-1.96345800	4.06968400	-0.06348800	C	-0.76495300	-0.47993500	2.42087200	
H	-2.08130400	4.67022800	-0.96602300	C	0.44951400	-1.18885300	2.43703800	
H	-2.90453000	4.01814300	0.49113300	C	1.11377500	-1.64024400	1.30157300	
H	5.27734200	2.10725600	-0.42412900	C	1.36465000	0.17158300	0.20512200	
H	5.01373900	0.26769300	1.58200500	C	0.34186000	0.87583600	0.06748300	
TS13a				C	-0.44892500	1.95822500	-0.46579200	
C	-2.05495800	-1.77301700	-0.89526700	O	-0.84743100	2.01781900	-1.61583500	
O	-2.43068800	-0.47196500	-0.81282600	O	-0.69562900	2.90992200	0.46804700	
C	-2.79151700	-0.22382200	0.48868000	C	-1.43356300	4.05520300	0.00235300	

H	-1.52714300	4.70668100	0.87181400		H	-2.11406400	-2.66417100	-1.06676600
H	-2.41870000	3.75319200	-0.36416700		H	-1.50317400	-2.79548800	0.56487000
H	-0.88902200	4.55995000	-0.80031100		H	1.18138200	-0.32718100	2.13752800
C	2.78473500	0.10378000	-0.15129800		H	3.74208600	0.11958500	3.02709800
O	3.62864300	0.88435600	0.24072700		TS16a			
O	3.04205800	-0.93775300	-0.97318100		C	1.50009600	-0.90782400	1.00361600
C	4.40890600	-1.06119200	-1.41430500		C	0.41540300	-0.05836100	0.12485900
H	4.42292100	-1.94192300	-2.05667100		C	1.51853500	-0.02916500	-1.48311500
H	5.07596700	-1.19340900	-0.55806600		O	2.11943300	-1.24490300	-1.15864400
H	4.70864200	-0.17072100	-1.97286200		C	2.70453800	-0.86433600	0.06973000
H	-2.29213400	0.58984700	1.44309900		C	3.26093500	0.46207100	-0.15040700
H	-0.95693400	0.14141900	3.29414300		C	2.51625600	0.99631600	-1.16366600
H	1.02587900	-1.12337200	3.35832200		H	0.92452800	-0.03857100	-2.39314100
H	2.12646200	-2.01849700	1.41110200		C	1.05128300	-2.31635900	1.29782100
H	0.58921800	-2.01431700	0.43259200		C	0.07717800	-2.93752800	0.63210600
H	-1.31723600	-3.20303200	0.54942900		C	-0.73016000	-2.23424100	-0.43931700
H	-2.73082200	-3.65672300	-1.74184800		C	-0.80136600	-0.75825300	-0.13798300
15a					H	1.68060800	-0.35137900	1.92700100
C	4.21175700	-0.02557700	0.89766900		H	1.61335000	-2.83357000	2.07293500
C	3.41953100	-0.02760200	2.00509000		H	-0.17314000	-3.97309400	0.85426200
C	2.08040700	-0.25946200	1.53988100		H	-1.73457200	-2.65544500	-0.50232200
O	3.45623700	-0.23611800	-0.22328200		H	-0.25501000	-2.40740100	-1.41892000
C	2.15503700	-0.37692500	0.18112600		C	-2.11331400	-0.10812300	0.00670700
H	5.27011300	0.10665200	0.73118400		O	-2.32398700	0.96015600	0.56595500
C	1.14852900	-0.66508700	-0.90660600		O	-3.12021800	-0.84088100	-0.54404200
C	1.09225600	-2.15507800	-1.18182500		C	-4.43823900	-0.28508400	-0.40933600
C	0.01729300	-2.91108800	-0.95262400		H	-4.49673400	0.68660900	-0.90780200
C	-1.27491200	-2.35983000	-0.42207300		H	-4.69597100	-0.16244700	0.64634600
C	-1.28807500	-0.85456100	-0.30976500		H	-5.10427200	-1.00381600	-0.88844300
C	-0.21159200	-0.08354000	-0.55251700		C	0.29639000	1.37606200	0.60679200
C	-0.35600500	1.40248900	-0.49334900		O	0.56513000	1.74537800	1.73193600
O	-1.31329600	1.99242600	-0.02485100		O	-0.05351800	2.21250700	-0.39272500
O	0.69826200	2.03695300	-1.04766700		C	-0.33794700	3.56666500	0.00225700
C	0.64510900	3.47528000	-1.03651800		H	0.54174000	4.02592600	0.46175400
H	1.56663300	3.79999300	-1.52016500		H	-0.60897800	4.08545100	-0.91813200
H	0.59662600	3.84320700	-0.00827100		H	-1.17087600	3.57371500	0.70960600
H	-0.22974600	3.82700000	-1.58960300		H	3.95932600	0.96931300	0.50363200
C	-2.65126100	-0.29385100	0.00661300		H	2.50775000	2.01560300	-1.52699500
O	-3.50162800	-0.09048600	-0.83478000	17a				
O	-2.84572300	-0.19232300	1.33295600		C	1.35882600	-0.96203100	1.03044000
C	-4.11851400	0.35106400	1.73805400		C	0.47943500	-0.04067500	-0.00555000
H	-4.09489200	0.35598800	2.82798100		C	1.50676500	-0.06523500	-1.28698600
H	-4.93585900	-0.27428400	1.36925400		O	2.10715400	-1.35867700	-1.10053500
H	-4.22559400	1.36610400	1.34743500		C	2.62324300	-1.06879300	0.18389300
H	1.51909600	-0.15743400	-1.80738700		C	3.36062300	0.21145200	0.00663200
H	2.00992300	-2.59993100	-1.56083500		C	2.66845700	0.85784600	-0.95232200
H	0.04930200	-3.98104300	-1.15026300		H	1.02404100	0.02368000	-2.25926000

C	0.75802800	-2.31718900	1.30531600		H	-4.56966700	0.94190600	-0.61106100
C	-0.17692200	-2.88683200	0.54109000		H	-4.49465800	0.25638500	1.03226800
C	-0.78802700	-2.15756700	-0.64428900		H	-5.21449600	-0.70650400	-0.30331900
C	-0.81950300	-0.69077000	-0.31389700		C	0.43322400	1.40473200	0.43721400
H	1.51303200	-0.40172100	1.95523200		O	0.58586800	1.69179700	1.60467400
H	1.17772400	-2.85348000	2.15446100		O	0.34473300	2.31302400	-0.55839000
H	-0.54209600	-3.88770000	0.76308100		C	0.23707700	3.68690600	-0.14034400
H	-1.79405700	-2.52507200	-0.84784000		H	1.11891200	3.98350400	0.43438100
H	-0.17700800	-2.34849000	-1.53861800		H	0.16355000	4.26442900	-1.06257800
C	-2.09529500	-0.02106300	-0.06130400		H	-0.66072300	3.81313800	0.46961300
O	-2.23108600	1.08904600	0.44185300		H	4.05011600	0.33112400	0.95154300
O	-3.16747300	-0.76507600	-0.45230500		H	3.03708500	1.62065400	-1.20974300
C	-4.45268900	-0.16482400	-0.22587200	1a-c				
H	-4.54133800	0.77254400	-0.78249600		C	1.94382100	-0.99268800	0.00001300
H	-4.59956000	0.03529200	0.83912800		C	2.76092800	0.17574000	0.00000700
H	-5.17868900	-0.89529700	-0.58510200		C	0.62916400	-0.57184300	-0.00000400
C	0.34982900	1.39000500	0.53435100		O	0.60900800	0.80282200	-0.00000500
O	0.50005500	1.71872700	1.69066100		C	1.90100200	1.23601500	0.00000200
O	0.14039500	2.26033700	-0.47646500		H	2.03589800	2.30724200	-0.00000100
C	-0.11934500	3.62047600	-0.08265500		C	-0.57066600	-1.36498900	-0.00001900
H	0.72860600	4.02630100	0.47583400		C	-1.90569400	-1.09358500	-0.00000700
H	-0.26760700	4.16832700	-1.01400600		C	-2.71441700	0.12399800	0.00002700
H	-1.01996800	3.65411000	0.53517400		C	-2.36484500	1.42526400	-0.00001700
H	4.17225100	0.57797700	0.62324200		H	-0.32020800	-2.42495900	-0.00003900
H	2.79175000	1.86986600	-1.31757500		H	-2.52011700	-1.99308300	-0.00001500
TS18a					H	-3.78375900	-0.09095700	0.00009400
C	1.22627300	-1.13890300	1.12424800		H	-3.13874200	2.18864900	0.00002600
C	0.43506400	-0.01043500	-0.13794200		H	-1.33667700	1.76097200	-0.00007400
C	1.60883200	-0.20880300	-1.25717700		H	3.84133000	0.22489600	0.00001000
O	2.07651800	-1.53500500	-0.95329600		H	2.27445500	-2.02280300	0.00002500
C	2.46606800	-1.22295900	0.36740500	1a-E				
C	3.30179500	-0.00653600	0.24521700		C	1.99741500	1.10954900	-0.00020400
C	2.79201700	0.63893000	-0.82406600		C	3.08473900	0.18388300	0.00032600
H	1.25519300	-0.13021200	-2.28507900		C	0.84273000	0.36730400	-0.00008000
C	0.43039300	-2.40964400	1.23481900		O	1.16633400	-0.96591800	0.00018700
C	-0.47427900	-2.84006000	0.35054800		C	2.52483700	-1.05576700	-0.00024600
C	-0.88859100	-2.02053700	-0.86199400		H	2.93036000	-2.05339700	-0.00035800
C	-0.84264600	-0.57185200	-0.45398300		C	-0.54256600	0.74751200	-0.00013100
H	1.28283700	-0.57648500	2.05766600		C	-1.59710200	-0.09610100	0.00002900
H	0.66608800	-3.01662800	2.10832300		C	-2.97536500	0.34535600	-0.00004600
H	-0.97326100	-3.79458400	0.50706500		C	-4.03678200	-0.47537900	0.00011200
H	-1.89184200	-2.30116200	-1.18373300		H	-0.71651600	1.82014000	-0.00032100
H	-0.19959400	-2.22568800	-1.69179100		H	-1.41744500	-1.16773200	0.00021600
C	-2.08289100	0.12296400	-0.08682100		H	-3.13994400	1.42137000	-0.00024000
O	-2.15233500	1.25041800	0.38789200		H	-5.04994800	-0.09238400	0.00005500
O	-3.19734900	-0.61105000	-0.35456200		H	-3.91850600	-1.55425500	0.00030600
C	-4.44717300	0.02063900	-0.03447300		H	4.13936300	0.40877900	0.00060700

H	2.05453400	2.18667200	-0.00032700	H	2.30159200	2.65221200	-0.50368700
Ia-E-c				H	1.49662500	3.27339900	-1.98370100
C	-0.74587500	0.27150400	-0.04672200	H	1.01741400	3.88509200	-0.36481200
C	-1.75103200	1.21108300	-0.09322100	H	-5.51555700	2.12615700	-0.01398500
C	-2.98830200	0.50261600	0.01176600	H	-5.57423300	0.72030000	-1.13229300
C	-2.65934000	-0.81771700	0.11438800	H	-5.85670900	0.47660400	0.61274600
O	-1.30550400	-0.97716500	0.08201100	TS13a'			
C	0.68701100	0.39247200	-0.10903400	C	3.59513800	-0.19020500	-1.63473800
C	1.56972100	-0.63391000	-0.08979100	O	2.75139800	-0.92016800	-0.85063200
C	3.02591300	-0.50567700	-0.13051500	C	2.80393800	-0.39344300	0.42221900
C	3.75491700	0.56872700	0.22301500	C	3.70968700	0.66873500	0.41956000
H	-1.61379700	2.27971200	-0.19163800	C	4.20514400	0.79394900	-0.90290500
H	-3.98692100	0.91792400	0.01095900	C	2.07852300	-0.95141300	1.49566100
H	-3.23550300	-1.72545600	0.21299400	C	1.19220400	-2.05877100	1.59720400
H	1.04662200	1.41631800	-0.19497300	C	0.29850600	-2.59146500	0.70103200
H	1.17787500	-1.64914800	-0.06241400	C	-0.12456300	-1.98839400	-0.59725400
H	3.55836900	-1.39543700	-0.46815000	C	-1.07231100	-0.78756200	-0.32019900
H	4.83768100	0.56515900	0.13636300	C	-0.62786800	0.38572600	0.05012600
H	3.30162100	1.47365200	0.62144600	H	3.65691600	-0.49658000	-2.66822800
TS14a-E				H	2.36978200	-0.51173700	2.44821900
C	2.65296200	-0.78335200	0.30155100	H	1.16041300	-2.49071100	2.59830400
C	3.35983800	0.03775600	1.15697400	H	-0.29753900	-3.43164000	1.05246100
C	4.61161600	0.30677300	0.53063100	H	-0.68420800	-2.71619000	-1.18926500
C	4.59058000	-0.36330700	-0.66157700	H	0.71961000	-1.62621500	-1.18084300
O	3.41519200	-1.02664600	-0.82062400	C	-2.53948300	-1.09729800	-0.42244500
C	1.34705000	-1.35261500	0.39853500	O	-2.98508200	-2.21595500	-0.59993800
C	0.76046800	-2.16896500	-0.54191000	O	-3.30947100	-0.00089800	-0.28861800
C	-0.58172800	-2.61728600	-0.46593300	C	-4.73158200	-0.21998300	-0.32994300
C	-1.46214800	-2.29802700	0.56006200	H	-5.03535400	-0.89451800	0.47497600
H	2.99988700	0.41344800	2.10479200	H	-5.17612100	0.76618400	-0.19465100
H	5.42152000	0.91394800	0.91137800	H	-5.02310100	-0.64825100	-1.29276400
H	5.30153100	-0.46931700	-1.46761600	C	-0.81609500	1.73199000	0.48908900
H	0.83956200	-1.13480400	1.33262300	O	-1.10209800	2.04964000	1.63673500
H	1.32622500	-2.40981600	-1.43868000	O	-0.58604400	2.62805300	-0.50658500
H	-0.98393400	-3.12110200	-1.34318000	H	-0.01749100	4.26227600	0.66603000
H	-2.46328900	-2.71301800	0.53277600	C	-0.71854500	4.01097200	-0.13516800
H	-1.08066200	-2.07172000	1.55127900	H	-0.48720300	4.57377300	-1.04021900
C	-1.93192900	-0.31006600	0.20785100	H	-1.73811400	4.22202600	0.19960400
C	-0.98918200	0.50976400	0.21795600	H	4.92191600	1.51426200	-1.27314400
C	0.02001100	1.50925400	0.30127600	H	3.96471700	1.27492200	1.27840100
C	-3.39618800	-0.31850800	-0.00582900	TS2a-c			
O	0.50793100	1.91343500	1.35048400	C	-0.15083000	-1.12630600	-0.12645600
O	-4.08650300	-1.29120800	-0.24257600	C	-0.97086300	0.60368900	-0.11685100
O	-3.88720300	0.93530400	0.08268300	C	-2.19811700	0.64203900	0.21571500
O	0.36777100	1.97857800	-0.92370300	C	-3.27907600	-0.18283000	0.65646900
C	1.36438200	3.01681000	-0.93196500	O	-3.30646200	-0.74581100	1.74681600
C	-5.30697700	1.06225700	-0.12891500	O	-4.28691000	-0.26102300	-0.25126600

C	-5.42083400	-1.05124900	0.14653200	C	-3.17137300	-1.12043600	-0.52251300
H	-5.12712800	-2.09023400	0.32277700	O	-2.84716600	-1.91737400	-1.39530500
H	-6.12068400	-0.98680000	-0.68749500	C	-2.46559000	0.07851200	-0.22032000
H	-5.86900500	-0.64550300	1.05780300	C	-1.54728900	0.74886900	0.33076300
C	0.02051700	1.61149500	-0.54923400	C	-1.02803100	2.13033100	0.22064200
O	0.92857000	1.40400700	-1.33285700	O	-0.09831700	2.58679500	0.86191200
O	-0.20996300	2.80658500	0.02749200	O	-1.72215500	2.84120700	-0.68873900
C	0.68250500	3.86661300	-0.36461900	C	-1.29693300	4.20502400	-0.86804700
H	1.71368000	3.61394800	-0.10321700	H	-1.39059000	4.76083800	0.06886900
H	0.34531100	4.74093200	0.19270000	H	-1.96558400	4.61169600	-1.62717700
H	0.61403600	4.04391800	-1.44138200	H	-0.25831900	4.23963900	-1.20809700
C	-0.13894400	-1.59721700	-1.47059300	H	-4.49526000	-3.34502200	0.13539000
C	1.18450300	-1.70137400	-1.87467700	H	-5.44306600	-2.40984000	-1.04996100
C	1.98073100	-1.34164700	-0.77871700	H	-5.90820100	-2.38173600	0.68503500
O	1.18845400	-1.05983700	0.28001000	12a-t			
C	3.40441700	-1.24013300	-0.73368600	C	3.53493000	-1.05662100	-0.07122600
C	4.29446400	-0.82451800	0.21816700	C	4.77845700	-1.42049900	-0.58298400
C	4.18935900	-0.32220900	1.58144500	C	5.49928700	-0.22105400	-0.82246400
C	3.14098000	-0.28440500	2.42952800	C	4.67104600	0.80381500	-0.44932400
H	-0.77407600	-1.52631400	0.66558700	O	3.48209400	0.31995600	0.00597900
H	3.84849900	-1.54890400	-1.67785900	H	4.77189400	1.87882300	-0.44440100
H	5.32684400	-0.85891700	-0.12803700	C	2.43673400	-1.84792000	0.33350700
H	5.13928700	0.05509300	1.96078100	C	1.18712700	-1.45777300	0.85576200
H	3.27388100	0.12204900	3.42867300	C	0.72784100	-0.18435800	1.12556000
H	2.15640300	-0.64863900	2.17041400	C	-0.63318200	0.08157800	1.66387200
H	-1.02661500	-1.77710200	-2.06295700	H	1.34810400	0.67910700	0.91087500
H	1.55718900	-1.95658500	-2.85747500	H	0.51258700	-2.28362500	1.08550900
TSIIa-t				H	2.60928600	-2.91553500	0.22110700
C	3.45647200	-1.19048900	-0.17421400	H	6.50092100	-0.12245600	-1.21829900
C	4.64931700	-1.54174700	-0.78016200	H	5.11292400	-2.43436500	-0.75750000
C	5.51168200	-0.41278500	-0.69086000	C	-3.91227200	-3.07408300	-1.25836700
C	4.79941300	0.55520400	-0.03829000	O	-3.19155000	-1.83081900	-1.16915300
O	3.55750100	0.10389300	0.28165100	C	-3.25214600	-1.20262600	0.02793000
H	5.02067100	1.56864600	0.26163300	O	-3.86970800	-1.63098700	0.99476000
C	2.25597500	-1.94259600	0.00777600	C	-2.54702400	0.05102100	0.02436200
C	1.06528100	-1.59800000	0.60066200	C	-1.56408000	0.71381900	0.58605400
C	0.71891500	-0.35775000	1.20298300	C	-1.26894000	2.14314000	0.25350400
C	-0.54749800	-0.10512000	1.73917200	O	-0.40119100	2.79527300	0.80614300
H	-0.63547300	0.71691500	2.44560700	O	-2.06563000	2.63286000	-0.71496800
H	-1.19488700	-0.95416600	1.94297400	C	-1.84656600	4.00998200	-1.07158200
H	1.43172000	0.45908400	1.17821500	H	-2.00687800	4.65852900	-0.20606600
H	0.29714800	-2.37025600	0.60779100	H	-2.57709900	4.22132500	-1.85280900
H	2.32927400	-2.94976400	-0.39719500	H	-0.82866600	4.14961900	-1.44568500
H	6.52449100	-0.32607800	-1.05953000	H	-4.97464900	-2.91365900	-1.05494600
H	4.86667400	-2.49932100	-1.23426500	H	-3.51359300	-3.80086700	-0.54506400
C	-5.07716400	-2.43185700	-0.01953100	H	-3.76245900	-3.41754300	-2.28218900
O	-4.27957100	-1.26747200	0.25577500	H	-1.10657100	-0.83061300	2.03706500

H	-0.58518800	0.81047400	2.48268300	H	4.85013500	0.10728100	0.00019800
TS12a-rot				H	3.86664600	-2.16905400	0.00015500
C	-4.27488500	-1.71131100	-0.62248500	H	1.42390900	-2.51296300	0.00005500
O	-3.25498300	-0.95418400	-0.12518300	C	-1.45885000	-1.17320700	-0.00017400
C	-3.79633900	0.23001000	0.31442200	C	-2.81237000	-1.01475000	-0.00006500
C	-5.15354800	0.21213600	0.09307200	C	-3.57482100	0.21905200	0.00015600
C	-5.46055900	-1.04553900	-0.51410400	C	-4.92287300	0.25096800	0.00018800
C	-2.94152400	1.23908600	0.89669000	H	-5.46948500	1.18958400	0.00037100
C	-1.60493000	1.20313600	1.08547400	H	-5.51642800	-0.66165700	0.00003300
C	-0.70314100	0.09979900	0.72935600	H	-3.02367600	1.15511200	0.00031600
C	0.02225000	-0.00386800	-0.55103300	H	-3.40327100	-1.93037600	-0.00015200
C	1.51512800	0.47974200	-0.36197900	H	-1.08645700	-2.19580600	-0.00030600
C	2.51867300	-0.35999300	-0.27037200	TS2b			
H	-3.99371700	-2.67967000	-1.00837400	C	-0.10190600	0.33148000	-0.91840500
H	-3.47810200	2.13051800	1.21546100	C	-1.06883300	-0.96007300	0.35851300
H	-1.14903400	2.08297600	1.54583800	C	-2.27002000	-1.19750900	0.07344300
H	-0.46199700	-0.63704700	1.49722200	C	-3.43257500	-1.11775900	-0.74451500
H	0.07100900	-1.03454700	-0.91308000	O	-3.62203200	-1.79275300	-1.74958400
H	-0.42884700	0.63180700	-1.31826000	O	-4.33476100	-0.21213900	-0.26930800
C	1.68954200	1.96385400	-0.29525100	C	-5.56613300	-0.12547700	-1.00740900
O	0.76416700	2.75466800	-0.33431700	H	-5.37894600	0.19161200	-2.03742500
O	2.97993400	2.33379000	-0.19067000	H	-6.16460600	0.61787300	-0.47915800
C	3.22291400	3.75171200	-0.13780000	H	-6.07528900	-1.09335200	-1.01725100
H	2.85307400	4.23627200	-1.04544100	C	-0.09047000	-1.29710700	1.40626700
H	4.30580700	3.85170500	-0.06062600	O	0.82464300	-0.58081000	1.76780100
H	2.73058200	4.19123700	0.73399900	O	-0.33821400	-2.51376600	1.93191300
C	2.77452700	-1.77802100	-0.28615400	C	0.54522900	-2.92196400	2.99371900
O	2.45371000	-2.50687800	-1.21607300	H	1.57707400	-2.96868600	2.63501900
O	3.43152200	-2.20111600	0.81607200	H	0.19365700	-3.91059600	3.28997000
H	2.83398400	-4.20563900	0.83052100	H	0.48368000	-2.22178700	3.83122000
C	3.74804800	-3.60601000	0.85544700	C	-0.11272600	1.63259900	-0.32862200
H	4.27886700	-3.75203200	1.79638600	C	1.24263400	1.97143000	-0.03518500
H	4.38221100	-3.87657700	0.00685200	C	2.03692800	0.90119700	-0.50367800
H	-6.43093900	-1.40568400	-0.82773900	O	1.23698700	-0.01981800	-1.08017200
H	-5.84462900	1.00802600	0.33692000	C	-1.15903500	2.51516800	0.01537800
Ib-t				C	-0.82897200	3.70648000	0.63294800
C	-0.40224000	-0.20690900	-0.00012800	C	0.52213900	4.04133700	0.93651600
C	0.98575100	-0.36880200	-0.00005300	C	1.55725700	3.18718600	0.61729500
C	1.56085400	0.96114800	-0.00003000	C	3.44786200	0.71467600	-0.42219600
C	0.49304700	1.83326600	-0.00009300	C	4.21535000	-0.33924200	-0.83064900
O	-0.67258200	1.13653200	-0.00017400	C	3.79259600	-1.57578500	-1.45224700
C	2.97969900	1.12868100	0.00006400	C	4.66549400	-2.54113200	-1.80851900
C	3.76790000	0.00669100	0.00012700	H	-0.69804600	0.00727200	-1.75994400
C	3.19838000	-1.31199000	0.00010200	H	-2.19392400	2.25627100	-0.18890700
C	1.83897000	-1.50853000	0.00003600	H	-1.61581100	4.40607000	0.90258500
H	0.40083000	2.90867000	-0.00013600	H	0.73310700	4.98381000	1.43424500
H	3.41776900	2.12324000	0.00008200	H	2.58444200	3.44158500	0.86349400

