

## Supporting Information

### On the Mechanism of Acceptorless Dehydrogenation of the 1,2,3,4-Tetrahydroquinoline catalyzed by <sup>t</sup>BuOK: A Computational Study

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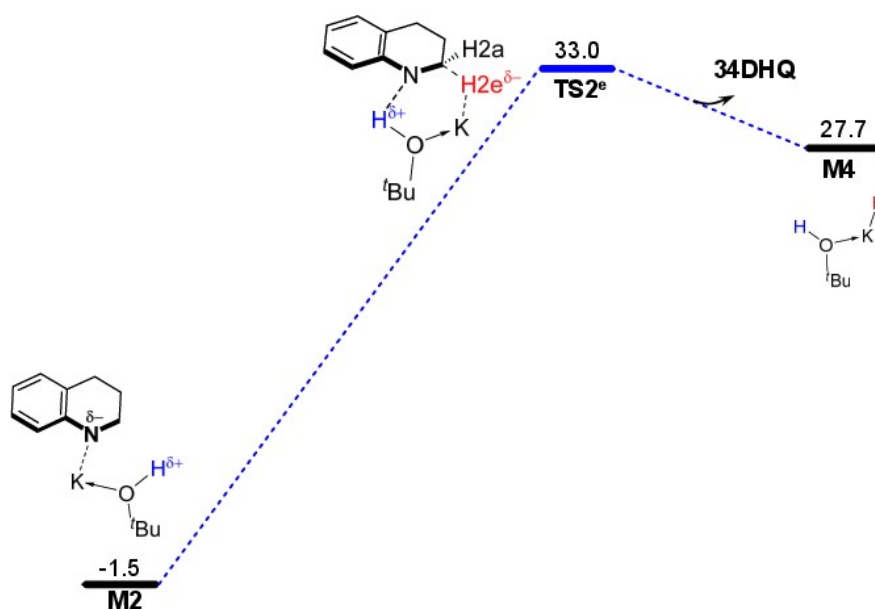
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### Contents

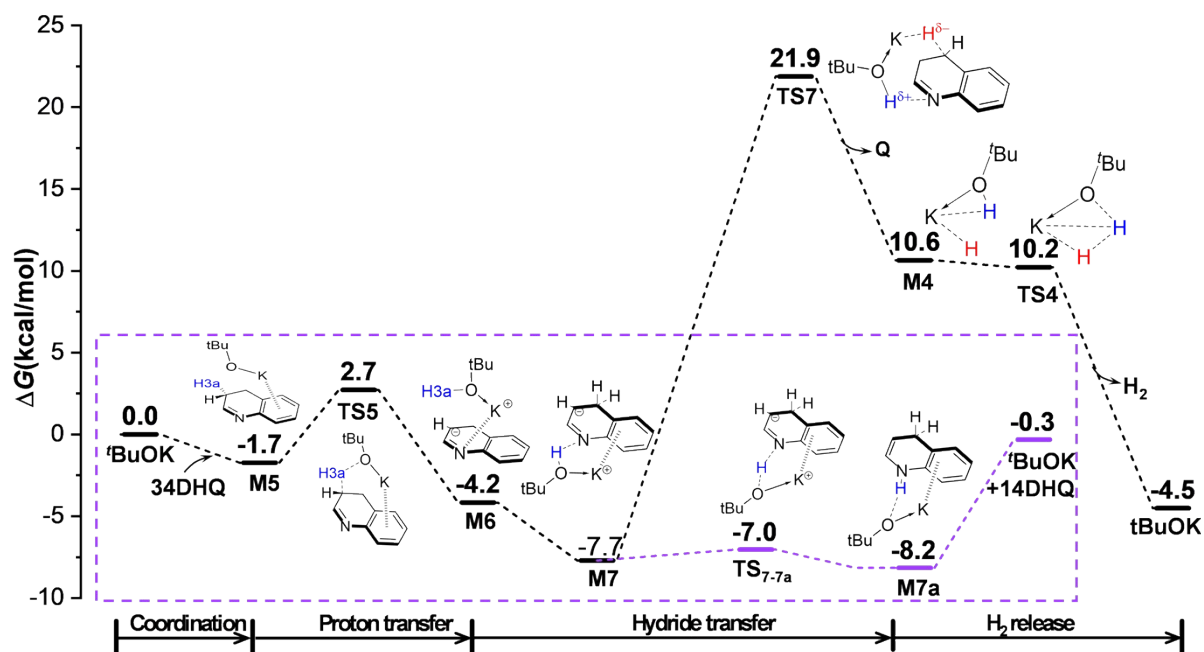
1. Supplementary data for the dehydrogenation of <b>THQ</b> catalyzed by <sup>t</sup> BuOK .....	S2
2. Mechanism details for the tautomerization between <b>34DHQ</b> and <b>14DHQ</b> .....	S3
3. Relative free energy profiles for the dehydrogenation of THQ catalyzed by <sup>t</sup> BuO <sup>-</sup> .....	S4
4. Supplementary data for the H <sub>2</sub> elimination process catalyzed by <sup>t</sup> BuOLi.....	S5
5. ETS-NOCV analysis.....	S6
6. Tables for the absolute energies of all the structures involved in this study .....	S7
7. Cartesian coordinates of all the optimized structures .....	S10