H	3.96417400	1.55294700	0.03916800	C	-0.88571500	-0.90813600	0.32296500
H	5.28777400	-0.24343600	-0.66214100	C	-2.13497400	-1.32929200	0.18549800
H	2.73240800	-1.72142800	-1.63399600	C	-3.10155500	-0.99888400	-0.80820400
H	4.33227900	-3.46434900	-2.27330000	O	-3.21065200	-1.53929600	-1.90958600
H	5.73612200	-2.43253700	-1.64472100	O	-3.97839700	-0.02208800	-0.38681900
3b-t				C	-5.08027400	0.23682600	-1.26857100
C	-0.32891900	0.13311400	-0.58315700	H	-4.73181500	0.60028900	-2.24044800
C	-0.99469700	-0.76989000	0.51115100	H	-5.67819600	1.00115600	-0.76829500
C	-2.20935100	-1.27348300	0.33740300	H	-5.67295700	-0.67014600	-1.42192700
C	-3.06992200	-1.21697900	-0.79681400	C	0.03044100	-1.30979800	1.41611200
O	-3.02695200	-1.97874100	-1.76433300	O	1.08918500	-0.74050800	1.66300400
O	-4.03209600	-0.23873400	-0.68208200	O	-0.40900700	-2.36285600	2.12965400
C	-5.03021900	-0.23334100	-1.71238900	C	0.42267400	-2.76736700	3.22612500
H	-4.58340800	-0.04718300	-2.69415300	H	1.41018500	-3.07676200	2.87065600
H	-5.71566600	0.57388600	-1.44696800	H	-0.09914900	-3.60840100	3.68467500
H	-5.56077300	-1.18998500	-1.74076500	H	0.54052300	-1.95026800	3.94396900
C	-0.18622500	-0.91968600	1.74535500	C	-0.13164100	1.54333900	-0.02771400
O	0.85522300	-0.30591300	1.95527000	C	1.23099300	1.90234000	-0.09778400
O	-0.69931400	-1.79743500	2.62681300	C	1.90350500	0.81896900	-0.74156700
C	0.04067000	-1.96434800	3.84488800	O	1.05296900	-0.11626700	-1.10601800
H	1.04907200	-2.33468200	3.63735800	C	-1.06284200	2.38856100	0.57479600
H	-0.52467400	-2.09593400	4.42371800	C	-0.60329100	3.59949700	1.09012100
H	0.11157500	-1.01671200	4.38691800	C	0.76225100	3.96141200	1.02724500
C	-0.13496200	1.56628400	-0.22844200	C	1.69430100	3.11843400	0.44196200
C	1.24040000	1.87012200	-0.27961800	C	3.30792000	0.69188300	-1.00710700
C	1.91419500	0.66603800	-0.66455900	C	3.95338000	-0.38401100	-1.52215800
O	1.04339900	-0.30077500	-0.89955300	C	3.38155400	-1.69456200	-1.90521900
C	-1.06648700	2.53509400	0.14221300	C	3.27827200	-2.74158800	-1.08256700
C	-0.59391600	3.81080500	0.44799400	H	-0.91859100	0.17922200	-1.53625700
C	0.78424100	4.11833800	0.40246700	H	-2.10865700	2.10236900	0.64433000
C	1.71579500	3.15408700	0.04611200	H	-1.30812700	4.28156700	1.55815800
C	3.31462000	0.45489100	-0.79157600	H	1.08176700	4.90918500	1.45090200
C	3.97397100	-0.70812800	-1.09471900	H	2.74580800	3.38886200	0.40921600
C	3.42531700	-2.01770000	-1.35235200	H	3.89349700	1.57380600	-0.76118200
C	4.21980500	-3.07220100	-1.63765300	H	5.02679300	-0.26663000	-1.68247000
H	-0.88744600	-0.02664700	-1.50681100	H	3.06755200	-1.79077700	-2.94695000
H	-2.12491000	2.29643700	0.19798700	H	2.87007100	-3.68632800	-1.43056100
H	-1.29896700	4.58690200	0.73364100	H	3.57138500	-2.68176600	-0.03745000
H	1.11512100	5.12114200	0.65710000	3b-c			
H	2.77663900	3.38688800	0.02639500	C	-0.27912100	0.17631900	-0.55883100
H	3.91681100	1.34141500	-0.61480200	C	-1.05691900	-0.58229100	0.56813500
H	5.06089100	-0.63978200	-1.14010200	C	-2.32734000	-0.93295200	0.41505200
H	2.34926900	-2.14717300	-1.31165300	C	-3.17621200	-0.82042000	-0.72389100
H	3.80558900	-4.05751300	-1.82914700	O	-3.22996400	-1.62663200	-1.65441400
H	5.30291300	-2.97637400	-1.68546600	O	-4.00655800	0.27452900	-0.65866400
TS3b-rot				C	-4.99556700	0.36079500	-1.69429100
C	-0.30547800	0.19616500	-0.63363900	H	-4.52811100	0.43637900	-2.68108400

H	-5.56735300	1.26416200	-1.47343800	H	1.43948700	0.07301200	-2.24891500
H	-5.64876900	-0.51703700	-1.67831400	H	3.65111300	0.31000700	-0.16572300
C	-0.26509800	-0.79633200	1.80466000	H	4.55787900	-1.01744900	1.73962400
O	0.85962700	-0.33818900	1.97826500	H	3.25581700	-2.87740900	2.72012400
O	-0.89275000	-1.54556700	2.72907700	H	1.02740300	-3.48545100	1.80352900
C	-0.16958100	-1.76859700	3.94857700	H	-0.89331700	-3.81137700	0.32143400
H	0.76815400	-2.29654000	3.75121500	H	-3.08679700	-3.74879400	-0.36456000
H	-0.83111800	-2.37938400	4.56430500	H	-4.31367200	-1.86969400	-1.00028200
H	0.05123800	-0.81944900	4.44569600	H	-3.46989800	0.16730300	-1.96403300
C	0.18278100	1.55706800	-0.24575300	H	-1.79846100	-0.58503600	-2.21106100
C	1.58678500	1.60619500	-0.34770700	C	-1.94906200	1.26619100	0.76821000
C	2.02257000	0.29077000	-0.72391400	O	-2.97967200	1.75486100	0.32698800
O	0.98345400	-0.50583400	-0.90173100	O	-1.61127900	1.30805100	2.08575700
C	-0.54676000	2.68585600	0.12373000	C	-2.50638200	2.05017700	2.92942300
C	0.15655600	3.86228100	0.38044100	H	-2.09787600	1.95445700	3.93672400
C	1.56440200	3.91486500	0.28490100	H	-2.53456600	3.10031900	2.62522100
C	2.29457100	2.79039900	-0.07339400	H	-3.51689600	1.63354400	2.88186200
C	3.36170700	-0.14156500	-0.89835000	C	0.69688700	2.22394900	-0.60485700
C	3.91274000	-1.35457900	-1.24358100	O	0.19580700	3.20543000	-0.09517200
C	3.40620300	-2.68115500	-1.53530800	O	1.90111200	2.26970600	-1.25310200
C	2.15210500	-3.18241400	-1.46165200	C	2.53180600	3.56226300	-1.29729400
H	-0.88341100	0.10590900	-1.46449800	H	1.89021600	4.28074900	-1.81430100
H	-1.62832500	2.64363000	0.21674600	H	2.73180500	3.92379400	-0.28493900
H	-0.38777200	4.75866900	0.66540600	H	3.46285900	3.41336500	-1.84614200
H	2.07923400	4.84656500	0.50120800	Sb			
H	3.37847200	2.82927800	-0.13235100	C	0.83375800	0.01415700	-1.29089600
H	4.07852400	0.65939300	-0.73790700	O	0.92295400	-1.41832400	-1.37503500
H	4.99888500	-1.30837900	-1.31678000	C	1.54327600	-1.85536400	-0.21650000
H	4.19215800	-3.36980900	-1.84368800	C	2.49902800	-0.81373400	0.16452500
H	1.98038500	-4.22573300	-1.71244300	C	2.08934600	0.36082800	-0.49173600
H	1.29439300	-2.59956100	-1.15728200	C	2.79981200	1.54560800	-0.33389100
TS4b				C	3.92782500	1.54370800	0.49849400
C	-2.78943300	-0.66128600	-1.79453600	C	4.32117100	0.37896000	1.17036500
C	-0.99183700	0.49674600	0.00116400	C	3.60678300	-0.81236600	1.01341400
C	0.11836700	0.85604300	-0.62055400	C	1.09201000	-2.94165800	0.44110000
C	0.97191800	-0.26391000	-1.32635400	C	-0.17213300	-3.62804700	0.21282600
O	0.05554100	-1.32910100	-1.64295400	C	-1.32144900	-3.19498400	-0.35760500
C	-0.10108300	-2.06052000	-0.51981000	C	-1.66521500	-1.90458000	-1.08453200
C	1.12213500	-1.95788900	0.25942100	C	-1.48504600	-0.54845600	-0.38572800
C	1.85888500	-0.89144500	-0.28929400	C	-0.48060600	0.33948900	-0.55156300
C	3.09167300	-0.52620600	0.24184800	H	0.83618200	0.41554600	-2.30864000
C	3.58709200	-1.26743700	1.31976000	H	2.49493600	2.45232300	-0.84578700
C	2.84848900	-2.32652000	1.87690700	H	4.50455600	2.45656100	0.62216600
C	1.60117900	-2.67543600	1.36210300	H	5.19799600	0.39877100	1.81226200
C	-1.15768800	-2.97624700	-0.32506000	H	3.92141200	-1.71812900	1.52482200
C	-2.48759400	-2.90067800	-0.69346100	H	1.68572000	-3.28684500	1.28486500
C	-3.24488100	-1.80328000	-1.20439900	H	-0.22826800	-4.61599100	0.66960300

H	-2.15140000	-3.89787600	-0.31488500	H	-5.04262600	-1.57652300	-1.45878600
H	-2.73231700	-1.96010500	-1.33567300	C	2.44740100	1.05205000	-0.79445100
H	-1.12472700	-1.87585500	-2.03276700	C	3.42035900	0.20935900	-1.24603500
C	-2.67227900	-0.21954700	0.48524400	C	3.27362400	-1.03316500	-1.97463300
O	-2.89387700	-0.77656600	1.53846000	C	4.33506900	-1.73904500	-2.41228900
O	-3.50654800	0.66237300	-0.10155200	H	2.77018000	1.93751100	-0.25189400
C	-4.65758900	1.04495100	0.67799200	H	4.44683100	0.50841900	-1.03557700
H	-4.33262900	1.54074400	1.59631700	H	2.27043700	-1.40220900	-2.16101300
H	-5.21872200	1.73197200	0.04394100	H	4.21244200	-2.67498200	-2.94926300
H	-5.25939900	0.16711300	0.92744100	H	5.35579400	-1.40348800	-2.23829500
C	-0.62667700	1.71884400	0.00273100	7b-t			
O	-1.18005200	2.02514600	1.03920300	O	1.02145600	0.31322100	-1.36631500
O	-0.07165500	2.62917800	-0.83621800	C	1.12835700	-0.07170600	0.02405400
H	0.33904300	4.14530100	0.54154300	C	-0.28093900	-0.74429900	0.19342100
C	-0.16655900	4.00440000	-0.41751100	C	-1.11061400	-0.04773900	-0.60276700
H	0.32301000	4.58023300	-1.20367400	C	-0.22714200	1.03492300	-1.25974800
H	-1.21470200	4.29852300	-0.32066600	C	0.13021600	2.03703400	-0.15813100
TS6b				C	0.98975200	1.32254800	0.68932000
C	-0.02144700	-1.04020000	0.98046200	C	1.51557400	1.89372100	1.83254300
C	1.02647400	0.95051800	-0.90664900	C	1.16746000	3.22986000	2.11479700
C	-1.02419300	-1.16917300	0.24317300	C	0.31446000	3.94289500	1.27179600
C	-0.92321600	0.02328500	-1.43391900	C	-0.22456500	3.34550000	0.11434500
O	0.43955300	-0.02847800	-1.63505700	H	-0.54837300	1.41694400	-2.22568200
C	0.02068600	1.85617200	-0.47282100	H	-0.88984900	3.90511900	-0.53881800
C	-1.22795000	1.30359500	-0.88288300	H	0.06259600	4.97339800	1.50852700
C	-2.43463700	1.97929000	-0.61046600	H	1.57161700	3.71064800	3.00180200
C	-2.36633500	3.19616400	0.04379300	H	2.17813300	1.34228900	2.49374400
C	-1.12225600	3.74641500	0.45986100	C	-0.55150800	-1.80267900	1.19549300
C	0.06822800	3.08911900	0.21763000	O	-0.20232700	-1.70087200	2.35823400
H	-1.49406800	-0.54338400	-2.15455800	C	-1.51563900	-3.91642800	1.59950900
H	-3.38746500	1.55152800	-0.90659200	H	-1.97930300	-4.69209500	0.99049000
H	-3.28022800	3.74677300	0.25084700	H	-0.62220700	-4.29633900	2.10177600
H	-1.11466100	4.70126100	0.97841200	H	-2.22095700	-3.53319000	2.34116200
H	1.01335600	3.51252900	0.54597300	C	-2.57988300	-0.14153300	-0.70703300
C	1.16807500	-0.95941700	1.75003700	O	-3.30177000	-0.83249100	-0.01500600
O	2.18186400	-1.60868700	1.52551600	O	-3.04127300	0.67609600	-1.68602200
O	1.05055300	-0.07754800	2.78245100	C	-4.46913100	0.68297600	-1.87317500
C	2.19417800	0.00773600	3.64877100	H	-4.81938600	-0.31505500	-2.14943400
H	2.40006200	-0.96258400	4.10984400	H	-4.97000000	1.00103000	-0.95496700
H	1.92249100	0.74218700	4.40824500	C	2.31358300	-0.89650700	0.39752400
H	3.07795500	0.33533100	3.09384900	H	-4.65055500	1.39326700	-2.68012400
C	-2.29320000	-1.91604100	0.22989200	H	2.28324200	-1.21520100	1.43768500
O	-2.52876600	-2.87075200	0.94098200	C	3.37375500	-1.27102000	-0.34555900
O	-3.18919500	-1.41942000	-0.66143600	C	3.66564800	-0.98332400	-1.74595300
C	-4.45932400	-2.09790300	-0.69900200	C	4.78048200	-1.42775500	-2.35244200
H	-4.32138900	-3.14798400	-0.96946000	H	4.12650300	-1.87327700	0.16549700
H	-4.95039400	-2.03785100	0.27576800	H	2.94737000	-0.38755900	-2.29939200

H	4.98778200	-1.20518900	-3.39537400	H	2.10510000	3.70992200	-0.07771600
H	5.51997100	-2.02751100	-1.82406000	C	1.62351900	1.97464200	-1.28725100
O	-1.16305600	-2.87046400	0.67151000	C	-0.85569900	1.20994000	-0.63756900
7b-c				C	-1.89343900	0.25533000	-0.04199400
C	-1.40911800	-0.44936900	0.52824800	C	-1.79544900	-0.92833300	-0.79408100
C	-0.89399300	0.64783000	-0.43440800	C	-0.69115600	-0.62785300	-1.80484000
O	-0.80246300	-0.13426700	-1.66521400	H	-0.67562500	-1.18445000	-2.73967100
C	0.01641200	-1.20171700	-1.13818500	O	-0.90956100	0.77771900	-2.03756200
C	-0.83366300	-1.63911600	0.05911900	C	0.61525800	0.63929800	-0.30322500
C	-1.05784500	-2.84659600	0.69574500	C	0.59473200	-0.59487200	-0.97157300
C	-1.89144200	-2.84334800	1.83208800	C	1.15617700	0.72535400	1.11728000
C	-2.45428400	-1.65632300	2.30334600	C	1.44213400	-1.75803100	-0.82712600
C	-2.21121800	-0.43078400	1.65287700	O	0.53869900	-0.17976900	1.90007000
H	-2.64735100	0.49316500	2.02183900	O	2.56350100	-1.51552700	-0.09253000
H	-3.09067500	-1.67623100	3.18426700	O	1.98889800	1.50455000	1.53068400
H	-2.09521800	-3.77761200	2.34899700	O	1.19723600	-2.85067300	-1.32768300
H	-0.61289100	-3.77207400	0.33789800	C	0.93239500	-0.18658300	3.28549400
H	0.25537900	-1.93671500	-1.90330100	H	0.72584500	0.78367000	3.74527500
C	1.18976900	-0.38126700	-0.56124900	H	1.99899300	-0.40966200	3.37272300
C	0.63666000	0.76445300	-0.12738000	H	0.33213800	-0.97000000	3.74849500
C	1.22672900	1.86701800	0.67186000	C	3.44513800	-2.63530100	0.08902900
O	0.80561300	2.17578300	1.77096700	H	2.93658700	-3.44034400	0.62739100
O	2.22157600	2.49279400	0.02915700	H	4.28337300	-2.25134900	0.67187400
C	2.90848500	3.51901400	0.77422000	H	3.78921500	-3.01276600	-0.87804100
H	2.20789400	4.29703500	1.08843400	H	2.65591500	1.63167500	-1.27619100
H	3.65278600	3.91988800	0.08647300	H	1.08717900	1.77743400	-2.20834600
H	3.38951000	3.07976500	1.65179200	H	-0.23711600	4.59349700	-0.10039500
C	2.57166300	-0.85797100	-0.36667600	H	-2.06164200	2.99423400	-0.19335300
O	3.43570000	-0.29397500	0.27697300	C	-2.79691900	0.36827200	1.00067600
O	2.76302700	-2.04258000	-0.99854000	H	-2.87593700	1.27663200	1.59328700
C	4.07787300	-2.61512600	-0.86902200	C	-2.57978400	-2.03267800	-0.50641600
H	4.31035500	-2.79665300	0.18366800	H	-2.48806000	-2.95591800	-1.07227500
H	4.04015700	-3.55222700	-1.42497200	C	-3.61973900	-0.73881500	1.28197200
H	4.82712900	-1.94217000	-1.29429800	H	-4.34928500	-0.67323800	2.08519400
C	-1.63336200	1.94110800	-0.57723100	C	-3.50987500	-1.91945400	0.54364000
C	-2.93847700	2.15100700	-0.84443500	H	-4.15549900	-2.76161800	0.77943500
C	-4.04410200	1.22431000	-1.11472800	9b			
C	-3.99006600	0.03580600	-1.73686900	C	0.03409900	-1.08582400	-0.06048400
H	-1.02590300	2.82941600	-0.42208000	C	1.25080600	-0.47729200	-0.92441800
H	-3.24194500	3.19915900	-0.83969200	C	-0.17611800	-2.58109400	-0.44846400
H	-5.02119400	1.60003400	-0.80670900	O	0.53128200	-0.23430400	-2.18329300
H	-4.89622600	-0.54528200	-1.88922500	C	-0.47082000	0.67110300	-1.65869400
H	-3.05955400	-0.37510800	-2.11375400	C	0.39971700	1.69884600	-0.94659500
TS8b				C	1.49868100	0.96112300	-0.48220400
C	-1.05101700	2.66807600	-0.42546900	C	2.51331500	1.56677500	0.24228200
C	-0.02777300	3.57075100	-0.40931900	C	2.41331100	2.94773400	0.48671000
C	1.32793400	3.17723600	-0.61948100	C	1.31179200	3.67970600	0.03188900

C	0.27712500	3.05538400	-0.68533600	C	-2.94172300	-1.95871600	-0.85013300
H	-0.58080900	3.62609000	-1.03200800	C	-3.20293900	-0.71580400	-1.36529900
H	1.25859300	4.74732500	0.22949800	H	-1.60801100	-3.11985800	0.38277300
H	3.20396200	3.45375600	1.03489300	H	-3.76829700	-2.64618900	-0.68296300
H	3.36464000	0.99927400	0.61046600	H	-4.23082100	-0.44886100	-1.59936800
H	-1.14168800	1.01926900	-2.44160500	H	-1.66444100	0.20937300	-2.49968600
C	2.41743700	-1.37737200	-1.08907100	H	-2.62228600	1.33170200	-1.53459100
C	2.30516600	-2.74721900	-0.89003100	C	0.26621700	0.80135400	-0.86622500
C	1.10367500	-3.35501300	-0.55502900	C	0.91985700	2.01097000	-0.39593900
H	3.36075200	-0.92977600	-1.38798000	O	2.21255900	2.09021300	-0.82961700
H	3.19603400	-3.36340000	-0.99403700	O	0.38262400	2.90383200	0.24650200
H	1.06419200	-4.42900600	-0.39434500	C	2.91915400	3.28386500	-0.45573900
H	-0.68897200	-2.60850500	-1.42144300	H	3.91526200	3.17900000	-0.88805700
H	-0.85674600	-3.04299400	0.27265600	H	2.97786800	3.36732900	0.63304700
C	-1.07404600	-0.19968200	-0.57710900	C	-1.45577300	0.74934300	0.94507200
C	-2.44609600	-0.24991400	-0.13623300	O	-0.79718700	0.51894700	1.93990700
O	-3.22036300	0.68836800	-0.75373400	H	2.41625100	4.16837700	-0.85704100
O	-2.88766600	-1.04391000	0.68878200	O	-2.67729300	1.32581300	0.97995400
C	-4.60814500	0.69105400	-0.38023300	C	-3.13325000	1.73360700	2.28246700
H	-5.06173300	1.49693100	-0.95844700	H	-3.21665100	0.86792900	2.94526900
H	-4.71552300	0.87710300	0.69211400	H	-4.11006900	2.18947800	2.11683600
C	0.26720000	-0.98948600	1.45255200	H	-2.43561500	2.45601300	2.71402600
O	0.80584900	-1.85056700	2.11655400	TS11b			
H	-5.07249900	-0.26830300	-0.62594600	C	1.65841000	-1.26537400	0.09154900
O	-0.17940100	0.17219300	1.96582500	C	2.97483900	-0.87726500	-0.22103300
C	0.00600000	0.34990600	3.38255500	C	3.35782100	0.12063800	0.74907600
H	-0.51329600	-0.43951000	3.93195600	C	2.26325600	0.27662000	1.57881000
H	-0.42354500	1.32624600	3.60756000	O	1.26146500	-0.54267000	1.18872900
H	1.07043900	0.32885500	3.63107000	H	2.06051400	0.89306800	2.44190200
TS10b							
C	-1.02814000	0.35547500	-0.44592700	C	0.83855300	-2.24153700	-0.51905600
C	-0.48787100	-1.55851700	-0.57803200	C	-0.44842400	-2.71092600	-0.32495800
C	-2.15846300	0.33882100	-1.53338800	C	-1.53417700	-2.33293300	0.51619400
O	-0.02979800	-1.27859000	-1.89560000	C	-1.71163200	-1.21872200	1.33730600
C	1.00902700	-0.32269300	-1.60414700	H	-2.52483500	-1.27571000	2.05652600
C	1.76019600	-1.01757200	-0.47739000	H	-0.86110500	-0.62595500	1.63945700
C	0.76969400	-1.75129800	0.19610500	H	-2.41021300	-2.96979100	0.41109800
C	1.06904000	-2.46005400	1.35402500	H	-0.68942500	-3.54979300	-0.97601400
C	2.39414500	-2.44762600	1.80875300	H	1.37735900	-2.74602300	-1.31957300
C	3.38070900	-1.71872800	1.13212700	C	0.49422800	3.73600700	0.17783800
C	3.06853400	-0.97413600	-0.01459400	O	-0.62144200	2.86589600	0.42347900
H	3.82789900	-0.38588100	-0.52122500	C	-0.81353500	1.89051100	-0.51165800
H	4.40193700	-1.72637900	1.50443700	O	-0.10234400	1.75604000	-1.50044000
H	2.65897200	-3.00700300	2.70210800	C	-1.94892700	1.08976100	-0.21582700
H	0.30547200	-3.00737300	1.90011600	C	-2.62836600	0.10927900	0.18372200
H	1.55301000	-0.07189400	-2.51334400	C	-4.03114700	-0.34695200	0.07569900
C	-1.66970000	-2.32120500	-0.35365400	O	-4.48176900	-1.37645500	0.54432300
				O	-4.77412200	0.53732900	-0.61984900

C	-6.16161800	0.18905100	-0.78340200	C	1.15089600	3.99777000	-0.25406900
H	-6.25696600	-0.75888900	-1.31985600	C	1.75842600	2.76961500	-0.16859800
H	-6.59140500	1.00619300	-1.36339200	H	2.83941300	2.68893700	-0.21166300
H	-6.65181700	0.10519400	0.19038200	H	1.75811300	4.89413800	-0.34927200
H	0.38767000	4.23682100	-0.78849800	H	-0.71598700	5.11390500	-0.31172900
H	1.43223100	3.17110700	0.18543400	H	-2.16752500	3.14367000	-0.16075100
H	0.47594300	4.46264200	0.99144400	C	-2.35152700	-0.10338500	0.06351000
C	3.89328800	-1.27147700	-1.22798100	C	-2.78369200	-1.40755600	0.00365500
H	3.62044600	-2.01557800	-1.97105400	C	-1.98411800	-2.61096100	-0.12921900
C	4.65421700	0.71343200	0.70287000	C	-2.48513900	-3.85573300	-0.27648500
H	4.94569300	1.46491300	1.43154300	H	-0.90671900	-2.48999300	-0.10681700
C	5.51703800	0.30741000	-0.28452300	H	-1.82564400	-4.71371200	-0.37247500
C	5.13722500	-0.68290400	-1.24808700	H	-3.55201900	-4.05951300	-0.30981700
H	5.85394400	-0.96858600	-2.01322900	C	2.44524200	-0.55058000	0.04949500
H	6.51134000	0.74154800	-0.34534100	C	3.66187400	-0.00077600	0.50494800
1b-c				C	2.43793700	-1.89739100	-0.37205100
C	0.48817500	0.26348600	-0.00352300	C	4.82795400	-0.76467300	0.51873100
C	-0.90769100	0.38251800	-0.00611900	H	3.68771800	1.01602100	0.88236900
C	-1.44269300	-0.96180100	0.01281000	C	3.60574500	-2.65681100	-0.34969600
C	-0.34813800	-1.80148000	0.02487200	H	1.51318000	-2.33825700	-0.73031000
O	0.79470700	-1.07162600	0.01431900	C	4.80928500	-2.09552000	0.09025600
C	-2.85493700	-1.17388600	0.01537900	H	5.75280300	-0.32132300	0.87937900
C	-3.67751800	-0.07644400	0.00030400	H	3.57733600	-3.69096100	-0.68387000
C	-3.14815200	1.25770800	-0.01737300	H	5.71931700	-2.68932500	0.10426700
C	-1.79456200	1.49509600	-0.02030100	C	-3.53668200	0.85050900	0.14787700
H	-0.22436400	-2.87369900	0.03915500	C	-4.30151100	-1.46608800	0.03220800
H	-3.26181900	-2.18147700	0.02908800	C	-4.72210100	-0.06541900	0.51729100
H	-4.75615700	-0.21003400	0.00179900	H	-3.69885300	1.34635900	-0.82168900
H	-3.84153100	2.09448300	-0.02873900	H	-3.38675800	1.64357100	0.88898300
H	-1.41105700	2.51183500	-0.03384000	H	-4.84541600	-0.07759100	1.60698700
C	1.48700800	1.28437800	-0.00546600	H	-5.66931000	0.27313200	0.08417200
C	2.85329400	1.30294200	0.02150600	H	-4.67736300	-2.26326500	0.68529900
C	3.89578900	0.28315200	0.04420000	H	-4.69097000	-1.68017400	-0.97611700
C	3.83343000	-1.05889000	-0.07467800	1c-c			
H	4.74897000	-1.64384900	-0.04122200	C	-1.10384500	0.27848700	0.04406400
H	2.90607100	-1.59908200	-0.20856600	O	0.03168000	-0.48288800	0.05531700
H	4.89155600	0.71231900	0.16324000	C	1.14541900	0.30430400	0.02463200
H	3.26286100	2.31200500	0.03550700	C	0.73759300	1.63634900	-0.02409200
H	1.02378100	2.26984000	-0.02064000	C	-0.71146800	1.62602800	-0.00437500
1c-t				C	-1.41689000	2.86439200	-0.06769300
C	-1.01681600	0.42464800	0.01474900	C	-0.70497800	4.03705000	-0.14764900
O	0.04532700	-0.44021600	0.04500200	C	0.72510600	4.04186800	-0.18680800
C	1.22726500	0.24184600	0.01927100	C	1.44174800	2.87242600	-0.13127600
C	0.94332100	1.60472200	-0.05198800	H	2.52466400	2.89136600	-0.19011600
C	-0.50017700	1.72785700	-0.05227600	H	1.24748800	4.99099200	-0.27398800
C	-1.09089600	3.02196000	-0.14670900	H	-1.23621800	4.98408200	-0.19569800
C	-0.27427500	4.12364900	-0.23706200	H	-2.49963600	2.89104800	-0.06198100

C	-2.39177700	-0.36428600	0.05189100	C	-1.26124400	1.89343700	0.04274900
C	-2.73996700	-1.68224200	-0.09886500	C	0.15193100	1.71777500	0.07756100
C	-1.96528400	-2.91475300	-0.24693700	C	1.01618500	2.77137700	-0.27197300
C	-0.85083600	-3.30206600	0.39586200	C	0.46017300	3.98751600	-0.62863100
H	-2.43543900	-3.64428300	-0.91166400	C	-0.94692400	4.16951000	-0.66678300
H	-0.42883700	-4.28827000	0.21856200	C	-1.80983600	3.13892200	-0.34933300
H	-0.34254900	-2.67011800	1.11524400	H	2.09160300	2.62188600	-0.28525900
C	2.43248000	-0.37348800	0.02167000	H	1.10893600	4.81582100	-0.90093300
C	3.60845300	0.28609500	0.43511000	H	-1.34917200	5.13247600	-0.96935300
C	2.53316900	-1.71614700	-0.40095800	H	-2.88060300	3.28683200	-0.41823900
C	4.83993200	-0.36760400	0.40635900	C	-3.19504100	0.20877800	0.48342600
H	3.55590800	1.30216800	0.81127300	C	-3.68092200	-1.07680100	0.60793700
C	3.76625700	-2.36381400	-0.42354600	C	-2.93016700	-2.31677800	0.62710400
H	1.63736800	-2.24096800	-0.71743500	C	-3.49025300	-3.54428300	0.67359600
C	4.92868800	-1.69434400	-0.02510100	H	-2.87113900	-4.43675300	0.67318700
H	5.73217700	0.15953500	0.73510600	H	-4.56492500	-3.70018500	0.71263500
H	3.82116400	-3.39681000	-0.75847100	C	1.39763300	-0.07388900	1.49466600
H	5.88921600	-2.20238800	-0.04393200	C	1.64518400	-1.43534200	1.73259500
C	-3.64289600	0.50955700	0.11823300	C	2.03077900	0.87991800	2.30464300
C	-4.25473400	-1.81970300	-0.20590800	C	2.50111800	-1.83197500	2.75803000
C	-4.78943200	-0.49202600	0.35552000	H	1.18097300	-2.18466200	1.09958000
H	-3.77744700	1.05486800	-0.82853500	C	2.89995500	0.48117600	3.32438800
H	-3.58616900	1.26156800	0.91324100	H	1.83862300	1.93691000	2.15107300
H	-4.96681000	-0.59631300	1.43287900	C	3.13563800	-0.87492800	3.55596600
H	-5.73186300	-0.17577300	-0.10429100	H	2.68967000	-2.88975700	2.91921600
H	-4.63343000	-2.69431100	0.33789200	H	3.38483400	1.23458800	3.94025200
H	-4.54345600	-1.95978100	-1.26141400	H	3.81238800	-1.18545500	4.34793900
TS2c				H	-1.84924100	-2.24286000	0.59398900
C	0.43307100	0.34043100	0.42542400	C	-4.34022600	1.21062200	0.40324200
C	1.10684400	-0.49061200	-1.19689800	C	-5.19876100	-1.06036600	0.63774700
C	2.34169600	-0.72849400	-1.31607100	C	-5.55399900	0.41173800	0.92103900
C	3.72539800	-0.84669600	-1.04154500	H	-4.15838300	2.11275100	0.99722500
O	4.27311400	-1.83707200	-0.567774300	H	-4.49101800	1.53346900	-0.63786200
O	4.41552200	0.27639400	-1.41705000	H	-5.65465100	0.56233000	2.00259300
C	5.83871100	0.20301900	-1.24411500	H	-6.49502000	0.72267400	0.45611200
H	6.09372600	0.06267800	-0.18946900	H	-5.61044700	-1.74464700	1.38893200
H	6.22205500	1.15800600	-1.60744800	H	-5.59327100	-1.39159500	-0.33600600
H	6.25685400	-0.62405900	-1.82574800	5c			
C	-0.03367900	-0.65370100	-2.12816500	C	1.01063600	-1.38819100	0.94288000
O	-0.82714400	0.21995300	-2.42598800	C	1.92758200	-1.49842500	1.97916600
O	-0.09322600	-1.90951800	-2.61718000	C	1.66569600	-2.42019800	3.00372000
C	-1.13918200	-2.15747100	-3.57542200	C	0.50067800	-3.19671300	2.98466400
H	-1.03101700	-1.49430800	-4.43795400	C	-0.42663300	-3.07884100	1.94266700
H	-1.01241700	-3.19919100	-3.87161600	C	-0.15945200	-2.17165600	0.91364800
H	-2.12030500	-2.00247600	-3.11803300	C	-0.88615900	-1.77839400	-0.29554300
O	-0.84440900	-0.23315300	0.65936200	O	0.04340200	-1.17199000	-1.12898700
C	-1.83556600	0.64090100	0.39281800	C	0.99146300	-0.47245200	-0.29147400

C	0.32125900	0.89221000	0.04716800	TS6c				
C	-0.58845500	1.48434700	-0.75561900	C	-0.44982300	-0.99262800	1.28809800	
C	-1.02662900	1.01884900	-2.14921700	C	-1.08025700	0.10389300	-0.94752400	
C	-2.34264300	0.26082900	-2.25758400	C	0.77564600	-0.74859900	1.15931600	
C	-2.78381200	-0.87789000	-1.67406300	C	1.12196500	0.24343200	-0.59783200	
C	-2.19486200	-1.71976400	-0.61556600	O	-0.08169800	0.93734800	-0.57022200	
H	-3.05717400	0.74530200	-2.92117400	C	-0.48969600	-0.99612000	-1.66046000	
H	-1.13993600	1.92572500	-2.75440600	C	0.91825300	-0.87458700	-1.49226000	
H	-0.22073700	0.43688200	-2.59782100	C	1.78912300	-1.83540500	-2.03538300	
H	2.82658700	-0.88926000	1.99522400	H	2.85802800	-1.78136800	-1.86043200	
H	2.37760000	-2.53599000	3.81680500	C	1.24707100	-2.87011600	-2.78239300	
H	0.31805800	-3.91036300	3.78412500	H	1.90420300	-3.61327500	-3.22635100	
H	-1.31732600	-3.69929100	1.92802700	C	-0.15069800	-2.98433800	-2.96662700	
C	-1.27340500	2.75949700	-0.34974700	H	-0.54453600	-3.81069100	-3.55208000	
O	-2.44352400	2.99589100	-0.57582200	C	-1.02501900	-2.07055600	-2.40192800	
O	-0.43577800	3.65116500	0.22577800	H	-2.09354000	-2.19007200	-2.53211100	
C	-1.03270100	4.89292400	0.64443200	C	2.03380100	-0.97574000	1.88897100	
H	-1.80505800	4.70808500	1.39611700	O	2.20567400	-0.70755700	3.06111300	
H	-0.21384300	5.47843900	1.06339400	O	2.98094100	-1.52863300	1.09997100	
H	-1.47816000	5.40683300	-0.21140800	C	4.24712900	-1.78582000	1.73676900	
C	0.70038400	1.46106500	1.38625700	H	4.68383900	-0.85220400	2.10096000	
O	1.83717800	1.74751800	1.70802100	H	4.11818200	-2.47821300	2.57279000	
O	-0.35439700	1.53962900	2.22102800	H	4.87385300	-2.22935000	0.96246700	
C	-0.07230100	2.04126400	3.54165700	C	-1.67822800	-1.50857800	1.80345800	
H	-1.03045100	2.03356900	4.06187700	O	-2.32391700	-0.59380000	2.57407300	
H	0.33219600	3.05557400	3.48467500	O	-2.11863200	-2.62698500	1.57295300	
H	0.64740200	1.39192400	4.04674600	C	-3.54973500	-1.04511600	3.17357200	
C	-3.29970000	-2.49757300	0.08576400	H	-3.92329900	-0.19022100	3.73859000	
C	-4.20353600	-1.39212800	-1.88513600	H	-4.26948200	-1.34625400	2.40689100	
C	-4.60699800	-1.90352400	-0.48804200	H	-3.36075600	-1.89238200	3.83886800	
H	-3.24586300	-2.41356800	1.17856700	C	-2.44822900	0.55732700	-0.88205300	
H	-3.22648600	-3.56855200	-0.15453100	C	-2.92803200	1.79818800	-0.54552600	
H	-4.93262800	-1.05702000	0.12921800	C	-2.17098300	2.98877000	-0.19802600	
H	-5.42483900	-2.63181200	-0.51450500	C	-2.72132400	4.19351800	0.05417300	
H	-4.88009800	-0.62712400	-2.27925900	H	-3.79327700	4.36916800	0.02462700	
H	-4.19670300	-2.23013500	-2.59954100	C	2.30460000	1.12775700	-0.45743800	
C	2.31576700	-0.37714900	-1.04252800	C	3.34759200	1.11377600	-1.39663600	
C	3.03631600	0.81645100	-1.15769800	C	2.37302200	2.02882100	0.61937700	
C	2.82872900	-1.54281300	-1.63404900	C	4.44032500	1.97194200	-1.25461600	
C	4.25043300	0.84452700	-1.85280000	H	3.29503500	0.45018800	-2.25349900	
H	2.66539900	1.72339000	-0.69330000	C	3.46139600	2.89022000	0.75465000	
C	4.03605700	-1.51254800	-2.33082200	H	1.57423000	2.04357400	1.35543700	
H	2.27090200	-2.47126600	-1.55545500	C	4.50217500	2.86193900	-0.17916900	
C	4.75305800	-0.31608900	-2.44218900	H	5.23777200	1.95189400	-1.99322700	
H	4.79979400	1.77936300	-1.93074600	H	3.50008700	3.57773100	1.59557400	
H	4.41666900	-2.42254700	-2.78799300	H	5.35238300	3.53043200	-0.07074700	
H	5.69503300	-0.29154700	-2.98445100	H	-1.09234600	2.89223200	-0.14943400	

H	-2.09785200	5.04856600	0.29964500	C	2.28388300	-1.10815300	-0.70253000
C	-3.58559500	-0.38495100	-1.25434800	C	2.80880700	-2.31866900	-0.23322700
C	-4.44362300	1.81986200	-0.65275900	C	2.84091200	-0.53287800	-1.85350500
C	-4.83742000	0.33072700	-0.70588500	C	3.88815800	-2.92556000	-0.88180900
H	-3.46006400	-1.38839100	-0.83353300	H	2.36782200	-2.80046500	0.63337400
H	-3.64513600	-0.49682500	-2.34796500	C	3.91635700	-1.13723900	-2.50446900
H	-5.04605600	-0.02884700	0.30855200	H	2.42435300	0.38966700	-2.24936000
H	-5.73081100	0.14426300	-1.31070400	C	4.44861700	-2.33458400	-2.01592600
H	-4.91390200	2.34801600	0.18515600	H	4.28430400	-3.86415900	-0.50242100
H	-4.74612500	2.35332500	-1.56771000	H	4.33568600	-0.67604900	-3.39509700
7c-t				H	5.28775200	-2.80619700	-2.52114900
O	-0.12208900	-0.91357800	-0.77867000	C	-3.44301000	0.68710300	-0.98326100
C	-1.11297800	-0.16614100	-0.02809300	C	-4.44970500	-1.52685000	-1.30874800
C	-0.46780400	1.25630200	-0.15515000	C	-4.80137300	-0.03203100	-1.15064000
C	0.86300300	1.05986100	-0.15567200	H	-3.51286700	1.51671700	-0.27137700
C	1.07129700	-0.48167500	-0.06367400	H	-3.08574900	1.11606700	-1.93250000
C	0.64832800	-0.82658600	1.38185300	H	-5.40019000	0.10948000	-0.24288700
C	-0.73960200	-0.61991900	1.40651100	H	-5.38525100	0.35983100	-1.98987900
C	-1.47785500	-0.78268900	2.56287100	H	-4.41231600	-1.83003400	-2.36618000
C	-0.79216600	-1.16609400	3.73185900	H	-5.18338300	-2.18126300	-0.82273000
C	0.59004300	-1.35172500	3.71826500	7c-c			
C	1.33332800	-1.17299300	2.53416600	O	-0.05764800	-0.90104400	-0.88908300
H	2.41204000	-1.30196000	2.53724100	C	-1.12832000	-0.29896100	-0.11173500
H	1.10429700	-1.63576000	4.63285400	C	-0.60999200	1.18157000	-0.13225400
H	-1.34669400	-1.30947000	4.65554400	C	0.73414600	1.10761200	-0.11472600
H	-2.55231800	-0.62169700	2.57413400	C	1.07787700	-0.41334300	-0.12000400
C	-1.17214000	2.55582600	0.03525300	C	0.66213800	-0.88180600	1.29290400
O	-1.65657200	2.89146800	1.09899400	C	-0.73780400	-0.79667500	1.30197000
C	-1.80553900	4.58966500	-0.97704000	C	-1.47043200	-1.05124600	2.44498000
H	-1.77229900	5.00527200	-1.98403100	C	-0.76946900	-1.42222900	3.60791600
H	-2.83534000	4.52592700	-0.61546000	C	0.62329100	-1.50143600	3.60621700
H	-1.20919900	5.19399100	-0.28903500	C	1.36149300	-1.21565800	2.44063900
C	1.87107600	2.11917800	0.06204600	H	2.44730200	-1.25105400	2.45415200
O	1.68929300	3.30807100	-0.13000300	H	1.14875100	-1.77786600	4.51681800
O	3.02523500	1.60906300	0.54223400	H	-1.32061200	-1.63895600	4.51937600
C	4.06399500	2.56292600	0.83126600	H	-2.55359600	-0.96894200	2.44907400
H	4.34263600	3.10611300	-0.07563500	C	-1.44590200	2.38164800	0.14605200
H	3.72593900	3.27349400	1.59025800	O	-2.06959000	2.51789100	1.18171600
C	-2.50955300	-0.41808000	-0.52276100	C	-2.15235200	4.48942600	-0.64024800
H	4.90195100	1.97106300	1.19992500	H	-2.05672700	5.04923800	-1.57045400
C	-3.06492100	-1.64501600	-0.69512700	H	-3.20320700	4.29651700	-0.40753300
C	-2.44755600	-2.93810300	-0.42068500	H	-1.68478900	5.03031200	0.18625300
C	-3.03597200	-4.12743300	-0.64212300	C	1.64359700	2.22525400	0.22252000
H	-1.43755300	-2.92162000	-0.02274900	O	1.35895400	3.40765100	0.16401600
H	-2.51817400	-5.05630400	-0.41971700	O	2.84093200	1.76915700	0.65079000
H	-4.03793000	-4.21815700	-1.05362400	C	3.78919800	2.77332100	1.05570100
O	-1.22878000	3.27308200	-1.09348100	H	4.00928300	3.44572000	0.22228500

H	3.39289600	3.35305000	1.89373800	O	-2.64779200	2.15525500	-0.94841000
C	-2.48346400	-0.62466200	-0.67322600	O	2.43192800	2.30651100	-0.04007200
H	4.68113800	2.22173800	1.35342700	C	-2.17349000	3.41496100	1.33592400
C	-3.09062100	-1.83654800	-0.66290900	H	-3.20215300	3.07016300	1.47218400
C	-2.66648300	-3.13966300	-0.12911200	H	-2.16043700	4.23803100	0.61642800
C	-1.46734200	-3.72306300	-0.26767400	H	-1.73973000	3.72309000	2.28741800
H	-3.46254300	-3.70471300	0.36169000	C	1.28751900	4.28136500	-1.38862200
H	-1.28631300	-4.71539200	0.13860000	H	1.37643700	4.71896400	-0.38982800
H	-0.64851200	-3.23235100	-0.78306500	H	0.61960000	4.87713200	-2.01254700
O	-1.45065900	3.25177000	-0.87126500	H	2.28146400	4.21896800	-1.84069300
C	2.35245000	-0.89206100	-0.76651700	H	-0.98746100	1.00585700	-3.06315000
C	2.96262900	-2.08657500	-0.36423800	H	-0.51323000	-0.66377400	-2.48845300
C	2.88593400	-0.19719400	-1.86104500	C	-1.28253900	-0.57899100	2.73351400
C	4.09934200	-2.56253600	-1.02408100	H	-2.36577600	-0.65011500	2.76048600
H	2.54281500	-2.65634400	0.45844100	C	1.54185300	-0.33680800	2.70437300
C	4.01931900	-0.67007200	-2.52253700	H	2.62275100	-0.23684800	2.69658200
H	2.40603600	0.71601000	-2.20292200	C	-0.56121800	-0.41895800	3.93071800
C	4.63403400	-1.85372200	-2.10190800	H	-1.09580100	-0.38633300	4.87671600
H	4.56120400	-3.49095500	-0.69757500	C	0.82954000	-0.30422400	3.91615600
H	4.41971500	-0.11760300	-3.36885700	H	1.37050800	-0.18764900	4.85182000
H	5.51775300	-2.22337500	-2.61592800	C	2.58083100	-1.04989400	-0.35974700
C	-3.30512000	0.38951700	-1.45845800	C	2.69951200	-2.20714700	-1.14437000
C	-4.42249800	-1.78204100	-1.39813400	C	3.74910700	-0.39900100	0.06584200
C	-4.69336600	-0.27640400	-1.58185000	C	3.95782400	-2.69980900	-1.49983800
H	-3.37858600	1.36530700	-0.97126100	H	1.80416500	-2.72472500	-1.46952900
H	-2.84440600	0.56567700	-2.44334100	C	5.00523200	-0.89685400	-0.28883900
H	-5.33957100	0.08288400	-0.77167600	H	3.67687600	0.51608600	0.64071100
H	-5.19336100	-0.04329400	-2.52764400	C	5.11669900	-2.04810200	-1.07245400
H	-4.32394100	-2.30350300	-2.36290600	H	4.02881400	-3.59722800	-2.10979400
H	-5.22033200	-2.30023300	-0.84953900	H	5.89867500	-0.37540000	0.04591600
TS8c				H	6.09586600	-2.43226300	-1.34785500
C	-2.25184000	-1.49374800	-0.28621900	C	-2.93782200	-2.53710800	0.57026000
C	-2.98006200	-1.22480500	-1.41431300	C	-4.28587400	-2.00022300	-1.41059300
C	-2.59175300	-0.22420400	-2.35123800	C	-4.01065900	-3.12235000	-0.38056400
H	-3.36484000	0.37211800	-2.82994300	H	-2.24083200	-3.29402900	0.95043400
C	-1.23726100	0.14161600	-2.45161000	H	-3.40661900	-2.08038100	1.45435700
C	-0.98970500	-0.78229800	0.07073300	H	-3.59882300	-3.99636100	-0.89934600
C	-0.57603700	-0.63906700	1.54276900	H	-4.91257000	-3.44759700	0.14793900
C	0.82470400	-0.51017100	1.53201800	H	-4.55146600	-2.38867800	-2.40018600
C	1.20795800	-0.55282600	0.04012100	H	-5.11287800	-1.34800100	-1.09021900
O	0.19078600	-1.45777600	-0.44819500	9c			
C	-0.74829300	0.63274300	-0.64634100	C	-2.32218700	-1.42862100	-0.35556700
C	0.64106900	0.79721500	-0.50306100	C	-3.00488900	-1.11008000	-1.53085800
C	-1.68553400	1.78756500	-0.30708200	C	-2.56023500	-0.15292600	-2.42427100
C	1.35697000	2.05417700	-0.57065900	H	-3.13383700	0.08329800	-3.31757600
O	-1.33882800	2.33672000	0.87317900	C	-1.24598700	0.54538600	-2.22320500
O	0.68354100	2.98062000	-1.31909100	C	-1.06258500	-0.74261200	0.02125000