## 1. Supplementary data for the dehydrogenation of THQ catalyzed by <sup>t</sup>BuOK



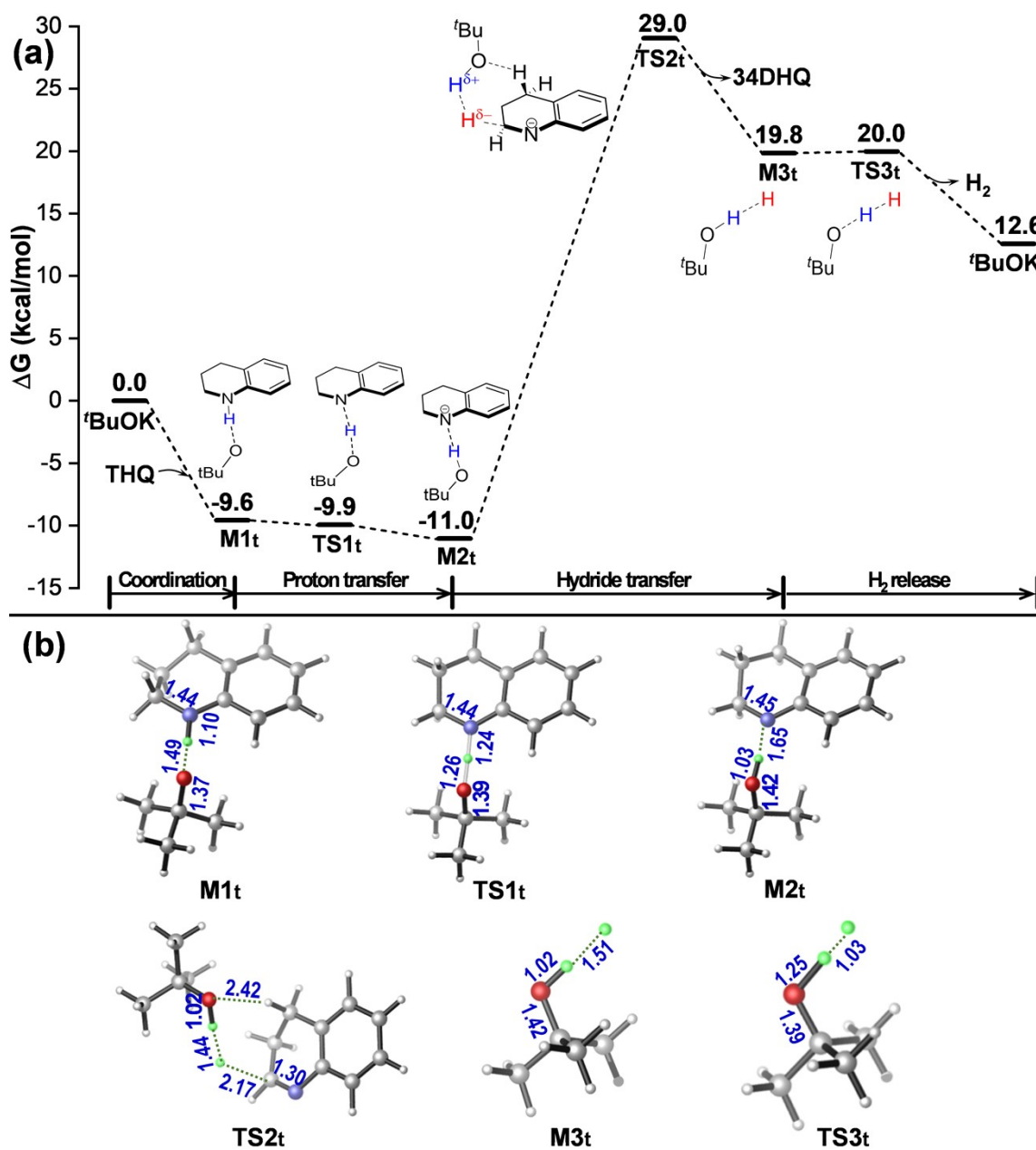
**Figure S1.** Relative free energy profile for the hydride transfer pathway from the equatorial of C2(sp<sup>3</sup>)-H2e bond catalyzed by <sup>t</sup>BuOK in *o*-xylene. The energies are given with respect to the intermediate separated <sup>t</sup>BuOK and THQ as shown in Fig. 1 of the main article.