C	-0.68831000	-0.58497000	1.49139600	H	-2.96279700	-2.53624800	1.43217300
C	0.71091300	-0.48880200	1.52718700	H	-4.03424400	-2.77112200	-2.44065500
C	1.15229700	-0.58461800	0.05557100	H	-5.12026300	-1.45511000	-1.99097600
O	0.11528400	-1.45284700	-0.46923800	TS10c			
C	-0.82014500	0.66327300	-0.72543600	C	-0.83405900	0.72286800	-0.78119600
C	0.68255400	0.75225500	-0.55417100	C	-0.98831200	-0.95202400	0.25994700
C	-1.59891200	1.81620400	-0.07701600	C	-1.16887300	0.14738700	-2.20709800
C	1.47573100	1.94495500	-0.77736700	C	-2.45779400	-0.59773400	-2.29742000
O	-0.93111900	2.37207200	0.95410200	C	-2.92309400	-1.38992500	-1.28347200
O	0.81767500	2.84938000	-1.55870900	C	-2.29211900	-1.47032800	-0.01117800
O	-2.70012300	2.18463000	-0.42941800	H	-3.08351600	-0.43160900	-3.17259100
O	2.59478800	2.15758300	-0.32784500	H	-1.16971100	0.99282900	-2.90375600
C	-1.60863200	3.43577700	1.64762800	H	-0.33837600	-0.50645100	-2.48137400
H	-2.54053000	3.06916600	2.08635300	O	0.12037000	-1.44685000	-0.48135100
H	-1.83071700	4.25628700	0.96001400	C	1.16435600	-0.50653600	-0.08420000
H	-0.91650000	3.75703300	2.42615600	C	0.54936100	0.86871200	-0.45979600
C	1.51273200	4.08350900	-1.80189800	C	1.15201600	2.15124500	-0.12959000
H	1.71148600	4.60254600	-0.85985200	O	0.62991500	3.24158900	-0.33855400
H	0.84487400	4.67151100	-2.43259300	O	2.40971600	2.03154400	0.37818400
H	2.46030200	3.89470500	-2.31428100	C	3.08143400	3.26527700	0.67403300
H	-1.26402500	1.54668000	-2.66226800	H	2.52803900	3.83149000	1.42861100
H	-0.45806600	-0.01220400	-2.75018700	H	4.06324800	2.97682100	1.05225200
C	-1.44236800	-0.48602300	2.65160800	H	3.18115000	3.87461100	-0.22896000
H	-2.52773400	-0.53677500	2.62782400	C	-1.77513800	1.79752700	-0.28872300
C	1.38679300	-0.29825900	2.72505300	O	-1.98378600	2.02122400	0.88745300
H	2.46891300	-0.22406300	2.76143100	O	-2.41844300	2.43566400	-1.29010500
C	-0.76517200	-0.31660800	3.87000400	C	-3.29493400	3.50138200	-0.88339000
H	-1.33182700	-0.25759000	4.79587300	H	-4.09391000	3.11654400	-0.24348400
C	0.62989900	-0.22809400	3.90512000	H	-3.70340200	3.90873000	-1.80906900
H	1.13721900	-0.10655200	4.85880400	H	-2.72897500	4.26314600	-0.34095600
C	2.52208900	-1.14321800	-0.27135600	C	0.96065000	-0.50240700	1.43147300
C	2.62369600	-2.29150000	-1.07063000	C	-0.41564200	-0.72116800	1.62045000
C	3.69601000	-0.56477100	0.23417700	C	-0.96773400	-0.65418800	2.89723100
C	3.87231000	-2.84911200	-1.35815400	C	-0.11275000	-0.41666300	3.98142400
H	1.72192600	-2.75086500	-1.45915700	C	1.25950100	-0.21898600	3.78746200
C	4.94194100	-1.12699700	-0.05202800	C	1.80896300	-0.223537800	2.49862800
H	3.64454900	0.34588900	0.81793600	H	2.86595200	-0.04591600	2.33913300
C	5.03670200	-2.27121600	-0.84822600	H	1.90379000	-0.03873500	4.64430800
H	3.93064100	-3.73927800	-1.97979600	H	-0.52420200	-0.37848800	4.98672800
H	5.84073500	-0.66132300	0.34460100	H	-2.03242300	-0.77009500	3.06482700
H	6.00815000	-2.70605400	-1.07021200	C	2.47788900	-0.95704600	-0.67040000
C	-4.22558700	-2.00441700	-1.67568100	C	3.13833000	-2.06416800	-0.11886100
C	-2.95321600	-2.61020800	0.33934300	C	3.02413700	-0.33481500	-1.79906900
C	-4.37585600	-2.64713800	-0.27460700	C	4.32522000	-2.53575300	-0.68236600
H	-4.79532800	-3.65795500	-0.31285400	H	2.71521700	-2.56146800	0.74940100
H	-5.04840400	-2.03386500	0.33811600	C	4.21159600	-0.80497500	-2.36510100
H	-2.39407900	-3.53166300	0.10279500	H	2.52136800	0.52533700	-2.23236100

C	4.86648400	-1.90599400	-1.80722500	H	1.64521100	2.70574600	0.28848600
H	4.82565900	-3.39590400	-0.24465400	H	0.57457500	1.28598900	-0.16344700
H	4.62449400	-0.30950600	-3.24024200	C	-3.20816300	1.67569700	0.02259600
H	5.79179300	-2.27127700	-2.24575800	C	-2.48750000	2.88264300	0.15229000
C	-3.27080400	-2.02295200	1.00381000	C	-4.59291600	1.74681100	-0.23674300
C	-4.28350400	-2.07248700	-1.22650000	C	-3.12924400	4.11065900	0.01289900
C	-4.26155400	-2.82285300	0.12435700	H	-1.42286400	2.84787900	0.35843800
H	-2.79114600	-2.63916300	1.77150400	C	-5.22665800	2.97974300	-0.38254200
H	-3.79470400	-1.20574900	1.52599100	H	-5.18254100	0.83804300	-0.28766800
H	-5.25262800	-2.91020800	0.58113200	C	-4.49995800	4.16811300	-0.26204100
H	-3.87388400	-3.83847700	-0.02198200	H	-2.55515300	5.02811400	0.11384900
H	-4.45397900	-2.74083900	-2.07799300	H	-6.29561000	3.01158500	-0.57722000
H	-5.08378300	-1.31909400	-1.24507800	H	-4.99666900	5.12798800	-0.37512400
TS11c				H	2.38738700	1.63706000	2.29835200
C	-2.53630300	0.39636300	0.17525000	C	0.65000400	-2.48214900	2.23748200
C	2.88618300	0.86414400	-0.61846400	C	2.23250900	-0.88215100	3.15011100
C	2.67938300	-0.25502000	-1.15210700	C	1.52759000	-2.21067000	3.47669000
C	2.14755600	-1.52366800	-1.49612000	H	-0.24448300	-3.06638300	2.47622700
O	2.39535100	-2.57377900	-0.90776800	H	1.21711000	-3.02926900	1.46680300
O	1.35375400	-1.45122500	-2.60085100	H	0.88597000	-2.08790600	4.35840500
C	0.82795100	-2.70191000	-3.07551900	H	2.22652300	-3.02719700	3.68451400
H	1.63997600	-3.40165200	-3.29266000	H	2.41938000	-0.26251700	4.03668100
H	0.28117100	-2.45301700	-3.98603100	H	3.21013200	-1.05998500	2.67731200
H	0.15399100	-3.14392000	-2.33633700	1d			
C	4.00018100	1.82982900	-0.50431200	C	-0.35338000	-2.18916700	2.12264800
O	4.05401200	2.76371700	0.27518100	C	-0.61416500	-2.53532700	0.85395500
O	4.98130600	1.54028100	-1.38290800	C	-1.61030200	-1.77615000	0.04636100
C	6.12820600	2.41018500	-1.34172100	O	-2.69314600	-2.50344800	-0.41476600
H	6.60426800	2.36737300	-0.35835400	C	-3.37671000	-3.33993600	0.52146600
H	6.79911400	2.03008400	-2.11258400	C	-1.52786300	-0.47693400	-0.35056100
H	5.83416600	3.44098800	-1.55729300	C	-0.31189800	0.30695500	-0.18417400
O	-1.35348800	0.40145900	0.84719200	C	-0.06167800	1.65719700	0.06575300
C	-0.85317700	-0.87052800	0.96167000	C	1.37893800	1.81355900	0.11625700
C	-1.75198700	-1.73836700	0.31481200	C	1.92231100	0.54998200	-0.10761900
C	-2.82596800	-0.92030100	-0.19963300	O	0.89107000	-0.32733600	-0.30000200
C	-3.86892500	-1.51636600	-0.96558400	C	-0.90482700	2.78627700	0.28522000
C	-3.84087200	-2.87431100	-1.17734500	C	-0.32853000	4.01274400	0.50655100
C	-2.78448200	-3.68475900	-0.65819800	C	1.09503100	4.17572900	0.51204700
C	-1.74898200	-3.13837300	0.06553200	C	1.93957900	3.10964900	0.32315700
H	-4.65970900	-0.91234500	-1.39710800	H	-0.95830700	4.88249600	0.67486100
H	-4.62651200	-3.34393100	-1.76318200	H	1.50939800	5.16876200	0.66623400
H	-2.79496400	-4.75337300	-0.85626500	H	3.01438600	3.25838500	0.31579100
H	-0.93783900	-3.76399300	0.42032100	H	-1.98473200	2.68042900	0.27977100
C	0.33537900	-1.08937600	1.71442200	H	-4.17291100	-3.82795200	-0.04476000
C	1.30363700	-0.19197300	2.15420600	H	-2.71712900	-4.09905900	0.95639000
C	1.64785700	1.11039200	1.69527900	H	-3.81276700	-2.74011800	1.33087300
C	1.38701300	1.66218000	0.44327500	C	3.26929200	0.01516600	-0.22326100

C	4.36952300	0.66919500	0.36950300	O	-0.26204800	-0.42119200	0.16819800
C	3.51000900	-1.18064200	-0.93345100	C	-1.45089700	0.06878900	-0.19416600
C	5.65964400	0.15615100	0.23960700	C	-1.45425900	1.47903700	0.04603400
H	4.21081800	1.56438700	0.96166100	C	-0.16015100	1.80841900	0.54246500
C	4.80057900	-1.69209400	-1.05235200	C	0.18383600	3.14759700	0.79882700
H	2.67711100	-1.69729100	-1.39963000	C	-0.77214500	4.13146000	0.59927900
C	5.88556700	-1.02584200	-0.47231200	C	-2.06408600	3.80848900	0.11933600
H	6.49082300	0.67652900	0.70930000	C	-2.40766700	2.50057100	-0.17034300
H	4.96148500	-2.61256700	-1.60842300	H	1.18622900	3.41228200	1.12103300
H	6.89179000	-1.42462300	-0.57006400	H	-0.52391000	5.17021900	0.80142200
H	0.37357600	-2.73543200	2.71994300	H	-2.78790000	4.60260000	-0.04158600
H	-0.83991700	-1.33817700	2.59208600	H	-3.39056700	2.28233900	-0.56929600
C	0.04998700	-3.71262300	0.17496100	C	-2.45241700	-0.85528700	-0.65897900
H	-0.68642200	-4.40360000	-0.25316800	C	-2.09617400	-2.07596000	-1.20524200
H	0.67564000	-3.36430400	-0.65665200	C	-0.80644400	-2.42147800	-1.84556600
H	0.68301500	-4.26771600	0.87483700	C	-0.27869800	-1.60513900	-2.77214600
C	-2.69965000	0.18045400	-1.07299100	O	-2.97434200	-3.11568100	-1.32033800
H	-2.35089700	1.10152000	-1.55353400	C	-3.79758300	-3.51789700	-0.21662800
H	-3.02882600	-0.48379100	-1.88180500	H	-3.36741300	-3.17592200	0.72939500
C	-3.91501800	0.49676300	-0.17889600	H	-3.82200600	-4.61063600	-0.24028100
H	-3.60210200	1.12598300	0.66701600	H	-4.81676100	-3.13414900	-0.32212500
H	-4.29054300	-0.43719600	0.25820200	H	0.65620800	-1.85679600	-3.26663500
C	-5.04972300	1.19396600	-0.94151600	H	-0.74319100	-0.66371100	-3.04557500
H	-5.35900300	0.56102900	-1.78604200	C	1.41000600	0.14456900	1.77293600
H	-4.67177800	2.12776800	-1.38351000	C	1.86721300	-1.18349100	1.82990800
C	-6.26774600	1.50253400	-0.06240000	C	1.69458300	0.99968300	2.84865700
H	-7.05937300	1.99941200	-0.63618500	C	2.58847900	-1.63940800	2.93485900
H	-6.69196900	0.58426600	0.36393000	H	1.64925400	-1.86441600	1.01477400
H	-5.99857900	2.16150300	0.77329200	C	2.42733100	0.54405400	3.94637500
TS2d				H	1.33207400	2.02144000	2.84740900
C	0.64398600	0.59917400	0.57318700	C	2.87812000	-0.77749300	3.99521500
C	1.97138900	0.67679700	-0.84910800	H	2.92816300	-2.67183700	2.96005200
C	3.00837900	-0.04799800	-0.79574700	H	2.63635100	1.22407100	4.76854500
C	3.96533100	-1.04530900	-0.52166800	H	3.44478700	-1.13213900	4.85248100
O	3.87544900	-2.22260100	-0.87525700	C	-0.18603700	-3.75171100	-1.48045300
O	5.05375100	-0.55269800	0.14413200	H	-0.82828200	-4.58578600	-1.78671600
C	6.08564700	-1.50781600	0.42235600	H	0.79019700	-3.86473000	-1.96010800
H	5.70475600	-2.32295800	1.04515200	H	-0.03886000	-3.83316600	-0.39568400
H	6.85704800	-0.94946900	0.95553000	C	-3.91588600	-0.44052700	-0.55463900
H	6.48800200	-1.92631600	-0.50540900	H	-4.52594700	-1.17507700	-1.08698700
C	1.49916200	1.56888500	-1.92956900	H	-4.04503200	0.48537200	-1.13020400
O	0.36669400	1.59173900	-2.38141200	C	-4.47704900	-0.22685000	0.86455900
O	2.48608100	2.36987600	-2.38762500	H	-3.86882500	0.51607500	1.39670400
C	2.13433800	3.22246400	-3.49125600	H	-4.38698400	-1.15784600	1.44025200
H	1.31931600	3.89634400	-3.21204500	C	-5.94333700	0.22770200	0.85927600
H	3.04098200	3.78535300	-3.71640400	H	-6.55335100	-0.51344900	0.32180200
H	1.82827900	2.62489300	-4.35463700	H	-6.03165800	1.16376600	0.28820700

C	-6.51401300	0.43455800	2.26735800	H		1.08238400	3.48194300	3.24241500
H	-7.56024200	0.76041400	2.22991500	H		-0.58619300	3.19922200	1.37734800
H	-6.47471200	-0.49365000	2.85167000	C		-2.46895700	-0.86876300	1.38308800
H	-5.94640600	1.19603900	2.81705800	C		-2.45672500	-2.02291100	2.18174200
Sd				C		-3.51942200	0.04340100	1.53082100
C	0.39855300	-3.74166100	-1.97755800	C		-3.47447500	-2.25960500	3.10559400
C	-0.99903300	-3.72771600	-1.90662200	H		-1.64059200	-2.73313900	2.08289400
C	-1.66265100	-2.75521900	-1.14643800	C		-4.54255700	-0.19357300	2.45442500
C	-0.90251800	-1.81781700	-0.45962900	H		-3.54610600	0.94272700	0.92345000
C	0.50352800	-1.83651700	-0.50986400	C		-4.52400200	-1.34467500	3.24359900
C	1.16290000	-2.79983000	-1.28022300	H		-3.44812500	-3.15721900	3.71835900
C	-1.31508900	-0.62929100	0.42136400	H		-5.35172000	0.52540700	2.55470800
O	-0.10125700	-0.46690400	1.21536500	H		-5.31895900	-1.52890300	3.96191800
C	0.96928900	-0.75639700	0.37464400	C		3.24880500	-0.28812900	-0.53810700
C	2.07550800	0.01967700	0.38180100	H		2.85537400	-0.66862400	-1.49002300
C	2.18873200	1.23761300	1.21864600	H		3.75738200	0.65375800	-0.77108700
C	1.27314900	2.19299500	1.51377100	C		4.29458100	-1.28405600	0.00301500
C	-0.22443900	2.17530200	1.21268000	H		3.79754000	-2.21479800	0.31374000
C	1.66993200	3.41505100	2.31461100	H		4.75863500	-0.86804700	0.90505000
C	-1.40586200	0.63827300	-0.47045500	C		5.39141200	-1.60530400	-1.02196900
C	-0.77615500	1.79009300	-0.15582200	H		5.87773200	-0.66959000	-1.33352200
C	-2.11845300	0.56018200	-1.78474000	H		4.93314600	-2.02584000	-1.92975800
O	-1.78752900	1.14110600	-2.80081800	C		6.45019600	-2.57750400	-0.48785200
O	-3.22578500	-0.20964700	-1.70717300	H		6.00023600	-3.53599400	-0.19783200
C	-3.99162200	-0.33084200	-2.92105000	H		7.21929200	-2.78537800	-1.24160500
C	-0.77233800	2.95744900	-1.11570700	H		6.95339800	-2.16724800	0.39713500
O	-1.66280100	3.78235500	-1.17369200	TS6d				
O	0.38460000	3.03443500	-1.78879800	C		-0.27895500	1.35642000	1.36538100
C	0.49189800	4.12017300	-2.73120300	C		0.66684600	-0.34275400	-0.54061500
O	3.50844300	1.45696500	1.64608400	C		-1.46224900	1.12695600	1.00772700
C	3.81538500	0.83234300	2.89250800	C		-1.57018400	-0.18487600	-0.52533000
H	0.90009000	-4.50496900	-2.56692700	O		-0.46621400	-0.94010100	-0.12622500
H	-1.57466200	-4.48030900	-2.43926400	C		0.32285200	0.61337700	-1.55236600
H	-2.74606000	-2.74110200	-1.08703900	C		-1.09867500	0.66940100	-1.59155300
H	2.24532000	-2.84887100	-1.31660200	C		-1.75339500	1.54499900	-2.47670000
H	-0.71055400	1.56009100	1.97381200	H		-2.83373400	1.63897400	-2.46659500
H	2.72984000	3.42263800	2.56908800	C		-0.98509500	2.30095800	-3.34793200
H	1.45076200	4.32782400	1.74275600	H		-1.47340000	2.97128300	-4.05045100
H	-3.38720500	-0.79415600	-3.70559500	C		0.42858300	2.21726900	-3.34065600
H	-4.32805100	0.65367200	-3.25553900	H		1.00092200	2.81338300	-4.04632300
H	-4.84213400	-0.96238500	-2.66237400	C		1.08969100	1.39275900	-2.44728500
H	1.48941900	4.02852500	-3.16118100	H		2.17274700	1.34172000	-2.45332400
H	0.37428500	5.08063100	-2.22242700	C		-2.81046200	1.57595200	1.40092700
H	-0.27484900	4.01594000	-3.50309800	O		-3.23069600	1.58304400	2.54019800
H	4.88573900	0.98058800	3.06022500	O		-3.52598000	2.00566100	0.33645600
H	3.24905200	1.29325400	3.71362500	C		-4.85709700	2.46989100	0.63051200
H	3.59279300	-0.24260000	2.86920600	H		-5.45003000	1.66569500	1.07400800

H	-4.82018000	3.31738600	1.32010100	H	7.01201100	-0.56782800	-1.56821500
H	-5.27546800	2.77306500	-0.32987900	7d			
C	0.89170900	1.73658600	2.06832300	O	-0.01912600	0.91022500	-0.54332400
O	1.32742100	2.97706500	1.70079200	C	-1.37702800	0.68516000	-0.10193700
O	1.47536300	1.04273800	2.89690200	C	-1.19529300	0.87147500	1.42254000
C	2.48926400	3.45700200	2.39476200	C	0.09962100	0.40118600	1.69689100
H	2.65376700	4.46588700	2.01337500	C	0.67097400	-0.04628400	0.31923500
H	2.31349500	3.47819500	3.47398100	C	0.54277900	0.28153600	3.00365100
H	3.35701200	2.82386100	2.18511100	C	-0.31510200	0.69401100	4.04232100
C	1.94396400	-0.83105000	-0.05715600	C	-1.59194400	1.17913900	3.76446300
C	2.08186200	-2.12322700	0.38387400	C	-2.05539100	1.25424500	2.43690100
O	3.12854800	-2.56207300	1.14106900	H	-3.06553600	1.59382600	2.22425100
C	3.60848400	-1.80128000	2.26357200	H	-2.24298900	1.48710300	4.57856900
H	4.52189800	-1.25919400	1.99608500	H	0.02307900	0.62320700	5.07302900
H	3.84645700	-2.53564700	3.03787100	H	1.52078900	-0.12917400	3.23669400
H	2.84544200	-1.10502800	2.62347500	C	2.16083300	0.02970300	0.05891100
C	1.20462400	-3.27055100	0.01943900	C	2.78941200	-0.69451400	-0.89810600
C	0.99066800	-3.56330700	-1.27195100	C	2.22430700	-1.67451900	-1.86567900
H	1.41611700	-2.96297600	-2.07139100	C	1.23766400	-1.33145100	-2.70823600
H	0.37913500	-4.41394800	-1.56379900	O	4.17412500	-0.58363000	-0.97089400
C	0.66497100	-4.11055600	1.15232600	C	4.71670700	-0.18147200	-2.23061000
H	0.07845500	-4.95215100	0.77070500	H	4.43919200	-0.86935700	-3.03837100
H	1.48079700	-4.50506200	1.76869900	H	4.37958800	0.82965800	-2.49288000
H	0.02086700	-3.51003500	1.80751600	H	5.80168700	-0.18473500	-2.10388900
C	-2.84500800	-0.94276600	-0.43968100	H	0.82825600	-2.04964900	-3.41559200
C	-3.18710500	-1.58974100	0.76042900	H	0.79815000	-0.33939100	-2.69517600
C	-3.71113200	-1.05541000	-1.53835000	C	-0.19337000	-1.31485900	0.02037400
C	-4.36766600	-2.32619700	0.85840300	C	-1.43148800	-0.87192600	-0.25372500
H	-2.52750400	-1.50598400	1.61930200	C	-2.66113900	-1.69773500	-0.43733200
C	-4.89742100	-1.78555800	-1.43534900	O	-3.09159100	-2.05097200	-1.51548000
H	-3.44950800	-0.59232500	-2.48418400	O	-3.25412100	-1.96092000	0.74082300
C	-5.23081800	-2.42330900	-0.23757600	C	-4.44408700	-2.77532900	0.67591400
H	-4.61705600	-2.81683500	1.79570300	H	-4.77801400	-2.87517000	1.70879500
H	-5.55453600	-1.86552000	-2.29783600	H	-4.20286600	-3.75151800	0.24818300
H	-6.15284000	-2.99367700	-0.15919300	H	-5.20663100	-2.28443800	0.06567600
C	3.09844600	0.16677300	-0.04940700	C	0.10385000	-2.72174700	0.35623400
H	2.71839700	1.15041900	-0.34074400	O	-0.55609100	-3.67727000	-0.00961600
H	3.47516400	0.30927200	0.96755300	O	1.17132600	-2.82438600	1.17967400
C	4.26889300	-0.23023600	-0.97026200	C	1.46294000	-4.14813400	1.66429900
H	3.90212300	-0.34682300	-2.00063100	H	2.35501200	-4.03829300	2.28150400
H	4.64797800	-1.21714900	-0.67299500	H	1.64888900	-4.83006000	0.83055900
C	5.41643600	0.78892600	-0.94878700	H	0.62560400	-4.52581700	2.25766000
H	5.78229500	0.90225500	0.08241700	C	2.87371400	-3.04259100	-1.89897400
H	5.03374600	1.77694300	-1.24503200	H	3.92923200	-2.98185300	-2.19018500
C	6.58469100	0.39917300	-1.86260000	H	2.85294300	-3.51131000	-0.90860700
H	6.25961300	0.31274300	-2.90741000	H	2.35843400	-3.69898500	-2.60701500
H	7.38794500	1.14468900	-1.82414200	C	2.94641700	1.08970200	0.81788600

H	2.56583600	1.19188400	1.83666800	H	-3.64724900	-4.21014200	-1.44625400
H	3.98962800	0.77166500	0.89859200	H	-4.63311400	-2.72586200	-1.66853000
C	-2.33484600	1.56990800	-0.85761500	H	-0.06479200	-2.20053000	-2.55160800
C	-2.92987500	1.14295100	-2.05358700	H	0.48191300	-0.47625600	-2.28154800
C	-2.56485200	2.88313900	-0.41845400	C	0.60785500	0.04815500	2.93305200
C	-3.75894800	2.00286500	-2.77869900	H	1.52078800	-0.50558400	3.13624500
H	-2.75173400	0.13839400	-2.42253000	C	-1.81655700	1.43016700	2.44052900
C	-3.39029600	3.74283700	-1.14502700	H	-2.75358800	1.94669800	2.25699700
H	-2.08496200	3.23915300	0.48791500	C	-0.17819700	0.52293300	3.99831900
C	-3.99539200	3.30268900	-2.32562400	H	0.14773000	0.35271400	5.02133500
H	-4.21673300	1.65338900	-3.70055500	C	-1.36785900	1.21118400	3.75451100
H	-3.55699100	4.75680500	-0.79013700	H	-1.95912900	1.57808300	4.58971000
H	-4.64115900	3.97032600	-2.89062100	O	4.08063400	-1.34173500	-0.90955700
C	2.89917400	2.48314700	0.15075000	C	4.75782700	-0.89791000	-2.08765400
H	3.30003400	2.40691100	-0.86987400	H	5.79706100	-1.21643200	-1.97959500
H	1.85533100	2.80506600	0.04520900	H	4.33309200	-1.34330800	-2.99576500
C	3.69097300	3.53809200	0.93476500	H	4.71502000	0.19570000	-2.17082500
H	3.28408900	3.61270000	1.95404400	C	2.40006500	-3.32882000	-2.12306200
H	4.73312800	3.20330600	1.04554500	H	3.08458800	-3.24874500	-2.98079400
C	3.66698300	4.92225000	0.27480800	H	2.95003800	-3.81714600	-1.31294400
H	2.64020300	5.29845500	0.18056500	H	1.56809400	-3.96988400	-2.42353200
H	4.23882900	5.65454500	0.85799900	C	3.13896800	0.66360700	0.81562300
H	4.09971700	4.88812300	-0.73354300	H	2.78812000	0.77581400	1.84504900
TS8d				H	4.13185500	0.20615000	0.85633700
C	2.20933900	-0.23995700	0.03679300	C	-2.01052100	2.00345100	-0.82374100
C	2.71224600	-1.12164400	-0.88533600	C	-1.38646000	2.84680700	-1.75552100
C	1.89588000	-1.97088400	-1.72401000	C	-3.36739000	2.20902100	-0.52985800
C	0.59804500	-1.52079000	-2.01971700	C	-2.10223100	3.87078200	-2.38126000
C	0.72214900	-0.09638200	0.24992500	H	-0.33679200	2.70235100	-1.98480000
C	0.18366100	0.30057700	1.63736100	C	-4.07883200	3.23586200	-1.15514200
C	-1.02909200	0.97076400	1.39667100	H	-3.87745900	1.54322500	0.15550300
C	-1.20485000	0.92371200	-0.13344600	C	-3.45153800	4.07159100	-2.08251800
O	0.17868300	0.99662000	-0.54456400	H	-1.60028700	4.51271800	-3.10130900
C	-0.23527000	-1.25221900	-0.28915900	H	-5.13084100	3.37548200	-0.91847300
C	-1.47174600	-0.59071500	-0.40186700	H	-4.00879800	4.86900600	-2.56810200
C	-0.17776500	-2.61507700	0.39329200	C	3.25997300	2.08187200	0.20384600
C	-2.76683800	-1.22864800	-0.47826900	H	3.63303600	2.00031700	-0.82719900
O	-0.93058000	-2.61174700	1.50940300	H	2.26507300	2.53845700	0.13665400
O	-2.67605300	-2.50166900	-0.97683800	C	4.19290900	2.98908500	1.01737800
O	0.48404900	-3.57122100	0.04790300	H	3.81385000	3.06543900	2.04676600
O	-3.84065800	-0.73709200	-0.15112100	H	5.18607700	2.52167100	1.08996500
C	-0.91744000	-3.82765900	2.28086000	C	4.33066000	4.39497900	0.42052600
H	0.09822600	-4.05670400	2.61472200	H	4.99922400	5.02097100	1.02395300
H	-1.29761400	-4.65946900	1.68171800	H	4.73950200	4.35631900	-0.59759000
H	-1.56956600	-3.63168700	3.13212500	H	3.35761700	4.89952700	0.36799200
C	-3.90809300	-3.23653800	-1.02836900	9d			
H	-4.33366800	-3.34799900	-0.02655600	C	2.23194000	-0.30211000	0.07978500

C	2.70969200	-1.27477700	-0.80714100	H	-4.99908000	3.55782300	-0.75256500	
C	1.89360500	-2.06251900	-1.62432600	H	-1.47864000	4.56099100	-3.01619000	
C	0.43367500	-1.71863200	-1.72123200	H	-3.85264500	5.02063300	-2.41245900	
C	0.75234500	-0.14689500	0.26784700	C	2.39171100	-3.24759900	-2.39230800	
C	0.20113300	0.21200700	1.64957400	H	3.44193000	-3.46262800	-2.18300800	
C	-1.00513500	0.89264400	1.42329800	H	1.80080500	-4.13289200	-2.11927600	
C	-1.16410000	0.92057200	-0.10677600	H	2.27124500	-3.10962400	-3.47844800	
O	0.22508600	0.97166800	-0.51196600	C	3.16749100	0.64556400	0.79029300	
C	-0.16683600	-1.31145900	-0.34312500	H	2.84429500	0.79119700	1.82744600	
C	-1.46654700	-0.55013000	-0.46010800	H	4.16349900	0.19259100	0.82731500	
C	-0.25780500	-2.56406800	0.54217300	C	3.27189400	2.04706300	0.13707600	
C	-2.76532900	-1.14859700	-0.69111100	H	3.58862400	1.93869100	-0.91013200	
O	-1.18000900	-2.43932900	1.51527900	H	2.27906100	2.51185400	0.10983300	
O	-2.65626300	-2.40624900	-1.21101500	C	4.25408400	2.96479100	0.87739100	
O	0.42258500	-3.55885600	0.39728100	H	5.24787200	2.49351700	0.90168300	
O	-3.84849000	-0.62871300	-0.45359700	H	3.93653400	3.06221800	1.92590300	
C	-1.30982100	-3.55752600	2.41276900	C	4.36420800	4.35894900	0.24802600	
H	-0.36977400	-3.72759100	2.94436900	H	5.07110300	4.99168300	0.79862100	
H	-1.58039600	-4.45972700	1.85771600	H	4.71112000	4.29916600	-0.79187300	
H	-2.10075600	-3.27618100	3.10807300	H	3.39248100	4.86895100	0.24395200	
C	-3.89687900	-3.09383000	-1.44218500	TS10d				
H	-4.44531600	-3.22005700	-0.50425100	C	0.17921400	-1.46258900	-0.12938500	
H	-3.61701400	-4.06232100	-1.85842600	C	-0.76333300	0.22897400	0.05842900	
H	-4.51811000	-2.53546100	-2.14811900	C	-0.08594200	-2.07505200	1.27822300	
H	-0.13762500	-2.55825200	-2.12597700	C	-1.49407700	-2.05875600	1.78752900	
H	0.29410600	-0.87018300	-2.40355000	C	-2.37519500	-1.06775000	1.43493400	
C	0.63094500	-0.06743700	2.93935500	C	-2.11917700	-0.08269800	0.42151600	
H	1.55042100	-0.61741900	3.12245600	O	-3.68012900	-1.13954900	1.91871600	
C	-1.79901100	1.31908100	2.48036700	C	-3.90422800	-0.36540600	3.09866500	
H	-2.73305300	1.84558000	2.31273100	H	-3.66345700	0.69257500	2.93327800	
C	-0.15435600	0.38005800	4.01347900	H	-4.96583200	-0.46743300	3.33748900	
H	0.17358200	0.19232500	5.03281500	H	-3.30116500	-0.74058200	3.93670000	
C	-1.34997500	1.06860900	3.78591000	H	0.28126000	-3.10816900	1.25159700	
H	-1.93991900	1.41649500	4.63008100	H	0.54189100	-1.53481400	1.99100500	
O	4.08142200	-1.51641600	-0.81231200	O	0.14331400	0.56605400	1.10834400	
C	4.79276900	-0.97208000	-1.92305900	C	1.41430300	0.57186100	0.39356100	
H	4.75123500	0.12513100	-1.91953800	C	1.45847200	-0.83104100	-0.26865100	
H	5.83048100	-1.29693100	-1.81191000	C	2.46622300	-1.27277400	-1.21605000	
H	4.39621800	-1.34030400	-2.87815900	O	2.44630500	-2.35094900	-1.80254300	
C	-1.94327600	2.04551700	-0.75737300	O	3.50350600	-0.39736400	-1.33631200	
C	-3.28104800	2.30763900	-0.42581800	C	4.56587700	-0.80695300	-2.21013300	
C	-1.30573600	2.86984000	-1.69652700	H	4.19660800	-0.92771000	-3.23262100	
C	-3.96102200	3.37398400	-1.01832100	H	5.30585800	-0.00672600	-2.16050200	
H	-3.80731400	1.65816600	0.26258400	H	4.99911200	-1.75289300	-1.87217700	
C	-1.99013100	3.93366300	-2.29019400	C	-0.34246300	-2.25719600	-1.30308700	
H	-0.27076700	2.67837200	-1.95572500	O	-0.57449400	-1.77384700	-2.39331900	
C	-3.31995800	4.19223500	-1.95196400	O	-0.60027200	-3.54745200	-0.99486200	

C	-1.07088800	-4.36153100	-2.08444200	O	1.55416200	0.59519500	-0.62367700
H	-2.02302800	-3.97973700	-2.46308100	C	-0.20795300	-0.93836200	-1.19460800
H	-1.19465400	-5.36103100	-1.66577100	C	-0.99227700	0.01926900	-1.83690200
H	-0.33340100	-4.36709700	-2.89109300	C	-1.30024500	1.36261600	-1.40866300
C	1.03524400	1.41727300	-0.81694200	C	-1.19134000	1.77849300	-0.07856600
C	-0.32075100	1.13337300	-1.06645700	H	-0.55222700	1.24428600	0.61036800
C	-0.92270400	1.65709100	-2.21087300	C	-1.71194600	-2.19607600	3.95180400
C	-0.17437900	2.49193000	-3.05049800	O	-2.05475900	-0.99823300	3.23866700
C	1.16551000	2.78434600	-2.77484700	C	-2.49620300	-1.17550700	1.95989200
C	1.79318200	2.22365200	-1.65705700	O	-2.58103700	-2.27738500	1.42296500
H	2.84257500	2.40943400	-1.45037800	C	-2.87128700	0.05900500	1.37477900
H	1.72484500	3.43879700	-3.43855900	C	-2.91955700	1.15011700	0.75730500
H	-0.64665500	2.91287300	-3.93436500	C	-3.90444500	2.22908100	0.53175900
H	-1.94807200	1.43602000	-2.47607200	O	-3.65166200	3.36695700	0.18031500
C	-1.88926300	-3.20473600	2.67371500	O	-5.15624100	1.79554400	0.78784500
H	-1.25701800	-3.23948000	3.57355300	C	-6.19664800	2.77986100	0.64062300
H	-2.93537400	-3.15158500	2.97967700	H	-6.22596800	3.15475800	-0.38615000
H	-1.72733400	-4.15533300	2.14618600	H	-7.11989200	2.25441800	0.88640800
C	-3.30379400	0.45696900	-0.34883200	H	-6.03174300	3.61523800	1.32654200
H	-4.17869700	-0.15138300	-0.10577800	H	-2.55583500	-2.89163000	3.96511100
H	-3.12759100	0.32351900	-1.42237900	H	-0.84631100	-2.68270400	3.49306800
C	2.50455900	1.02823000	1.32864500	H	-1.46835100	-1.86635900	4.96278900
C	3.40768500	0.11974600	1.89315300	C	1.38559900	-2.42504500	1.41439200
C	2.58179500	2.37935100	1.69587200	H	0.57694800	-3.09759500	1.15166600
C	4.37528700	0.55170300	2.80352800	C	3.50185200	-0.66103000	2.18739100
H	3.35833500	-0.92883400	1.61297200	H	4.28583400	0.01332900	2.51502000
C	3.54799400	2.81366200	2.60502100	C	3.28056800	-1.84371900	2.85094000
H	1.87715800	3.08940900	1.27218800	C	2.22802700	-2.72810600	2.45881600
C	4.44932600	1.90042100	3.16073300	H	2.08725200	-3.65445200	3.00972900
H	5.07166700	-0.16550900	3.23080800	H	3.90729100	-2.11232100	3.69716400
H	3.59584200	3.86423900	2.88056300	O	-1.75662600	-0.37713800	-2.92887000
H	5.20385500	2.23819600	3.86682000	C	-1.04343200	-0.66182700	-4.13418100
C	-3.63769800	1.93974100	-0.06388400	H	-1.80046900	-0.90916600	-4.88247400
H	-3.86550700	2.05701400	1.00445900	H	-0.35926200	-1.50921500	-4.01387000
H	-2.75958700	2.56707200	-0.26150000	H	-0.47187400	0.21496500	-4.46632100
C	-4.82764400	2.44108500	-0.89366300	C	-0.51934200	-2.41288000	-1.38052300
H	-5.70167200	1.80269100	-0.69919500	H	-0.86191200	-2.79559700	-0.40596600
H	-4.59806200	2.32569900	-1.96327100	H	-1.39332400	-2.49758200	-2.03091500
C	-5.18665900	3.90345900	-0.60457100	C	0.61923200	-3.30232000	-1.91785500
H	-4.34194500	4.56957000	-0.82165300	H	1.49172500	-3.24674700	-1.25507000
H	-6.03691100	4.23316800	-1.21373300	H	0.95725000	-2.92199300	-2.89263500
H	-5.45772200	4.04458300	0.44971700	C	0.19035500	-4.76853300	-2.06790100
TS11d				H	-0.68037400	-4.82683200	-2.73700900
C	0.90958700	-0.58845100	-0.36326700	H	-0.15160600	-5.14699700	-1.09363800
C	1.58824100	-1.21217800	0.69811600	C	1.30882400	-5.67013700	-2.60361800
C	2.66518600	-0.32750700	1.08337500	H	0.97231400	-6.70950700	-2.69900000
C	2.60309500	0.77236200	0.22229000	H	1.64744500	-5.33760900	-3.59353900

H	2.18002400	-5.66136900	-1.93599000		H	-5.63881300	-0.78623800	0.14217200
H	-1.31751800	2.83543500	0.13795800		H	0.14395100	1.70648400	1.59630600
C	-2.01642200	2.25359700	-2.39663100		H	1.14450100	4.50195300	0.28118000
H	-1.47109600	2.30116900	-3.34699400	3b1-t				
H	-3.01482800	1.86397700	-2.63259900		C	0.50526400	1.41000700	-0.43073500
H	-2.12939100	3.26438000	-2.00019600		C	0.55653500	2.48908000	0.65543500
C	3.39769900	1.97607000	0.03824200		C	0.71926800	3.76896100	0.41407000
C	4.73524200	2.04437100	0.47900600		C	1.54759900	0.33367500	-0.26288400
C	2.84310700	3.10407500	-0.60336400		C	0.88792600	-0.88477500	-0.01426700
C	5.48329100	3.20757100	0.30108800		C	-0.53334700	-0.63642800	-0.04266100
H	5.20249200	1.17531900	0.92991500		O	-0.75307900	0.69094900	-0.33010200
C	3.59863400	4.25985200	-0.78369000		C	2.93451300	0.41250800	-0.29629000
H	1.81384000	3.06650000	-0.94595400		C	3.67523400	-0.75824000	-0.08913400
C	4.92040100	4.32191000	-0.32798800		C	3.02392100	-1.97885900	0.15833200
H	6.51446200	3.23790100	0.64378200		C	1.63307700	-2.05704100	0.20115900
H	3.15154800	5.12003600	-1.27548300		C	-1.58207900	-1.52594800	0.16581300
H	5.50580100	5.22699300	-0.46602600		C	-2.96176900	-1.30916800	0.14461500
C2H2					C	-3.66294200	-0.08568200	-0.09896700
C	-0.60382400	0.00038000	-0.00010400		C	-5.02020100	0.01168000	-0.09178100
H	-1.67103400	-0.000068600	0.00052600		H	0.52824200	1.88118700	-1.41869700
C	0.60385000	-0.00045100	-0.00005200		H	3.43667200	1.36046400	-0.47340200
H	1.67087800	0.00111600	0.00041100		H	4.76078100	-0.72245900	-0.11606400
TS2b1					H	3.61486800	-2.87669600	0.31994200
C	0.48296200	1.28747700	-0.70475700		H	1.14080200	-3.00587000	0.39589700
C	0.48570400	2.42855300	0.86341500		H	-1.25713100	-2.54357200	0.37212500
C	0.80279200	3.64510300	0.83110500		H	-3.58142900	-2.18417800	0.33974800
C	1.51935900	0.31502700	-0.48610700		H	-3.07308500	0.80455200	-0.29805400
C	0.87874300	-0.86043800	0.00567500		H	-5.52211700	0.95606900	-0.28003700
C	-0.52014700	-0.62510000	-0.04819600		H	-5.65332400	-0.85197900	0.10331200
O	-0.72816700	0.61301700	-0.59104900		H	0.45988000	2.10824500	1.67372800
C	2.92205400	0.38456400	-0.57417600		H	0.83247500	4.40802900	-0.45390800
C	3.66166800	-0.72308600	-0.19328700	TS3b1-rot				
C	3.02693500	-1.89545700	0.30021700		C	0.32074500	1.37003900	-0.52223600
C	1.65149200	-1.97551000	0.41015400		C	0.19213900	2.45419800	0.55711400
C	-1.60138700	-1.46068900	0.32885800		C	0.24114000	3.74290100	0.31575500
C	-2.95631700	-1.24311000	0.27163500		C	1.45382100	0.40815200	-0.27131700
C	-3.65590700	-0.06543900	-0.18473200		C	0.89944400	-0.86576100	-0.02545700
C	-5.00435600	0.03142400	-0.19524300		C	-0.52702500	-0.75620900	-0.14847900
H	0.47131000	2.02361000	-1.49722800		O	-0.86147400	0.52811200	-0.49499400
H	3.41248200	1.28629400	-0.93078600		C	2.82512400	0.62202200	-0.22462900
H	4.74562600	-0.69895900	-0.26559000		C	3.66279500	-0.46528400	0.05935100
H	3.63981900	-2.74220500	0.59781400		C	3.11861000	-1.73819500	0.30604900
H	1.17760800	-2.87467800	0.79450600		C	1.74273700	-1.95356700	0.27105200
H	-1.27765900	-2.42460000	0.71602400		C	-1.50740200	-1.75520400	0.00629600
H	-3.58665000	-2.06144400	0.61869500		C	-2.87578800	-1.66550300	-0.09156300
H	-3.06215600	0.77552200	-0.53089000		C	-3.69282900	-0.45578200	-0.34527600
H	-5.50625100	0.93022100	-0.54117900		C	-4.15333200	0.36907600	0.60091900