## 2. Mechanism details for the tautomerization between 34DHQ and 14DHQ.



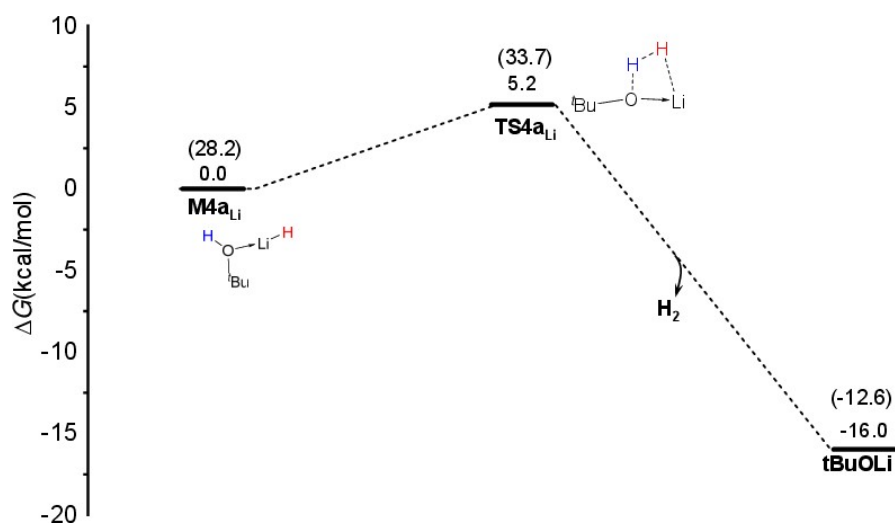
**Figure S2.** Mechanism details for the tautomerization between 34DHQ and 14DHQ via a reversible proton transfer pathway (in square brackets). Energies are in kcal/mol.