H	0.35812100	1.83942300	-1.51009600	C	1.06839300	-0.72157300	-0.14510700
H	3.24304100	1.61061700	-0.39880100	C	1.45556400	0.61475600	-0.36037200
H	4.73938300	-0.32338400	0.09402500	C	2.77282600	1.02031100	-0.17768100
H	3.78352500	-2.56854300	0.52976000	C	3.71758100	0.06339500	0.21413700
H	1.33508900	-2.94123600	0.46829000	C	3.33568500	-1.27037400	0.43418500
H	-1.09592400	-2.74115800	0.21579700	C	2.01137100	-1.67430300	0.26691700
H	-3.42845100	-2.60107700	0.00262300	C	-1.24413500	-1.80960700	-0.03379500
H	-3.96747000	-0.26397000	-1.38650600	C	-2.63968900	-1.81456000	0.15493600
H	-4.77237500	1.22693600	0.34921100	C	-3.61556400	-0.77692000	0.21995100
H	-3.91680200	0.22246700	1.65260500	H	-1.83392600	2.78340600	1.88823800
H	0.34483900	4.38467200	-0.55147100	H	0.45373700	3.13771400	0.62113400
H	0.06775400	2.06506900	1.56904000	H	0.31152300	1.97049900	-1.64731200
3b1-c				H	3.07265500	2.05348600	-0.33712100
C	0.37425500	1.40062800	-0.42183100	H	4.75545800	0.35510300	0.35018100
C	0.37851700	2.47400000	0.67111300	H	4.08349800	-1.99776700	0.73897300
C	0.49531600	3.76038700	0.43783300	H	1.72376300	-2.70703400	0.44461500
H	0.58899500	4.40873700	-0.42551600	H	-0.74765400	-2.74510100	0.21925300
H	0.29068100	2.08381100	1.68669500	H	-3.02431800	-2.79046000	0.44748600
C	1.45698000	0.36563100	-0.25768500	H	-4.55220100	-1.10710600	0.67270000
C	0.84558900	-0.87846500	-0.02237600	H	-4.41790000	1.18415500	0.04935000
C	-0.58986200	-0.68774700	-0.05302700	H	-2.75832400	0.95311700	-0.73830100
O	-0.85424800	0.63103400	-0.33109600	Sb1			
C	2.84015300	0.50113300	-0.28521100	C	0.01324300	-1.29184100	0.68550900
C	3.62611900	-0.64015800	-0.08493300	O	-0.71617900	-0.14163400	1.16839300
C	3.02317200	-1.88767300	0.14945100	C	-0.24789300	0.94379700	0.45264000
C	1.63620900	-2.02097600	0.18622200	C	1.17665900	0.69799600	0.19286100
C	-1.57229100	-1.64626200	0.14674700	C	1.36430600	-0.68880100	0.33049600
C	-2.97629300	-1.63755000	0.15660100	C	2.60008100	-1.27321400	0.08357500
C	-3.98371900	-0.62621600	-0.00237900	C	3.66817900	-0.44309100	-0.28768700
C	-3.88831000	0.71767800	-0.19995400	C	3.48340800	0.93901700	-0.42549200
H	0.38128700	1.87860500	-1.40686700	C	2.23281200	1.52327600	-0.19551700
H	3.30405900	1.47007400	-0.45263100	H	2.09637500	2.59607000	-0.30439300
H	4.70948600	-0.56080800	-0.10706600	H	4.32389600	1.56651000	-0.71058600
H	3.64853100	-2.76275300	0.30603900	H	4.64883200	-0.87557700	-0.46785300
H	1.18259500	-2.99066900	0.37152900	H	2.74669200	-2.34673700	0.17979000
H	-1.14071800	-2.62921300	0.32775400	H	0.05563400	-2.02298700	1.50093200
H	-3.39537900	-2.62736600	0.33080400	C	-0.71621400	-1.81423500	-0.54458000
H	-4.99519000	-1.03093100	0.05739500	C	-1.98806100	-1.52909800	-0.86267000
H	-4.79438500	1.31119800	-0.28864800	C	-3.05202000	-0.84525000	-0.00961400
H	-2.94097700	1.23458900	-0.27416000	C	-3.34768000	0.63605300	-0.20001800
TS4b1				C	-2.54839500	1.73068500	-0.16932800
C	-3.56389300	0.54287900	-0.15219500	C	-1.09821200	1.85354000	-0.06508900
C	-1.38179900	2.21775600	1.08315800	H	-0.65382400	2.73275900	-0.52775700
C	-0.26019100	2.33193500	0.40869800	H	-3.05831500	2.67872900	-0.34405600
C	0.21353800	1.39768000	-0.71743900	H	-4.40550000	0.84976600	-0.35202200
O	-0.76357000	0.37252100	-0.95421900	H	-3.98959500	-1.38009800	-0.21040500
C	-0.36264400	-0.79973800	-0.37463600	H	-2.82165300	-1.01219400	1.04764900

H	-2.34221600	-1.89146800	-1.82809100	H	-4.71870000	-1.58403800	-0.39156100
H	-0.11217000	-2.39470000	-1.24087600	H	-1.87556400	-0.73575500	-1.24676200
TS6b1				H	-3.66589000	-0.02936500	1.20017300
C	0.29617400	2.15430700	1.24125200	H	-1.89459200	1.28776100	2.02576700
C	0.48526500	1.52233900	-0.73596900	H	0.34255300	2.61472200	1.94720900
C	-0.42187500	-0.32972200	0.01851800	H	2.07642400	3.21230800	-0.03952000
C	-0.18952700	1.20227100	1.88087400	H	1.26180300	1.69665400	-2.15154000
H	-0.59644900	0.61437900	2.67708700	H	0.02664900	-1.64386800	1.96744600
H	0.67543200	3.16118300	1.23351500	H	1.91053900	-3.19277500	1.41473300
O	-0.67663100	0.79386900	-0.71954700	H	3.49516100	-2.64779100	-0.40087900
C	0.99106500	-0.57419900	-0.04588100	H	3.24924300	-0.53745700	-1.71348400
C	1.57402400	0.60497900	-0.58623600	7b1-c			
C	2.96796100	0.71501100	-0.73956800	C	-0.44371700	-0.18257300	-0.43231100
C	3.75412300	-0.36898800	-0.37906900	C	-1.40855000	0.25021900	0.49199500
C	3.17492600	-1.54698400	0.15674500	C	-2.56624500	-0.47217600	0.71300400
C	1.80475000	-1.65825900	0.33732300	C	-2.75051200	-1.66423100	-0.01880800
H	1.37523000	-2.56472600	0.75609300	C	-1.79549900	-2.08881900	-0.94189400
H	3.82107100	-2.37855700	0.42593600	C	-0.62001100	-1.34117300	-1.16286600
H	4.83199400	-0.32107800	-0.51012400	C	0.65577600	0.91032700	-0.39625600
H	3.41789400	1.62055100	-1.13911000	O	0.56459600	1.26932800	1.02565400
H	0.44638200	2.40709900	-1.35972900	C	-0.85052200	1.57635200	1.02854800
C	-1.47061200	-1.27225700	0.32108700	C	-0.92041600	2.58617200	-0.13268000
C	-2.81646000	-1.17569800	0.15358800	C	-0.00420100	2.17204500	-1.00998300
C	-3.57599500	-0.06512500	-0.39180300	H	0.12821000	-1.68166600	-1.87414400
C	-4.91759700	-0.08796300	-0.51697500	H	-1.95424800	-3.01151100	-1.49447400
H	-1.09379400	-2.19221900	0.76450600	H	-3.64694300	-2.25810100	0.14098100
H	-3.40560300	-2.03696600	0.46881700	H	-3.31634100	-0.14432600	1.42951600
H	-3.02571600	0.81762800	-0.70372300	H	-1.17752900	1.90629900	2.01444700
H	-5.46550800	0.75794900	-0.92200600	H	-1.63786500	3.39354500	-0.22139800
H	-5.50522400	-0.95446400	-0.21821000	H	0.22002600	2.55585400	-1.99910300
7b1-t				H	2.41634300	1.31310400	-1.61599800
C	1.01221100	1.43107300	-1.12455500	H	3.81706700	-0.41859500	-1.08507100
O	-0.41606400	1.25014600	-0.96674500	C	2.72933600	-1.50423800	0.41767200
C	-0.39004300	0.95790100	0.46807400	C	2.03283400	-1.51116000	1.56579000
C	0.43190900	2.17433800	0.96040000	C	2.87165900	-0.40148200	-0.54011700
C	1.28680000	2.47030200	-0.02099100	H	3.30965500	-2.39217300	0.16143700
C	0.60568700	-0.23332900	0.43980500	H	2.02331800	-2.39691900	2.19628800
C	1.50531600	0.07730500	-0.59348700	H	1.47372600	-0.64491600	1.90378300
C	2.55151300	-0.76792500	-0.91130200	C	2.04137000	0.60820300	-0.87567600
C	2.68694600	-1.95943500	-0.16700100	TS8b1			
C	1.79305300	-2.26661300	0.85776900	C	-1.44454500	1.43555000	0.63270200
C	0.73007400	-1.39462100	1.17680400	C	-2.76146700	1.55969000	0.26866200
C	-1.73836300	0.76004100	1.08664900	C	-3.47027600	0.51822000	-0.38610700
C	-2.74852100	0.00436200	0.61088700	H	-4.27039600	0.78258600	-1.07616900
C	-2.76081000	-0.77942800	-0.61834900	C	-2.95589200	-0.80299900	-0.35131400
C	-3.81233000	-1.52933700	-0.99248800	C	-0.61261100	0.25973800	0.27734600
H	-3.79977000	-2.10936600	-1.91090800	C	0.88884000	0.49401600	0.06041500

C	1.50817500	-0.75580900	0.25287700	H	-0.17989700	-2.62971500	-1.38220800
C	0.33837100	-1.69386500	0.56694200	TS10b1			
H	0.54313200	-2.59655800	1.14304600	C	1.30867600	-0.73490100	1.02158900
O	-0.52702800	-0.80836500	1.30232200	C	0.56111400	0.43536800	-0.29683500
C	-1.13736200	-0.63185600	-0.91175100	C	2.75361100	-0.88256900	0.43407400
C	-0.39393900	-1.81016100	-0.76845000	C	3.46353800	0.40061300	0.14762200
H	-3.42310300	-1.54060400	-1.00376100	C	2.80779600	1.52867900	-0.26412900
H	-2.69511100	-1.19722300	0.62587400	C	1.39693100	1.58397500	-0.37705800
H	-0.93541300	2.27448800	1.10028800	H	0.91105000	2.55618300	-0.32007300
C	1.63187000	1.61171800	-0.27535700	H	4.53434900	0.44526700	0.33406600
H	1.16331500	2.58034900	-0.43224800	H	3.33477600	-1.48513100	1.14579500
C	2.87579600	-0.91313800	0.10368200	H	2.66848400	-1.47205400	-0.48350300
H	3.35794500	-1.87790700	0.24434700	O	0.65304000	-0.63503700	-1.25772200
C	3.02765800	1.46566900	-0.41065400	C	-0.22691600	-1.59013200	-0.62734700
H	3.63499000	2.33196200	-0.66042100	C	0.35908700	-1.76251000	0.77712900
C	3.63850800	0.22496500	-0.22482000	H	-0.34569500	-2.46115600	-1.27321800
H	4.71695600	0.13540800	-0.32859500	C	-1.45227000	-0.73000500	-0.34397400
H	-3.24717600	2.52574400	0.40145300	C	-0.91950200	0.54492900	-0.08268900
H	-1.26881000	-0.18843900	-1.89621800	C	-1.74483500	1.58942200	0.31348100
H	-0.15886900	-2.53331300	-1.54122000	C	-3.12401000	1.34416900	0.41878500
9b1				C	-3.64976200	0.07443400	0.15688200
C	-1.17753800	-0.61326500	-0.83806200	C	-2.80960600	-0.98882200	-0.21413500
C	-0.62247900	0.23556200	0.36911200	H	-3.22129900	-1.97794700	-0.40141000
C	-2.71914700	-0.76265300	-0.76197400	H	-4.72087300	-0.09128700	0.24017800
O	-0.50580700	-0.81175100	1.39771600	H	-3.79134500	2.15267400	0.70603300
C	0.37585800	-1.69195400	0.65658300	H	-1.34680700	2.57732800	0.53241700
C	1.50321200	-0.73225500	0.28436100	H	3.36752400	2.45299600	-0.39447400
C	0.85731500	0.50104400	0.09479000	H	1.32919700	-0.33442900	2.03880100
C	1.56302600	1.62346200	-0.30824100	H	-0.28678200	-2.15805600	1.55678100
C	2.95126400	1.49890200	-0.50262300	TS11b1			
C	3.59272800	0.27108300	-0.31621500	C	-0.08341900	-0.59472600	-0.20350700
C	2.86747900	-0.87014600	0.06949600	C	-1.47103200	-0.45593500	0.01284500
H	3.37216500	-1.82392900	0.20673300	C	-1.82222500	0.89175000	-0.36807800
H	4.66706800	0.19828300	-0.46618800	C	-0.64698400	1.48472500	-0.79237100
H	3.53204400	2.36893300	-0.79843800	O	0.37852500	0.59669100	-0.70062900
H	1.06723700	2.57864000	-0.46537200	H	-0.39789100	2.45650400	-1.19094500
H	0.63196500	-2.57271700	1.24667300	C	0.75881700	-1.70479100	0.02344300
C	-1.47274000	1.38053800	0.78362700	C	2.12647300	-1.94128600	-0.08350800
C	-2.77882300	1.51032400	0.32238700	C	3.25685100	-1.16218600	-0.42851700
C	-3.40130700	0.53922500	-0.45399200	C	3.38009600	0.20984800	-0.72706700
H	-1.03928800	2.12688600	1.44377300	H	4.29347000	0.50542500	-1.24175700
H	-3.33864300	2.40420300	0.59284800	H	2.50528500	0.75784900	-1.04530900
H	-4.42732500	0.68617900	-0.78296300	H	4.19598200	-1.71152900	-0.35270900
H	-2.96484200	-1.48947200	0.02823900	H	2.38524800	-2.96849200	0.17118200
H	-3.09494500	-1.19259400	-1.69906300	H	0.18529500	-2.56417200	0.36600800
C	-0.41477700	-1.89552400	-0.61850700	C	2.96083100	1.94053800	1.41831200
H	-0.92352400	-0.12675400	-1.79022200	C	3.79707300	1.14091900	0.91729400

H	1.97114300	2.36069300	1.40275000	C	-3.73227100	0.70832100	0.01818400
H	4.79831200	0.81060900	1.14678300	H	-1.57830000	2.98443200	-0.13635500
C	-3.17207600	1.33947500	-0.25953100	H	-4.36922300	1.58883700	0.00218900
C	-2.47045200	-1.33709000	0.49632100	H	-5.34708100	-0.67859500	0.11737900
H	-2.22176000	-2.35388500	0.78855400	H	-3.90998100	-2.70021400	0.15013100
C	-3.76648900	-0.87832900	0.58972300	H	-1.44979400	-2.52666300	0.07358400
H	-4.54652300	-1.53937000	0.95767200	C	1.06933300	-0.64886600	-0.08949400
C	-4.11466700	0.45807800	0.21204600	C	2.37766400	-0.29837600	-0.22440400
H	-5.15047300	0.77448900	0.30318900	C	3.00699900	1.02561200	-0.29449100
H	-3.44307000	2.35241200	-0.54481400	C	2.71412900	2.10749200	0.44242000
1b2-t				H	0.89915300	-1.72266800	-0.06090700
C	-0.20600400	0.14694900	-0.04979800	O	3.24303300	-1.36250800	-0.44171100
O	-0.19820400	1.50505700	0.12525200	C	4.38457800	-1.44182200	0.41491300
C	-1.47708800	1.95659300	0.22987800	H	4.94724600	-2.31743300	0.08397700
C	-2.35559700	0.90001600	0.12527700	H	5.01924900	-0.55061100	0.33876200
C	-1.53629500	-0.28133900	-0.05704300	H	4.07450300	-1.57492100	1.46020600
C	-2.15287000	-1.55608000	-0.20225500	H	3.82763700	1.08553900	-1.01146000
C	-3.52386500	-1.63134700	-0.16479300	H	3.25354100	3.03971900	0.29632900
C	-4.33602400	-0.46037300	0.01647900	H	1.93501500	2.10231500	1.19753100
C	-3.77954500	0.78454600	0.15970600	TS2b2-t			
H	-1.59145400	3.02067500	0.36901700	C	-0.58643700	0.32350500	-0.92539200
H	-4.40130200	1.66546000	0.29559900	C	-1.65843900	-0.96938100	0.35181500
H	-5.41680600	-0.57382000	0.03841700	C	-2.86269600	-1.13460700	0.04241000
H	-4.01408700	-2.59496400	-0.27528700	C	-4.02108000	-0.99553100	-0.77205200
H	-1.55170200	-2.45064500	-0.34246800	O	-4.25292400	-1.66263800	-1.77352000
C	1.00832000	-0.59641600	-0.18480800	O	-4.87052100	-0.03846900	-0.29763300
C	2.31154200	-0.19409600	-0.21232400	C	-6.09638900	0.11404300	-1.03331500
C	2.80882500	1.17109900	-0.11316200	H	-5.89414500	0.41246800	-2.06609600
C	4.09362600	1.52657200	-0.30385500	H	-6.64951500	0.89461600	-0.50915500
H	0.84920500	-1.66531500	-0.30635100	H	-6.66132200	-0.82250800	-1.03537500
O	3.26212300	-1.18417500	-0.42171000	C	-0.69435200	-1.36042800	1.39018000
C	3.85308600	-1.71339900	0.76895700	O	0.26527100	-0.70136300	1.74617500
H	4.61968600	-2.42029900	0.44234100	O	-1.01005700	-2.56122200	1.91947000
H	4.31464600	-0.92160800	1.37222400	C	-0.14477300	-3.02077700	2.97426000
H	3.10281900	-2.23970300	1.37437000	H	-0.15908700	-2.31908200	3.81278100
H	2.07069600	1.93281400	0.11599700	H	-0.55109800	-3.98752600	3.27301600
H	4.40107400	2.56507100	-0.22374500	H	0.88024700	-3.12772600	2.60867400
H	4.85721100	0.79893800	-0.56200500	O	0.74739100	-0.06553200	-1.06544000
1b2-c				C	1.56186500	0.82088800	-0.45966700
C	-0.14681100	0.10654000	-0.06064300	C	0.78679600	1.90955300	0.00487300
O	-0.16173200	1.47152300	-0.11341100	C	-0.57115800	1.61326600	-0.32215000
C	-1.44791500	1.91385200	-0.09609800	C	-1.59790000	2.52454600	0.01224600
C	-2.31013700	0.84094200	-0.02753500	C	-1.24696100	3.69668600	0.65335400
C	-1.47062600	-0.34003500	-0.00334400	C	0.10640300	3.98801000	0.99050300
C	-2.06621400	-1.63158300	0.05897600	C	1.12150900	3.10637600	0.68062600
C	-3.43612700	-1.72336600	0.10122700	H	-1.18160000	0.01092500	-1.77140400
C	-4.26799900	-0.55235400	0.08189100	H	-2.63536500	2.29939600	-0.21737700

H	-2.01904400	4.41523700	0.91611300	C	2.72988100	0.43783800	-0.60542500
H	0.33466700	4.91697900	1.50575200	C	3.50131600	-0.70448900	-0.75208100
H	2.15012100	3.32850700	0.95246900	C	2.98769600	-2.06594600	-0.85198200
C	2.96306900	0.61279600	-0.33123200	C	3.77232400	-3.14950100	-0.99486100
C	3.73159500	-0.45646800	-0.72686200	H	3.23767600	1.39073200	-0.52353400
C	3.23582400	-1.66008200	-1.38747900	H	1.91205800	-2.17291700	-0.80354100
C	4.01522300	-2.68682800	-1.77035400	H	3.33007600	-4.13885300	-1.06078700
O	5.07457700	-0.49356700	-0.52406800	H	4.85405100	-3.08056700	-1.04706100
C	5.73811600	0.59062100	0.11628000	O	4.84489900	-0.64577000	-0.80762500
H	5.62758200	1.51787400	-0.45970300	C	5.53589600	0.60328700	-0.74206500
H	6.79103000	0.30721300	0.15300300	H	5.24478700	1.25459600	-1.57387100
H	5.36115600	0.73707800	1.13602000	H	6.59336300	0.35106200	-0.82471300
H	3.45829500	1.43912100	0.16482600	H	5.34966300	1.10339600	0.21518100
H	2.16819600	-1.69411500	-1.56379900	TS3b2-rot			
H	3.58007500	-3.55497400	-2.25647100	C	-0.76446300	0.21024000	-0.54739200
H	5.08862600	-2.68828200	-1.61141900	C	-1.49139400	-0.83797000	0.34171800
3b2-t				C	-2.72249100	-1.25880500	0.04624500
C	-0.89512900	-0.11479800	-0.45487500	C	-3.49784200	-0.92999200	-1.10201300
C	-1.57473400	-0.91136000	0.70611100	O	-3.46999300	-1.51750000	-2.18585300
C	-3.61817200	-1.38322000	-0.62661800	O	-4.38098400	0.10784300	-0.86583700
C	-2.80032300	-1.39707400	0.53800400	C	-5.33221300	0.35364100	-1.90919900
O	-3.55632900	-2.19284500	-1.55494800	H	-4.83446400	0.63892700	-2.84162600
O	-4.56762200	-0.38257700	-0.59958100	H	-5.95682700	1.17272800	-1.54614500
C	-5.53278600	-0.42271600	-1.65909800	H	-5.94291900	-0.53573600	-2.09404700
H	-6.07946300	-1.37067800	-1.64827700	C	-0.74320000	-1.22655400	1.55761200
H	-6.21261400	0.40915900	-1.46374000	O	0.32148900	-0.71521700	1.90059000
H	-5.05374000	-0.30241100	-2.63611700	O	-1.33347600	-2.20188900	2.27558400
C	-0.85972600	-1.04281500	2.00505900	C	-0.66087600	-2.58880500	3.47982800
O	-1.13677500	-1.80079100	2.90917300	H	0.33461200	-2.98747100	3.26010800
O	0.19690500	-0.16756900	2.09975900	H	-1.29079400	-3.36140500	3.92336800
C	0.91436600	-0.20847000	3.34211800	H	-0.56132300	-1.73761300	4.16022200
H	1.69831800	0.54617600	3.25343300	C	-0.56525900	1.56362000	0.04515500
H	1.34961600	-1.19903500	3.50354300	C	0.81143100	1.84672300	0.10313400
H	0.24919300	0.02706100	4.17763900	C	1.48886500	0.70203500	-0.44440600
O	0.51728400	-0.49935000	-0.67042200	O	0.62625500	-0.18877200	-0.87740100
C	1.32216800	0.54313400	-0.54663500	C	-1.50188900	2.47523400	0.53001400
C	0.55686000	1.74604700	-0.35189000	C	-1.02939500	3.67566200	1.06037400
C	-0.79640900	1.36307600	-0.29543200	C	0.35166900	3.96125600	1.12470600
C	-1.79968100	2.30948100	-0.08900400	C	1.28694000	3.04911800	0.65418500
C	-1.42046100	3.64453500	0.04504400	C	2.89165900	0.51024700	-0.54430200
C	-0.06381900	4.03338200	-0.00842900	C	3.52296500	-0.63107300	-0.97552000
C	0.93790600	3.09165500	-0.20004000	C	2.86188400	-1.89757700	-1.38175300
H	-1.39617900	-0.42492000	-1.37401400	C	2.57341300	-2.87536500	-0.52241500
H	-2.84142900	2.00667200	-0.02849400	H	-1.27319300	0.22376400	-1.51308200
H	-2.18255200	4.40374000	0.19922800	H	-2.56372300	2.24718000	0.49953200
H	0.19582700	5.08192500	0.10689100	H	-1.73817000	4.40725800	1.43931700
H	1.98141400	3.39379100	-0.23002600	H	0.68292700	4.90262500	1.55375500