### 3. Relative free energy profiles for the dehydrogenation of THQ catalyzed by $t\text{BuO}^-$ .



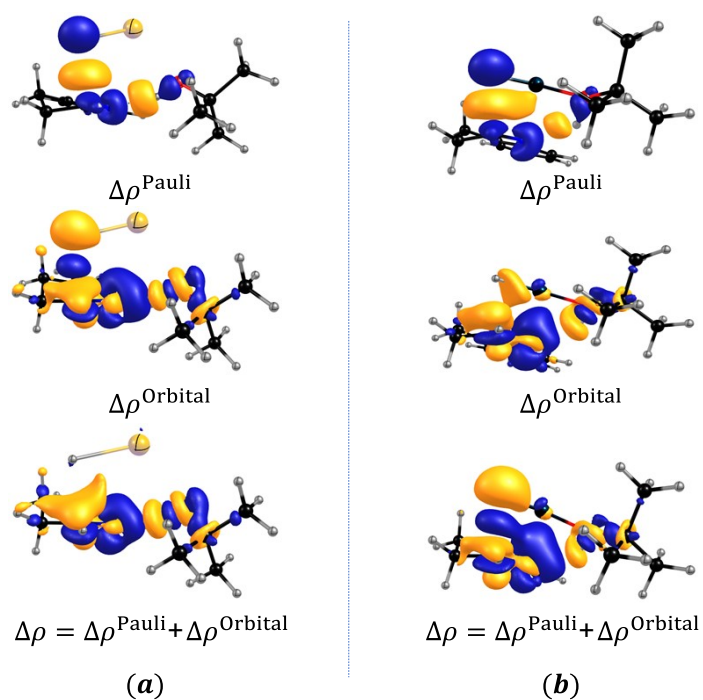
**Figure S3.** (a) Relative free energy profiles for the dehydrogenation reaction of THQ catalyzed by a  $t\text{BuO}^-$  anion in *o*-xylene. (b) Geometrical information. Energies are in kcal/mol, bond distances are in angstroms.

#### 4. Supplementary data for the H<sub>2</sub> elimination process catalyzed by <sup>t</sup>BuOLi



**Figure S4.** Relative free energy profile for the hydrogen release process from the isolated dihydride species LiO<sup>t</sup>Bu(H)(H) in *o*-xylene. Shown in parentheses are the free energies plus the **34DHQ** with respect to the separated <sup>t</sup>BuOLi and **THQ** as shown in Fig. 4 of the main article.

## 5. ETS-NOCV analysis



**Figure S5.** ETS-NOCV analysis on the transition states of hydride transfer along the first dehydrogenation of THQ catalyzed by **<sup>t</sup>BuOK (a)** and **<sup>t</sup>BuOLi (b)**. The blue/yellow contours correspond to regions the increased/lowered of election density (i.e., acceptor/donor moieties), the isosurface value was set as 0.002 au.

## 6. Tables for the absolute energies of all the structures involved in this study.

**Table S1.** The absolute electronic energies ( $E+ZPE$ , Hartree), the thermal enthalpies ( $H$ , Hartree) and free energies ( $G$ , Hartree) with zero-point correction at 298.15 K in *o*-xylene, as well as the imaginary frequencies ( $I.F.$ ,  $\text{cm}^{-1}$ ), obtained at B3LYP-D3/def2-TZVP level of theory.

Species	$E+ZPE$	$H$	$G$	$I.F.$
Hydrogen	-1.169055	-1.165750	-1.180547	
THQ	-404.335787	-404.327022	-404.368081	
<sup>t</sup> BuOK	-833.029703	-833.020562	-833.063045	
<sup>t</sup> BuOLi	-240.631901	-240.623233	-240.662985	
34DHQ	-403.135700	-403.127472	-403.167502	
14DHQ	-403.135817	-403.127292	-403.168010	
12DHQ	-403.131831	-403.123424	-403.163771	
Q	-401.963029	-401.955444	-401.994141	
THNap	-388.276977	-388.268076	-388.309880	
DHNap	-387.248205	-387.070106	-387.110404	
M1	-1237.384933	-1237.371143	-1237.437724	
TS1	-1237.370021	-1237.369077	-1237.434839	-787.0016
M2	-1237.689355	-1237.366174	-1237.433498	
TS2	-1237.335016	-1237.316107	-1237.383093	-379.8821
TS2 <sup>a</sup>	-1237.330910	-1237.312163	-1237.378510	-482.7764
M3	-1237.378639	-1237.359696	-1237.426314	
TS3	-1237.333984	-1237.315313	-1237.381950	-502.1387
M4	-834.184965	-834.174728	-834.219455	
TS4	-834.186272	-834.176375	-834.220126	-1064.6668
M5	-1236.184890	-1236.166400	-1236.233312	
TS5	-1236.178663	-1236.160755	-1236.226213	-1291.3443
M6	-1236.190397	-1236.172003	-1236.237193	
TS6	-1236.147202	-1236.129127	-1236.193922	-660.5151

<b>M7</b>	-1236.194362	-1236.175911	-1236.242839	
<b>TS7-7a</b>	-1236.194688	-1236.176683	-1236.241772	-965.6717
<b>M7a</b>	-1236.194169	-1236.175607	-1236.243557	
<b>TS7</b>	-1236.148816	-1236.130603	-1236.195684	-748.7849
<b>M8</b>	-1236.177580	-1236.157489	-1236.227281	
<b>M9</b>	-1236.188421	-1236.170132	-1236.235797	
<b>TS8</b>	-1236.187747	-1236.169699	-1236.234602	-934.4584
<b>M10</b>	-1236.186099	-1236.167582	-1236.234484	
<b>TS9</b>	-1236.151231	-1236.133030	-1236.198476	-657.7448
<b>M11</b>	-1236.179953	-1236.161322	-1236.227169	
<b>TS10</b>	-1236.149166	-1236.130952	-1236.197038	-829.9286
<b>M1<sub>Nap</sub></b>	-1221.325936	-1221.306767	-1221.375542	
<b>TS1<sub>Nap</sub></b>	-1221.304171	-1221.285615	-1221.351379	-1232.5244
<b>M2<sub>Nap</sub></b>	-1221.303705	-1221.284714	-1221.351171	
<b>TS2<sub>Nap</sub></b>	-1221.258555	-1221.239420	-1221.305998	-729.5667
<b>TS3<sub>Nap</sub></b>	-1221.259113	-1221.240367	-1221.306730	-795.4914
<b>M3<sub>Nap</sub></b>	-1221.293098	-1221.273098	-1221.341844	
<b>M1<sub>t</sub></b>	-637.472814	-637.456185	-637.516979	
<b>TS1<sub>t</sub></b>	-637.474763	-637.458594	-637.517558	-1028.3583
<b>M2<sub>t</sub></b>	-637.475145	-637.458484	-637.519313	
<b>TS2<sub>t</sub></b>	-637.412550	-637.396280	-637.455439	-320.5911
<b>M3<sub>t</sub></b>	-234.273122	-234.264844	-234.302616	
<b>TS3<sub>t</sub></b>	-234.273148	-234.265154	-234.302396	-1187.7696
<b>M1<sub>Li</sub></b>	-644.989456	-644.971254	-645.037689	
<b>TS1<sub>Li</sub></b>	-644.977997	-644.960525	-645.024128	-867.2042
<b>M2<sub>Li</sub></b>	-644.976443	-644.958630	-645.021878	
<b>TS2<sub>Li</sub></b>	-644.932521	-644.914648	-644.978361	-501.0166
<b>M3<sub>Li</sub></b>	-644.969201	-644.951617	-645.013580	
<b>TS3<sub>Li</sub></b>	-644.918209	-644.900625	-644.962946	-1159.7698
<b>M4<sub>Li</sub></b>	-644.944190	-644.925468	-644.991341	



<b>TS4<sub>Li</sub></b>	-644.944202	-644.925843	-644.990623	-1122.7034
<b>M4a<sub>Li</sub></b>	-241.785448	-241.775037	-241.818062	
<b>TS4a<sub>Li</sub></b>	-241.777776	-241.768242	-241.809829	-1165.0216
<b>M5<sub>Li</sub></b>	-644.952005	-644.931553	-645.001542	

**Table S2.** The absolute electronic energies ( $E_{\text{BS-2}}$ , Hartree) calculated at B3LYP-D3/def2-QZVP level of theory, the thermal correction to Gibbs free energy ( $G_{\text{corr}}$ , Hartree) obtained at B3LYP/def2-TZVP level of theory, as well as the refined single-point free energies ( $G_{\text{BS-2}}$ , Hartree) for the critical rate-determining intermediates and transition states at 298.15 K in *o*-xylene.