H	2.35022000	3.26384300	0.71797400	H	2.08920700	-3.89641500	-0.61584300
H	3.48515500	1.36211700	-0.23477900	H	1.57514200	-2.36679900	0.28606300
H	2.64118100	-1.99924500	-2.44397700	O	4.90078400	-0.64033800	-1.15196900
H	2.10488700	-3.79451100	-0.86221300	C	5.55028600	0.63349700	-1.12490300
H	2.76717200	-2.78123700	0.54286400	H	5.07721100	1.32647400	-1.82958000
O	4.85604200	-0.72878600	-1.09111200	H	6.57807800	0.43607100	-1.43001200
C	5.69863700	0.39259900	-0.79018000	H	5.54173900	1.05508100	-0.11345400
H	6.71333800	0.05138800	-0.99455400	TS4b2c			
H	5.45204700	1.24404300	-1.43393600	C	1.57286100	-2.07925900	-1.60317200
H	5.60456700	0.67252100	0.26470700	C	-0.51894600	-1.16959500	0.05689700
3b2-c							
C	-0.83720200	-0.05634600	-0.47071800	C	-0.69384400	0.96526300	-1.24356600
C	-1.58972100	-0.95506100	0.56066200	C	-0.58959900	2.06245600	-0.22477500
C	-3.62632100	-1.09368500	-0.85357400	C	0.71561700	2.01335600	0.29610300
C	-2.84488100	-1.32390400	0.31266000	C	1.43400100	1.00944700	-0.47150600
O	-3.63737600	-1.79994100	-1.86411800	O	0.69256500	0.68013700	-1.54074800
O	-4.45890500	0.00204900	-0.72618100	C	2.75066000	0.58521800	-0.27191600
C	-5.41236600	0.17381700	-1.78323400	C	3.37713800	-0.61372600	-0.62515200
H	-6.06224800	-0.70306500	-1.86375600	C	2.79315400	-1.85514200	-1.05271800
H	-5.99675500	1.05401900	-1.50708000	H	0.97035000	-1.29648900	-2.02927100
H	-4.91392600	0.33319400	-2.74476700	H	1.22254100	-3.09934500	-1.72331000
C	-0.93134900	-1.29972900	1.84895800	H	3.42164100	-2.71055900	-0.81111100
O	-1.33491000	-2.07941000	2.68452600	O	4.69617800	-0.78978000	-0.35187000
O	0.24831000	-0.60837300	2.02915300	C	5.50508700	0.28122300	0.12925900
C	0.90012400	-0.82927500	3.28910700	H	5.23526000	0.55078700	1.15765500
H	1.80047000	-0.21225500	3.26531100	H	5.42541300	1.15891600	-0.52251400
H	1.15954100	-1.88476300	3.41212500	H	6.52658800	-0.10114000	0.11380500
H	0.25020900	-0.52673700	4.11511500	H	3.31222600	1.24407500	0.38179600
O	0.55770600	-0.48620000	-0.72652000	H	-1.18447500	1.22015300	-2.18114100
C	1.41331400	0.47933700	-0.45385200	C	-1.53664700	2.93308200	0.30833700
C	0.71149800	1.68638100	-0.09319400	C	-1.14519400	3.76870700	1.35819100
C	-0.66043200	1.37763900	-0.10527800	C	0.15696500	3.71331300	1.88794500
C	-1.61466100	2.34067900	0.22139500	C	1.09806100	2.82657700	1.37070900
C	-1.16475800	3.61942000	0.54878000	H	2.09889300	2.77677800	1.79106300
C	0.21155800	3.93396200	0.56505700	H	0.42853200	4.36787100	2.71146200
C	1.16346800	2.97310000	0.25043500	H	-1.86102500	4.46972800	1.77934100
H	-1.33561300	-0.20439800	-1.43060600	H	-2.55057400	2.95752600	-0.07791700
H	-2.67220500	2.09113100	0.22476000	C	-2.78885100	-0.44317500	-0.66479700
H	-1.88662800	4.39132000	0.80191900	O	-3.45865100	-1.35282700	-0.21969600
H	0.52638000	4.93882600	0.83203800	O	-3.35343100	0.62102200	-1.32190900
H	2.22233800	3.21638700	0.27520100	C	-4.78412400	0.57418600	-1.45899500
C	2.81501300	0.33207100	-0.54879700	H	-5.05493200	1.47907700	-2.00549000
C	3.57968000	-0.76782000	-0.90299100	H	-5.26196200	0.55801400	-0.47545500
C	3.20564400	-2.17193300	-1.07971800	H	-5.08473800	-0.31680300	-2.01677500
C	2.23555200	-2.83584800	-0.43256800	C	-0.82356300	-2.41063100	0.72460500
H	3.34404400	1.26083000	-0.37381500	O	-0.75389900	-3.52220600	0.21219000
H	3.87147400	-2.70900800	-1.75211200	O	-1.09581000	-2.22397100	2.04844300

C	-1.38995900	-3.41615200	2.79076100	H	3.54220500	2.52106900	-1.34195100
H	-1.56064000	-3.08268400	3.81601900	TS6b2			
H	-0.55033700	-4.11686000	2.74957800	C	-0.69475500	-1.05030900	1.07391900
H	-2.28471800	-3.90421100	2.39351800	C	0.76171900	0.72716800	-0.85396100
Sb2				C	-1.65321400	-1.08491100	0.27457700
C	-0.67497700	2.19191200	0.64643400	C	-1.28225600	0.07320200	-1.45794400
C	-0.18393900	3.48681400	0.51994000	O	0.06915500	-0.18867900	-1.56950400
C	-0.86226300	4.37319200	-0.32844000	C	-0.12718600	1.77360900	-0.48547200
C	-1.99249600	3.95961900	-1.04660100	C	-1.42284000	1.39033800	-0.94510800
C	-2.47906700	2.65437300	-0.92580300	C	-2.53120400	2.24204700	-0.74661700
C	-1.81735800	1.78108300	-0.06171700	C	-2.32003400	3.45279000	-0.11445100
C	-2.04026900	0.37676300	0.29367200	C	-1.02992800	3.83307200	0.35177300
O	-1.35703900	0.15201100	1.47462500	C	0.06282100	3.00659400	0.18059500
C	-0.18564800	0.98630400	1.44385000	C	-2.99337400	-1.67719900	0.15635800
C	0.92298000	0.19454300	0.71969000	O	-3.38036300	-2.62027000	0.81581000
C	0.88742800	-1.14116000	0.52601500	O	-3.76966000	-1.05291600	-0.76584300
C	-0.07804800	-2.14934800	1.17382400	C	-5.10617900	-1.57324900	-0.89635300
C	-1.27898300	-2.68656600	0.41661800	H	-5.07804800	-2.62379400	-1.19726200
C	-2.32439600	-2.06630100	-0.17788800	H	-5.57940700	-0.96313100	-1.66656600
C	-2.57332500	-0.64434100	-0.40307100	H	-5.64255500	-1.48420100	0.05202500
O	-3.22617600	-2.90551000	-0.83064000	C	0.45787200	-1.03439700	1.89901400
C	-4.57067600	-2.83169800	-0.36134500	O	1.44196500	-1.74641300	1.73540600
H	-4.63621700	-3.16216600	0.68478800	O	0.34289900	-0.13467500	2.91812600
H	-5.15351200	-3.50376600	-0.99559300	C	1.43649500	-0.11832700	3.84856800
H	-4.97672000	-1.81407900	-0.44024900	H	1.55081000	-1.09607400	4.32575200
H	-1.32522300	-3.77129200	0.35717200	H	1.17159900	0.63918500	4.58768800
H	0.53987800	-3.02186100	1.42114600	H	2.37185400	0.14493500	3.34610700
H	-0.40921400	-1.73093600	2.12666500	C	2.17344600	0.65545300	-0.67705300
H	0.09576400	1.22169900	2.47400900	C	3.04417600	-0.35432200	-1.00967900
H	0.70440900	3.80135200	1.05792000	C	2.67403100	-1.63129400	-1.61416200
H	-0.50560300	5.39480000	-0.43025900	C	3.56015000	-2.54604000	-2.04087800
H	-2.50192800	4.66397800	-1.69905300	O	4.38178000	-0.24684000	-0.80683300
H	-3.36063800	2.33826700	-1.47718300	C	4.93043300	0.92771400	-0.22188900
H	-3.14913700	-0.40181900	-1.29287600	H	4.54239800	1.08096700	0.79263700
C	1.93812500	-1.84953300	-0.28904000	H	6.00708700	0.75636300	-0.17779400
O	1.71861700	-2.36998200	-1.36101700	H	4.72311600	1.81149100	-0.83852600
O	3.11433600	-1.94099300	0.37057300	H	2.57611300	1.53942700	-0.19638800
C	4.15535800	-2.67020800	-0.30940600	H	1.61188200	-1.82197900	-1.69602500
H	4.39451000	-2.18861000	-1.26131700	H	3.21850000	-3.48499400	-2.46621200
H	5.01199900	-2.64468000	0.36457900	H	4.63167400	-2.38964300	-1.97131600
H	3.83903800	-3.69993500	-0.49602600	H	1.04253400	3.30153200	0.54712500
C	2.08446800	1.04010700	0.31849600	H	-0.90963000	4.79041900	0.85152200
O	2.48669300	1.96196700	1.00831400	H	-3.15465000	4.13257400	0.03631300
O	2.62892400	0.70564900	-0.86459000	H	-3.52115500	1.94824400	-1.08205800
C	3.78986700	1.45947700	-1.26427800	H	-1.88936400	-0.43460800	-2.19175000
H	4.07062000	1.05665100	-2.23752300	7b2-t			
H	4.59623300	1.32600600	-0.53807400	O	0.16588900	0.53454600	-1.67793300

C	-1.26557100	0.47589800	-1.48882400	O	0.10350300	0.59283700	-1.81171000
C	-1.48379500	1.75856600	-0.68007100	C	-0.23991400	2.92112300	0.91745000
C	-0.33667300	1.85705900	0.12291900	C	-1.32413500	3.81065400	1.06326100
C	0.52890400	0.63925600	-0.26923100	C	-2.49979500	3.63186900	0.33476400
C	-0.18200000	2.88877000	1.02961700	C	-2.63543600	2.55465400	-0.56511700
C	-1.20679400	3.85366500	1.10938700	C	-1.24935400	-0.73966200	-0.52166600
C	-2.34378300	3.75884300	0.30736100	C	-0.11069500	-0.56512800	0.16705100
C	-2.49924400	2.69328700	-0.60278200	H	-1.87727700	0.27637300	-2.44078900
H	-3.38936400	2.62110600	-1.22309400	H	-3.55533300	2.41676100	-1.12828800
H	-3.12038800	4.51548900	0.38339700	H	-3.32222100	4.33143900	0.46032500
H	-1.10692900	4.68238400	1.80547400	H	-1.24001400	4.64670200	1.75273600
H	0.69583000	2.96766000	1.66579400	H	0.66932600	3.06301500	1.49600000
C	1.99592300	0.73974400	-0.01565200	C	-2.32128300	-1.70843000	-0.24107500
C	2.96286300	-0.05912700	-0.51469300	O	-2.31584100	-2.52910200	0.65698200
C	2.75882500	-1.20314500	-1.40842600	O	-3.34540100	-1.56748900	-1.12044200
C	3.71452700	-2.09468800	-1.71358200	C	-4.45849700	-2.46041100	-0.93002700
O	4.26293300	0.18517800	-0.10403000	H	-4.89705200	-2.31442900	0.06077800
C	5.05181900	0.95175100	-1.02083900	H	-5.17326300	-2.20138600	-1.71162900
H	5.09768300	0.47388300	-2.00688900	H	-4.13286600	-3.49909700	-1.03125000
H	4.64255700	1.96501000	-1.12639300	C	0.39917400	-1.30730000	1.35464900
H	6.05421400	1.00375900	-0.58984400	O	0.96818800	-2.37610700	1.31543300
H	1.75915900	-1.31227300	-1.81726100	O	0.18424800	-0.59641200	2.47853900
H	3.50190800	-2.93715100	-2.36505400	C	0.64696300	-1.20317300	3.70315500
H	4.71883100	-2.02100600	-1.30640600	H	0.37387500	-0.50065400	4.49067400
H	2.31386100	1.53592400	0.65128800	H	1.73020100	-1.34644400	3.66873500
C	-0.25964100	-0.60829200	0.27034700	H	0.15363600	-2.16666800	3.85291200
C	-1.36350700	-0.69727100	-0.48859700	C	2.01606800	0.96481400	-0.26079700
C	-2.51806600	-1.59840600	-0.31203300	H	2.29946800	1.94901600	0.10181500
O	-2.68576100	-2.36189600	0.61801400	C	3.03053600	0.09857800	-0.47081400
O	-3.39928100	-1.45545400	-1.33411100	O	4.27369100	0.51894100	-0.04709000
C	-4.57340200	-2.28645000	-1.26466700	C	5.39551700	0.22297200	-0.88465400
H	-5.15744400	-2.03504800	-2.15034100	H	5.27906600	0.69358200	-1.86899500
H	-5.13705200	-2.07104800	-0.35299500	H	6.26200100	0.64811500	-0.37440100
H	-4.29044400	-3.34233100	-1.27344400	H	5.54008200	-0.85549300	-1.01257400
C	0.18831000	-1.44102700	1.41737200	C	2.95832200	-1.27578000	-1.00124500
O	0.47039700	-2.61649400	1.34543200	C	2.30916200	-1.64577000	-2.11200700
O	0.29824100	-0.69230600	2.53352900	H	3.50025900	-2.02179500	-0.42007300
C	0.77300700	-1.38519000	3.70699800	H	2.29286400	-2.68862500	-2.41856900
H	0.78712700	-0.63397100	4.49677400	H	1.76634600	-0.93282200	-2.72361800
H	1.77568700	-1.78231500	3.52904200	TS8b2			
H	0.09410300	-2.20311200	3.96058100	C	2.10284700	1.20933700	-0.38374900
H	-1.78890700	0.36498900	-2.43547100	C	3.08493800	0.25340700	-0.37267900
7b2-c				C	2.77707400	-1.12949500	-0.58272800
C	0.55572900	0.72644100	-0.42436700	H	3.31648900	-1.87137600	-0.00252600
C	-0.37724200	1.87792000	0.02135400	C	1.59603300	-1.48926600	-1.25845600
C	-1.56270900	1.69478100	-0.70723400	C	0.67371600	0.91847900	-0.61770100
C	-1.30177500	0.42869500	-1.53059900	C	-0.35453800	1.89371000	-0.03801100

C	-1.52193900	1.72071700	-0.80085900	O	0.32718700	0.62051500	-2.09470900
C	-1.14115100	0.63876300	-1.80911100	C	0.26329000	-0.63843400	-0.12703100
H	-1.69016100	0.58668500	-2.74725000	C	-1.03333000	-0.74790000	-0.89546100
O	0.24763900	0.94379000	-2.02852100	C	0.10068600	-0.66387900	1.39762300
C	0.19117500	-0.58714000	-0.29518700	C	-2.05911800	-1.75823400	-0.81704400
C	-1.03684600	-0.64180000	-0.97391600	O	-1.09484500	-0.18320500	1.78877400
C	0.29502900	-1.12692000	1.12443700	O	-1.74446600	-2.76736200	0.04276400
C	-2.14698900	-1.56188300	-0.84046600	O	0.94690600	-1.05844600	2.17332700
O	-0.64069500	-0.55409900	1.90451900	O	-3.10571800	-1.72649500	-1.45888100
O	-1.84108500	-2.66502600	-0.10299500	C	-1.32401800	-0.13194000	3.20908600
O	1.10886500	-1.92574300	1.53924900	H	-0.59179800	0.52401000	3.68741200
O	-3.24701300	-1.38660100	-1.35274400	H	-1.25091100	-1.13360300	3.64088400
C	-0.63301900	-0.94751800	3.28996100	H	-2.33169200	0.26807800	3.32239000
H	0.32496000	-0.69461700	3.75227900	C	-2.72931600	-3.80631300	0.17153200
H	-0.80544000	-2.02350700	3.37683800	H	-3.67383900	-3.39430300	0.53799900
H	-1.44539000	-0.38504000	3.75046400	H	-2.31220200	-4.51247600	0.89042400
C	-2.90374800	-3.61718300	0.06689300	H	-2.90059600	-4.29328500	-0.79274200
H	-3.74644800	-3.16086600	0.59421800	H	1.07919700	-2.65080600	-0.02124100
H	-2.47350400	-4.42790700	0.65620500	H	1.15321200	-1.92246000	-1.62111000
H	-3.24610700	-3.98615100	-0.90407200	H	2.56019600	2.07182200	-0.61847400
H	1.32026400	-2.54120100	-1.23906700	C	-0.12000200	2.91052000	0.66336100
H	1.37979900	-0.97860500	-2.18953400	H	0.79166400	3.08645400	1.22934600
H	2.37666500	2.22845300	-0.12672800	C	-2.51872200	2.44351000	-0.78933100
C	-0.30855400	2.80478200	1.00299800	H	-3.43960500	2.26054700	-1.33714900
H	0.58878200	2.94163500	1.60165700	C	-1.24246600	3.73911700	0.83648900
C	-2.67683400	2.43360900	-0.52529300	H	-1.19075600	4.57331100	1.53162100
H	-3.58688600	2.28288900	-1.09988200	C	-2.42372500	3.50696300	0.12398500
C	-1.46791400	3.55637500	1.27224000	H	-3.27732300	4.16352900	0.27228500
H	-1.45597300	4.29027900	2.07412300	O	4.41805300	0.43349600	-0.18643600
C	-2.63261100	3.37081700	0.52351600	C	5.42554900	-0.54208700	0.04269000
H	-3.51605200	3.96244300	0.74994400	H	6.35834200	0.01608600	0.14205900
O	4.33335600	0.66498300	0.00357500	H	5.23643900	-1.10322000	0.96710000
C	5.41306000	-0.26393600	-0.06682600	H	5.50820600	-1.23974500	-0.80148300
H	6.32115500	0.33069800	0.04874300	TS10b2			
H	5.36080300	-1.00096500	0.74405200	C	0.26066800	-0.92374900	-0.41836300
H	5.43013200	-0.78040600	-1.03449600	C	0.76931100	1.00977600	-0.49089000
9b2				C	1.30792000	-1.43220400	-1.47795700
C	2.20375500	1.04914400	-0.55053500	C	2.72583400	-1.04960300	-1.22970400
C	3.12050700	0.01699300	-0.35016500	C	3.10628600	0.15945300	-0.68687200
C	2.72611600	-1.31440600	-0.31309800	C	2.15915000	1.08665000	-0.20167100
H	3.44470400	-2.10588200	-0.13568700	H	2.45013300	1.77779300	0.58323300
C	1.30016900	-1.71951600	-0.55078400	O	4.45617900	0.32782800	-0.49614700
C	0.75798200	0.78659900	-0.69578000	C	4.92916500	1.54595000	0.06463900
C	-0.21530800	1.87352400	-0.25123900	H	4.67571300	1.62723900	1.13001700
C	-1.39524100	1.65184100	-0.97579800	H	6.01534200	1.51625800	-0.04061600
C	-1.08520500	0.43541500	-1.83757300	H	4.53085100	2.41502300	-0.47515100
H	-1.64979300	0.29841300	-2.75792000	H	3.50579800	-1.78584800	-1.40288100

H	1.22141800	-2.52362300	-1.51825100	C	0.49779200	-2.27798400	-0.55368200
H	0.97918800	-1.04193900	-2.44374000	O	-0.23363200	-1.98724200	-1.49289300
O	0.28757000	1.02583100	-1.82847500	C	1.70397000	-1.60079500	-0.22933800
C	-1.10134200	0.71296100	-1.60293900	C	2.47239800	-0.71436200	0.22647000
C	-1.05757300	-0.64724600	-0.88735500	C	3.90796100	-0.37317900	0.11513600
C	-2.25429000	-1.35773900	-0.46675900	O	4.46275400	0.54891300	0.68502800
O	-2.27262200	-2.40216900	0.17120300	O	4.54620000	-1.22775200	-0.70809200
O	-3.38973500	-0.76384400	-0.94003800	C	5.95396900	-0.98284200	-0.88727300
C	-4.61957000	-1.42982300	-0.61167200	H	6.11678400	0.00949900	-1.31636400
H	-4.75167700	-1.47392300	0.47300800	H	6.29068900	-1.76051200	-1.57327800
H	-5.40646200	-0.83007800	-1.07135700	H	6.47899200	-1.05537300	0.06906700
H	-4.62473300	-2.44630100	-1.01544000	H	-0.90186100	-4.48346900	-1.00709100
C	0.37955300	-1.52420400	0.95975300	H	-1.81867900	-3.44066800	0.10990100
O	-0.06956000	-0.99968600	1.95978900	H	-0.94627200	-4.87879900	0.74481000
O	1.09343300	-2.67005700	0.97741500	C	-3.76133000	1.13862700	-1.18610000
C	1.22581200	-3.29987800	2.26448500	H	-3.40786200	1.89077100	-1.88588600
H	1.75082200	-2.63917500	2.95982300	C	-4.72819200	-0.87226900	0.62190000
H	1.80279800	-4.20744300	2.08362100	H	-5.09775900	-1.63384600	1.30321300
H	0.23826600	-3.54078600	2.66643800	C	-5.51062100	-0.38993500	-0.39752200
H	-1.65783600	0.78933700	-2.53565300	C	-5.02823500	0.61322900	-1.30022100
C	-1.44974600	1.66750900	-0.46945700	H	-5.68318400	0.95871300	-2.09545400
C	-0.25470400	1.79027000	0.25830500	H	-6.51875900	-0.77268500	-0.53188700
C	-0.20814200	2.53001000	1.43432600	O	0.98690400	3.42569800	-0.78296900
C	-1.37865200	3.17660600	1.85240800	C	0.97589500	4.67166300	-0.08786800
C	-2.56749900	3.05685100	1.12134700	H	1.32632900	5.42407100	-0.79841200
C	-2.62150200	2.27933000	-0.04453500	H	-0.03991400	4.92497100	0.24793600
H	-3.55055400	2.16255800	-0.59451200	H	1.64693600	4.65233300	0.78231400
H	-3.46207700	3.56925400	1.46590800	1b3			
H	-1.36508600	3.77458300	2.75982000	C	3.39000900	-0.38110900	1.07907000
H	0.70189200	2.60832700	2.02322400	C	2.33674700	-0.08479800	0.01555900
TSIIb2				C	2.30745600	-1.05714100	-0.91207700
C	-1.61322900	0.97943200	0.25984100	C	3.30183700	-2.15606300	-0.62646800
C	-2.92512500	0.66601400	-0.14243800	C	4.22444000	-1.52298100	0.44830600
C	-3.40992200	-0.34619900	0.76579900	C	1.47630900	1.10554700	0.08681000
C	-2.37526900	-0.58559900	1.64945100	O	2.12683300	2.30959400	0.32379900
O	-1.31379900	0.19991100	1.34816400	C	3.16649400	2.65867200	-0.59191200
H	-2.25114500	-1.24077700	2.49862100	C	0.12040400	1.18232500	0.05021900
C	-0.72848700	1.94964400	-0.25887700	C	-0.89732400	0.17142900	0.03220700
C	0.58140000	2.32586000	-0.01634600	C	-2.28777100	0.30488400	0.02005700
C	1.62751900	1.77801500	0.77964700	C	-2.83542500	-1.03766300	0.03087500
C	1.70094600	0.57962700	1.49095400	C	-1.75007900	-1.88595900	0.04870800
H	2.52161000	0.50036200	2.19965800	O	-0.59782600	-1.16076600	0.04880300
H	0.79886100	0.05283900	1.76371100	C	-3.16366800	1.42768800	0.00564200
H	2.55787100	2.33537100	0.69772600	C	-4.51890700	1.20555000	-0.00024300
H	-1.19571700	2.54578700	-1.03959400	C	-5.06152200	-0.12504300	0.00794500
C	-0.93238000	-4.07526800	0.00699200	C	-4.25165600	-1.23129900	0.02348000
O	0.26016200	-3.32586100	0.28724400	H	-5.20404600	2.04918400	-0.01135100