<b>Species</b>	$E_{\text{BS-2}}$	$G_{\text{corr}}$	$G_{\text{BS-2}}$
<b>M1</b>	-1237.757317	0.258030	-1237.499287
<b>TS2</b>	-1237.694692	0.250361	-1237.444331
<b>TS3</b>	-1237.693205	0.249960	-1237.443245
<b>M1<sub>Li</sub></b>	-645.349019	0.260231	-645.088788
<b>TS2<sub>Li</sub></b>	-645.282282	0.255275	-645.027007
<b>TS3<sub>Li</sub></b>	-645.264138	0.253232	-645.010906

**7. Cartesian coordinates of all the optimized structures (obtained at the B3LYP-D3/def2-TZVP level of theory).**

<b>Hydrogen</b>				H	2.72126000	0.70753700	-1.32536700
H	0.00000000	0.00000000	0.37232900	H	1.25524800	0.15897800	-2.16138300
H	0.00000000	0.00000000	-0.37232900	H	1.26169800	1.71669300	-1.32629700
<b>THQ</b>				<b><sup>t</sup>BuOLi</b>			
C	1.33960100	-1.37896200	-0.05485600	Li	-1.93510300	-0.00400200	0.00380100
C	0.11467700	-0.69496500	-0.01766900	O	-0.32608500	-0.00267000	0.00081600
C	0.11607900	0.71299300	0.04300500	C	1.05372400	-0.00014800	-0.00053600
C	1.33735000	1.38135800	0.04901300	C	1.57590800	0.76582000	1.22996900
C	2.55009500	0.70280800	0.01163800	C	1.57812400	-1.44798300	0.04649900
C	2.54097600	-0.68865700	-0.03903900	C	1.57409500	0.68502000	-1.27880500
H	1.33564700	-2.46264600	-0.10403100	H	1.20782500	1.79476900	1.20760300
H	1.33166400	2.46582300	0.08638000	H	1.20347500	0.29436800	2.14296800
H	3.48471500	1.24867900	0.01898100	H	2.66887900	0.79144800	1.27628600
H	3.47325600	-1.23980200	-0.06860100	H	1.20626700	-2.00285100	-0.81863200
C	-1.19037500	1.47461900	0.11339500	H	2.67117900	-1.50018400	0.04616000
C	-2.37504500	0.63288100	-0.36434900	H	1.20975600	-1.94397600	0.94804600
C	-2.32512200	-0.74806700	0.27828300	H	2.66704300	0.71140300	-1.32618000
N	-1.07825500	-1.40124300	-0.08810000	H	1.20389100	0.15433700	-2.15962200
H	-1.11502400	2.39248600	-0.47480500	H	1.20291400	1.71204500	-1.32355100
H	-2.33806100	0.51626200	-1.45107300	<b>34DHQ</b>			
H	-3.15219200	-1.36866900	-0.07104000	C	0.49069600	-1.62604900	2.82696400
H	-1.01050900	-2.37486700	0.16417000	C	0.18635300	-0.48931100	2.07855500
H	-1.36872500	1.78863000	1.14810600	C	-1.14258300	-0.23317800	1.69930500
H	-3.31797500	1.12458900	-0.11751100	C	-2.13673600	-1.12555800	2.08141600
H	-2.42442300	-0.64584000	1.36960600	C	-1.83114000	-2.25534000	2.83589200
<b><sup>t</sup>BuOK</b>				C	-0.51492900	-2.50395000	3.21095600
K	-2.58235800	-0.04726800	0.00843900	H	1.52316300	-1.80285400	3.10128500
O	-0.28822500	0.01209600	-0.00084000	H	-3.16312800	-0.93258300	1.78959100
C	1.08554100	0.00609900	-0.00123700	H	-2.61917200	-2.93770900	3.12939500
C	1.62746600	0.76803600	1.22933000	H	-0.27209200	-3.38145000	3.79708100
C	1.61620500	-1.44479400	0.04648200	C	-1.41363300	0.98807600	0.85962000
C	1.62679200	0.68708100	-1.27888700	C	-0.42167800	2.09827100	1.20624000
H	1.26605100	1.79987400	1.20923600	C	0.97255700	1.54066700	1.30563500
H	1.25254300	0.29905400	2.14328400	N	1.25176100	0.36375200	1.70635900
H	2.72192400	0.78677800	1.27615600	H	-2.44142300	1.32854200	0.99252900
H	1.24273000	-1.99891400	-0.81913000	H	-0.67311100	2.54350000	2.17830300
H	2.71025900	-1.50382600	0.04721600	H	-1.30237700	0.72321300	-0.19902500
H	1.24475900	-1.94002600	0.94781800	H	-0.45325200	2.90666000	0.47428600