H	-6.14167600	-0.24745900	0.00249900	H	-3.20885600	2.03297600	-0.79018900
H	-4.67114800	-2.23396900	0.03069000	H	-3.01599600	4.40384300	-0.09505300
H	-2.76767700	2.43990700	-0.00110200	H	-0.83131800	5.37842800	0.55314300
H	-1.63162400	-2.95854800	0.06250900	H	1.23463800	4.01582900	0.49449800
H	-0.28016600	2.19249400	0.09791000	C	-1.20022800	-0.71200300	1.82493200
H	1.61718300	-1.08663700	-1.75022400	O	-0.07548700	-0.25693800	1.94190300
H	3.85137900	-2.48059500	-1.51955200	O	-1.89832500	-1.22611400	2.86035200
H	2.78185900	-3.04886500	-0.24272500	C	-1.22502200	-1.21230200	4.13220300
H	4.57573600	-2.24916000	1.18878500	H	-0.97990400	-0.18751800	4.42451100
H	5.11148800	-1.10082500	-0.04012700	H	-0.30696200	-1.80483600	4.08683100
H	3.99493700	0.49320800	1.34531900	H	-1.93431500	-1.65463200	4.83245700
H	2.88980200	-0.70315300	2.00529000	C	-3.06617600	-1.22120200	0.14466700
H	3.58286500	3.60093900	-0.22873200	C	-4.03065400	-1.52387100	-0.85615100
H	3.95592300	1.89823300	-0.62701700	O	-3.99290500	-2.50436900	-1.59008100
H	2.75905400	2.80038100	-1.60206000	O	-5.03374800	-0.59825200	-0.89346000
TS2b3				C	-6.08318700	-0.86774700	-1.83860200
C	-0.83888200	0.30093500	-0.88919400	H	-5.68935100	-0.89051300	-2.85885200
C	-1.97498200	-0.78241900	0.58063500	H	-6.79321300	-0.04820800	-1.71927400
C	-1.07058200	1.67162100	-0.58456200	H	-6.56150200	-1.82622800	-1.61761600
C	-2.24349900	2.45965700	-0.53314400	3b3			
C	-2.12835600	3.777759000	-0.13534800	C	-1.75634000	-0.78979800	0.46640600
C	-0.87257500	4.34070300	0.23360900	C	-1.13666800	0.24182600	-0.50740900
C	0.28175800	3.58510000	0.19796700	C	-1.31100900	1.68362100	-0.16030100
C	0.19000900	2.23854600	-0.22630700	C	-2.47799400	2.41509500	0.05482800
C	1.15731600	1.21715500	-0.40137200	C	-2.35144200	3.76351900	0.39057600
O	0.54380400	0.11235000	-0.85219900	C	-1.08626200	4.37260600	0.52239900
C	2.56491700	1.30417700	-0.20086000	C	0.07757300	3.64143100	0.31658300
C	3.54693900	0.34926800	-0.30400000	C	-0.04971500	2.28786500	-0.03462600
C	3.40165300	-1.10238700	-0.43726400	C	0.93397300	1.26073400	-0.29497600
C	4.32820100	-1.94491100	-1.30556900	C	2.33260800	1.43431400	-0.27592800
C	4.00872400	-3.39537900	-0.86073400	C	3.33867700	0.49249200	-0.45773000
C	2.61862600	-3.32099800	-0.17647900	C	3.24245500	-0.95734200	-0.38155700
C	2.48463000	-1.86483700	0.18609400	C	2.40404400	-1.63857300	0.42807000
H	1.71417500	-1.48484800	0.84864600	C	2.55812100	-3.12473100	0.27420500
H	2.53556300	-3.98438200	0.69380400	C	3.87681600	-3.27864400	-0.52819400
H	1.80501000	-3.61064600	-0.86078000	C	4.12688000	-1.89773400	-1.19066800
H	4.75597400	-3.72324500	-0.12809400	H	3.81342900	-1.88811900	-2.24514200
H	4.03429500	-4.10663200	-1.69265900	H	5.18225800	-1.60905400	-1.17277300
H	5.38364100	-1.68678800	-1.17460600	H	4.69804800	-3.50732700	0.16111300
H	4.09224300	-1.78287100	-2.36873300	H	3.83146700	-4.09035100	-1.26049800
O	4.86867100	0.68418300	-0.27286300	H	2.57569900	-3.64831400	1.23804300
C	5.26970400	2.04893700	-0.20874000	H	1.68653300	-3.52091000	-0.27068900
H	4.97085700	2.50496900	0.74333400	H	1.68282000	-1.18490200	1.10060900
H	6.35850000	2.03651600	-0.27881500	O	4.60437200	0.87694400	-0.71654900
H	4.84907400	2.62206700	-1.04425100	C	4.94069700	2.25427200	-0.91028200
H	2.87720600	2.31706500	0.02742000	H	4.83004000	2.81711000	0.02325000
H	-1.29585000	-0.28101600	-1.67563500	H	5.98796900	2.25310600	-1.21369800

H	4.32126100	2.69828400	-1.69702800	C	-1.11111100	3.47425600	0.95283800
H	2.63159300	2.46836100	-0.15391300	H	-0.28298000	4.04293300	1.36752800
H	1.05125400	4.10909500	0.43498100	C	-2.42536200	3.79195100	1.29016300
H	-1.02386100	5.42229500	0.79513900	H	-2.62363500	4.61703200	1.96875400
H	-3.24530000	4.35788300	0.56079800	C	-3.49810700	3.05538900	0.75974300
H	-3.45194200	1.94106400	-0.02991700	H	-4.51540100	3.32219800	1.03391300
H	-1.49203600	-0.00325800	-1.51038700	H	-4.10882400	1.40438300	-0.50138800
O	0.34190500	0.12863300	-0.61250100	C	-1.32651800	-0.78126600	-0.48446100
C	-1.16301400	-0.79124600	1.82031400	C	-2.61753400	-1.52076100	-0.39256000
O	-0.21141200	-0.08330000	2.15474700	O	-2.84997400	-2.47808300	0.31667600
O	-1.74698100	-1.64794500	2.68014600	O	-3.55720500	-1.00950700	-1.25053000
C	-1.20391300	-1.67518000	4.00571200	C	-4.82041100	-1.69681900	-1.26509100
H	-1.27862700	-0.69029500	4.47661600	H	-5.43082500	-1.16999800	-2.00045900
H	-0.15384600	-1.98401500	3.99203500	H	-5.28697500	-1.66158600	-0.27655300
H	-1.80807200	-2.40512600	4.54663400	H	-4.68191100	-2.74114000	-1.55741900
C	-2.79378200	-1.55492200	0.10650600	C	-0.00860000	-2.38283900	0.91101500
C	-3.39039100	-1.63345100	-1.18390600	O	0.36355200	-3.47744500	0.49128700
O	-3.04009700	-2.38329000	-2.09871700	O	-0.14016900	-2.11575200	2.24316000
O	-4.50053500	-0.81679400	-1.30571100	C	0.06015500	-3.23415300	3.11862800
C	-5.27430900	-1.00590500	-2.49664300	H	-0.65983600	-4.02784800	2.89872300
H	-4.68667800	-0.78044600	-3.39250500	H	-0.09818200	-2.84365600	4.12561300
H	-6.11504700	-0.31400700	-2.41034000	H	1.07480100	-3.63214500	3.01829500
H	-5.63699500	-2.03654500	-2.56391900	O	3.96414200	1.83787900	0.27978900
TS4b3				C	4.06604900	3.20060200	0.68274300
C	0.32549800	1.83921100	-0.48846700	H	3.52600600	3.38257400	1.62005400
C	-0.21320400	-1.21152200	0.10174000	H	5.13134800	3.37178400	0.84653100
C	2.06110300	-0.87520600	-1.23090600	H	3.69845800	3.87575600	-0.09877300
O	-0.02062400	1.01172700	-1.49455600	5b3			
C	1.62063500	2.09169000	-0.08871000	C	-3.76859200	2.87362300	1.01602300
H	1.69589600	2.95382900	0.56446000	C	-4.44238000	1.91044200	0.25432900
C	2.80246700	1.31682000	-0.21148200	C	-3.73502200	1.03084600	-0.57821400
C	2.96544800	-0.03366400	-0.59650400	C	-2.35239800	1.15192900	-0.64410000
C	4.23181000	-0.80678100	-0.23358800	C	-1.67806600	2.13351400	0.10302500
C	4.12012000	-2.11356500	-1.05318900	C	-2.37633800	2.99299900	0.95101400
C	2.61393300	-2.26311300	-1.37812500	C	-1.28318700	0.36072800	-1.39525400
H	2.42287800	-2.66755500	-2.38052500	O	-0.19041700	1.29925400	-1.41878500
H	2.09856200	-2.94125700	-0.68163000	C	-0.25369000	1.98869500	-0.21696300
H	4.52211800	-2.97948000	-0.51746400	C	0.84959200	2.21453300	0.51930700
H	4.69163300	-2.01189600	-1.98431500	C	2.18645100	1.67165900	0.28868400
H	4.24818200	-1.00572500	0.84853900	C	2.56461500	0.51384900	-0.30498100
H	5.14311700	-0.24440600	-0.45826400	C	1.71549200	-0.54987600	-1.02856200
H	1.21945000	-0.52965800	-1.79935700	C	2.75610000	-1.63427700	-1.44224200
H	-1.82855400	0.42478100	-2.27292600	C	4.05995600	-0.84896400	-1.61979500
C	-1.37834800	0.55790300	-1.28879400	C	4.03018600	0.13275900	-0.43681100
C	-1.96668100	1.67514700	-0.46218900	C	-0.81089700	-0.87086700	-0.59507100
C	-3.27890100	1.98267900	-0.11007800	C	0.48346500	-1.16834300	-0.34939300
C	-0.89462800	2.41913000	0.05895100	C	-1.89365600	-1.72228400	-0.00578600

O	-1.94512900	-2.13079200	1.13535100	H	0.33084200	-3.70838200	-0.92053100
O	-2.84267800	-1.98775600	-0.93589600	C	2.78821700	1.95816200	0.95193200
C	-3.93472300	-2.81764900	-0.49251200	O	2.94907700	2.65681800	1.93220700
C	0.78614300	-2.34420200	0.55296300	O	3.62235200	1.98458700	-0.11823800
O	0.60395100	-3.50811400	0.25959200	C	4.73794500	2.88801800	-0.00476600
O	1.35521000	-1.93160200	1.69841500	H	4.38528000	3.91479300	0.12342000
C	1.67708400	-2.96596200	2.64991700	H	5.36433400	2.61312500	0.84798300
O	3.19988400	2.39925300	0.91873300	H	5.29031700	2.78288600	-0.93926100
C	3.36649300	3.73891100	0.45803200	C	-0.13431900	-0.34450500	2.20117600
H	-4.33519700	3.54412400	1.65683300	O	0.34054400	-1.50586200	2.73743100
H	-5.52578200	1.84354500	0.30853900	O	-1.29265500	0.03581100	2.34059500
H	-4.25944500	0.27720600	-1.15745800	C	-0.58702400	-2.23069100	3.55847400
H	-1.85840500	3.75072400	1.53303600	H	-0.04046400	-3.11181300	3.89791100
H	-1.54587900	0.11566800	-2.42808400	H	-0.90261100	-1.62339300	4.41212200
H	0.73098400	2.80412900	1.42593700	H	-1.47039000	-2.52481200	2.98423500
H	1.35676700	-0.08663300	-1.94985300	C	-1.59266600	-1.26239600	-0.86878200
H	2.43447600	-2.17791800	-2.33700900	H	-1.65348900	-2.34206900	-0.78966100
H	2.89467000	-2.37746600	-0.64850700	C	-2.74672600	-0.55111500	-0.65783200
H	4.94557600	-1.49431500	-1.62165500	O	-3.91042100	-1.16875800	-0.31113900
H	4.04896100	-0.29626800	-2.56924300	C	-3.94070000	-2.56759700	-0.05352100
H	4.67683200	1.00448300	-0.56905500	H	-3.71509500	-3.14415600	-0.95971900
H	4.37305500	-0.37397300	0.47925500	H	-4.96080300	-2.78296900	0.26854500
H	-4.46682800	-2.33570500	0.33223800	H	-3.23608600	-2.83360000	0.74387200
H	-3.55817400	-3.78920600	-0.16326700	C	-2.96246100	0.89772600	-0.74358300
H	-4.58337300	-2.92977400	-1.36191200	C	-3.75905300	1.65710300	0.30914900
H	2.12220000	-2.44560100	3.49812200	H	-3.16193100	1.72347800	1.22866800
H	2.38423400	-3.67792400	2.21561700	H	-4.69545800	1.15472000	0.57165900
H	0.76677200	-3.49114200	2.94986500	C	-3.98957100	3.04111600	-0.34980500
H	4.15580100	4.17863700	1.07264300	H	-3.93519800	3.86320000	0.37121200
H	3.66955600	3.75508200	-0.59847700	H	-4.98767000	3.06982600	-0.80374200
H	2.44683700	4.32801000	0.57149100	C	-2.91710400	3.15363400	-1.46547400
TS6b3				H	-2.03959000	3.73174800	-1.13385100
C	0.86933400	0.35924200	1.49234600	H	-3.29179800	3.65303300	-2.36836700
C	-0.25055600	-0.82529700	-1.07217600	C	-2.52116300	1.71928200	-1.71114400
C	1.68921300	0.99554900	0.80079200	H	-1.91851600	1.41072700	-2.55872600
C	1.46277300	0.58318400	-1.29021600	7b3			
H	1.82571300	1.50426500	-1.72000700	C	1.35649300	0.96545400	-0.37789600
O	0.08852500	0.46111200	-1.30048200	C	1.67860300	0.02290500	-1.55794700
C	0.92452100	-1.62102700	-1.16603400	C	0.40016100	0.34035700	0.32817200
C	2.01219600	-0.72141700	-1.37988200	C	0.12803900	-1.01129000	-0.42144900
C	3.32665800	-1.21536500	-1.53381300	O	0.37847800	-0.55491500	-1.79222300
H	4.15889800	-0.53405100	-1.68219400	C	2.40746600	-1.18304300	-0.95560600
C	3.52111900	-2.58242900	-1.48614000	C	1.41857300	-1.83853500	-0.20612000
H	4.52141700	-2.98740000	-1.61648200	C	1.70740900	-2.97767300	0.52156500
C	2.43882200	-3.48059800	-1.26399800	H	0.95097100	-3.48467900	1.11507400
H	2.63726300	-4.54828000	-1.22571300	C	3.02651200	-3.47309300	0.47234100
C	1.14982200	-3.01566900	-1.09576500	H	3.27986900	-4.37320600	1.02650000

C	4.00767500	-2.82456000	-0.27710400	C	1.50213600	-0.35746900	-1.84265000
H	5.01754800	-3.22582900	-0.30329300	H	1.99526100	-0.10274400	-2.77874500
C	3.70608700	-1.65405100	-1.00343600	O	0.21983800	-0.97531800	-2.07713900
H	4.47494700	-1.14976300	-1.58391100	C	-0.05129700	0.38500300	-0.22252000
C	2.10058200	2.18053900	-0.00387500	C	1.11977700	0.79042600	-0.90258400
O	1.95670100	2.81264400	1.02506700	C	-0.20505700	0.68248500	1.26025200
O	2.99742100	2.51289800	-0.96713800	C	1.99081500	1.92000600	-0.69704600
C	3.79434900	3.68187900	-0.70066300	O	0.95357900	0.46062800	1.90820100
H	3.15336200	4.56057500	-0.59032700	O	1.46227600	2.87556500	0.12540300
H	4.37739800	3.54329200	0.21376200	O	-1.22749100	1.00743100	1.82930900
H	4.44978800	3.78753500	-1.56558600	O	3.09664400	2.03891800	-1.21833800
C	-0.19848200	0.71867900	1.63749100	C	0.92518900	0.64968600	3.33493600
O	-0.98851500	1.62216400	1.80771500	H	0.19086900	-0.01745500	3.79450000
O	0.22588300	-0.11624000	2.60540200	H	0.67214400	1.68641000	3.57302700
C	-0.29659300	0.13411800	3.92682900	H	1.93269200	0.40846900	3.67446800
H	-0.02949500	1.14294700	4.25097600	C	2.30606400	4.00891100	0.37941900
H	-1.38404600	0.02259900	3.93058100	H	3.22922300	3.69711300	0.87694200
H	0.17109100	-0.61549300	4.56523400	H	1.72342300	4.66515100	1.02783400
C	-1.15516500	-1.74569700	-0.24363600	H	2.55925200	4.51790400	-0.55506000
H	-1.06388100	-2.81357100	-0.06506000	H	-1.28140700	0.63447800	-2.05890200
C	-2.41601400	-1.26302600	-0.28042500	H	-1.43544000	-2.89654500	-0.28494000
C	-4.46094600	-2.33602600	-0.89406800	C	1.29448500	-2.86383900	0.79595600
O	-3.40855500	-2.16779500	0.05948300	H	0.47484600	-3.25601200	1.39377100
H	-4.06932200	-2.77304100	-1.82201500	C	3.45817000	-1.82163300	-0.72328800
H	-5.17361500	-3.02517100	-0.43594700	H	4.28880200	-1.411178900	-1.29169700
H	-4.96179100	-1.38881100	-1.12524100	C	2.60760300	-3.33001900	0.99564400
C	-2.86499300	0.11246600	-0.55110800	H	2.79576700	-4.10019200	1.73950800
C	-3.89217800	0.81968800	0.32755300	C	3.67107100	-2.81450500	0.25064200
H	-3.42582200	1.07492300	1.28866000	H	4.67724100	-3.18876100	0.42224200
H	-4.77098300	0.20507200	0.55343800	O	-3.85070500	-1.70127100	-0.03896400
C	-4.24069200	2.09064300	-0.48669300	C	-3.90438000	-3.10125700	0.21072400
H	-4.42843300	2.95926400	0.15245800	H	-4.94919400	-3.32180400	0.43509400
H	-5.14943900	1.91364200	-1.07610300	H	-3.58860600	-3.67269400	-0.67129800
C	-3.03981900	2.29979100	-1.44499900	H	-3.27676100	-3.37252600	1.06943300
H	-3.33820900	2.68967100	-2.42676800	C	-3.74601700	1.18929100	0.09044200
H	-2.31201600	3.01455700	-1.03029500	H	-4.65465600	1.12064400	-0.52972000
C	-2.41515400	0.92947800	-1.52117900	H	-4.04221500	0.89735500	1.10442400
H	-1.65524100	0.65609100	-2.24519100	C	-1.94172600	2.49672700	-0.99271300
H	2.08453200	0.47532400	-2.45986600	C	-3.11247400	2.60358400	0.02155100
TS8b3				H	-2.23920500	2.86762400	-1.98359300
C	-1.46549900	-1.82422500	-0.44028500	H	-1.06650200	3.07907000	-0.68819200
C	-2.64803400	-1.13958600	-0.35645400	H	-3.84143200	3.36519300	-0.27509100
C	-2.69537300	0.28682500	-0.48960100	H	-2.73030400	2.87488500	1.00817700
C	-1.63768700	1.00280000	-1.10345000	9b3			
C	-0.15947200	-1.16121500	-0.66719200	C	-1.62538900	-1.72088800	-0.52553800
C	1.08889900	-1.89769300	-0.17431300	C	-2.74827500	-0.95049300	-0.28890300
C	2.15831900	-1.39120400	-0.93246600	C	-2.67817600	0.45141400	-0.25718700

C	-1.40854400	1.17995700	-0.61152600	TS10b3				
C	-0.28788800	-1.10990400	-0.69829500	C	0.14441000	-0.66226500	-0.11321300	
C	0.91841000	-1.93250600	-0.25398400	C	0.13341500	1.31766700	-0.61183900	
C	2.00827800	-1.45422500	-0.99564300	C	1.38256500	-1.04222700	-1.01773800	
C	1.41290000	-0.35241300	-1.86192000	C	2.63006300	-0.24668500	-0.79069100	
H	1.92076700	-0.09468200	-2.78930000	C	2.62556100	1.11398600	-0.53231400	
O	0.08292200	-0.86053400	-2.10028200	C	1.43037500	1.82548600	-0.31763000	
C	-0.12498700	0.41014700	-0.14247300	C	3.84260200	-1.13260300	-0.79470900	
C	1.11779600	0.79027100	-0.90957100	C	3.29144500	-2.53316000	-0.44021600	
C	0.01785800	0.44169400	1.38058600	C	1.82756500	-2.53968600	-0.93769900	
C	1.98943900	1.93476700	-0.79321700	H	1.17389400	-3.12950600	-0.28953600	
O	1.30050900	0.32823600	1.77438400	H	1.76299300	-2.97925000	-1.94103100	
O	1.54694100	2.87390300	0.08500500	H	3.31646300	-2.67025000	0.64460900	
O	-0.91069700	0.52131300	2.15982500	H	3.88626400	-3.33623400	-0.88907400	
O	3.03171300	2.05828200	-1.43329000	H	4.62588500	-0.78055600	-0.11479200	
C	1.52733500	0.29697200	3.19541700	H	4.28986100	-1.13544100	-1.80361300	
H	1.01289200	-0.55709900	3.64372900	O	3.86147600	1.68525900	-0.33511100	
H	1.16705300	1.22043400	3.65671000	C	3.94244500	3.07338700	-0.03972800	
H	2.60702200	0.20081600	3.31118500	H	3.56276400	3.29667700	0.96624600	
C	2.38867700	4.02806100	0.23787600	H	3.39365300	3.67050900	-0.77967500	
H	3.37341200	3.73633800	0.61436000	H	5.00451600	3.32257700	-0.08262400	
H	1.87547600	4.66693800	0.95771000	H	1.02463800	-0.83514700	-2.02723300	
H	2.51000800	4.54468600	-0.71854800	H	1.46176700	2.73765600	0.27066600	
H	-1.67611100	-2.80131900	-0.58764300	O	-0.23409800	0.91924000	-1.92230500	
C	1.07701500	-2.94718400	0.67710300	C	-1.49853300	0.27774800	-1.66102200	
H	0.23727000	-3.31735800	1.26044200	C	-2.17442200	1.29341400	-0.75286500	
C	3.28707100	-1.95967400	-0.81312200	C	-1.11451800	1.89910700	-0.05593000	
H	4.13516000	-1.57319400	-1.37234300	C	-1.36056800	2.83268500	0.94581200	
C	2.36272100	-3.49024500	0.84641100	C	-2.69135000	3.17842800	1.21193000	
H	2.51343200	-4.30140100	1.55440000	C	-3.74495300	2.57699400	0.51092500	
C	3.45050600	-3.00230900	0.11450500	C	-3.49738600	1.60645300	-0.46995800	
H	4.43486800	-3.43976400	0.26099800	H	-1.98467000	0.01920400	-2.60038300	
O	-3.99432400	-1.46710300	-0.04332400	H	-0.55169300	3.28707900	1.51209200	
C	-4.15465200	-2.87908000	-0.03056600	H	-2.91010500	3.91885200	1.97684500	
H	-5.20934700	-3.05546300	0.18877300	H	-4.76940000	2.86267800	0.73563300	
H	-3.90594700	-3.31783100	-1.00569700	H	-4.31557600	1.11729200	-0.98979000	
H	-3.53592900	-3.34328800	0.74865500	C	-1.14829900	-0.86037900	-0.68549400	
H	-1.32985100	1.20684600	-1.70865300	C	-2.12708900	-1.82347000	-0.21430600	
C	-3.76390200	1.40994800	0.13152100	O	-3.35404700	-1.62813800	-0.78697200	
C	-1.65660000	2.62301000	-0.10786000	O	-1.89498700	-2.76167600	0.53738300	
C	-3.18380900	2.79116700	-0.25320000	C	-4.36463300	-2.58054300	-0.42183700	
H	-1.08903100	3.36601200	-0.67516600	H	-4.54600000	-2.55080600	0.65622600	
H	-1.37111500	2.71532300	0.94449400	H	-4.06014700	-3.59205100	-0.70600800	
H	-3.43766000	3.02160400	-1.29672300	H	-5.25887000	-2.28076400	-0.97053400	
H	-3.57796400	3.60438600	0.36591200	C	0.24925300	-0.81645200	1.37359800	
H	-3.94264600	1.34781900	1.21752000	O	-0.60172500	-0.43028100	2.15260800	
H	-4.72295600	1.18652900	-0.35183300	O	1.43212500	-1.33526000	1.78250400	

C	1.59984500	-1.44305700	3.20682200	H	2.58761200	-1.88343100	3.35032700
H	1.54565100	-0.45582700	3.67398800	H	0.82378600	-2.08536200	3.63142900