H	1.80838000	2.18723700	1.04128500
<b>14DHQ</b>			
C	-6.37946400	-3.60435600	3.40303900
C	-5.18689600	-2.90864600	3.62610000
C	-5.19433400	-1.72254300	4.37939600
C	-6.41111000	-1.26266000	4.87375300
C	-7.59961800	-1.95134200	4.65647400
C	-7.57630000	-3.13108400	3.91900500
H	-6.35862200	-4.51804200	2.81912500
H	-6.42287700	-0.34309200	5.44881400
H	-8.53071900	-1.57307600	5.05844100
H	-8.49144400	-3.68161300	3.73896900
C	-3.90279000	-0.97913500	4.66797100
C	-2.78513500	-1.43001900	3.76669900
C	-2.86631100	-2.56452800	3.06908000
N	-3.98848500	-3.38173900	3.09707600
H	-4.04751000	-4.11856500	2.41433100
H	-1.88188400	-0.83789200	3.71168700
H	-4.06968400	0.09808900	4.56374500
H	-2.05907900	-2.92045100	2.44277300
H	-3.62202000	-1.12677400	5.72101500

**12DHQ**

C	-6.37682000	-3.60938200	3.41331400
C	-5.17591600	-2.92394100	3.61881100
C	-5.18640200	-1.72090600	4.36279600
C	-6.39318400	-1.24612100	4.87278200
C	-7.58645100	-1.92791100	4.66021400
C	-7.56747900	-3.11363800	3.93141300
H	-6.37113000	-4.53573900	2.84950600
H	-6.38813100	-0.32630200	5.44698500
H	-8.51543800	-1.54410900	5.06116600
H	-8.48771800	-3.65864600	3.75887000
C	-3.91170500	-1.05178200	4.58876100
C	-2.80626600	-1.42864600	3.94228200
C	-2.84181200	-2.53007900	2.92139700
N	-3.96425400	-3.42648300	3.18157600
H	-4.03114800	-4.20930600	2.54931400
H	-1.86340300	-0.91839000	4.09569400
H	-3.88517500	-0.23104700	5.29707400
H	-2.89413400	-2.08918200	1.90940100
H	-1.91963000	-3.11478000	2.95806000

**Q**

C	1.20469400	-1.40070700	0.00000100
C	-0.02714000	-0.70415600	-0.00000100
C	-0.01439100	0.72279200	0.00000100
C	1.22699800	1.40267900	0.00000500
C	2.40399900	0.69969200	0.00000600
C	2.39100400	-0.71293800	0.00000400
H	1.17676900	-2.48280300	-0.00000100
H	1.23067100	2.48653400	0.00000600
H	3.35078000	1.22504200	0.00000900
H	3.32939900	-1.25343200	0.00000500
C	-1.26156600	1.38778500	0.00000000
C	-2.41480900	0.65068400	-0.00000400
C	-2.32102200	-0.75907900	-0.00000500
N	-1.18667900	-1.41946200	-0.00000400
H	-1.28831200	2.47135800	0.00000100
H	-3.22913000	-1.35488600	-0.00000900
H	-3.38795200	1.12386100	-0.00000500

**THNap**

C	-5.92982600	-3.35414600	2.80038200
C	-4.85946400	-2.68162300	3.38218600
C	-5.09896300	-1.52759200	4.14361100
C	-6.40341900	-1.07239300	4.30985200
C	-7.46921200	-1.74616900	3.71942200
C	-7.23187800	-2.88901300	2.96394400
H	-5.74467800	-4.24973500	2.21755500
H	-6.58759800	-0.18459000	4.90469400
H	-8.48093000	-1.38325300	3.85375500
H	-8.05773200	-3.42011400	2.50648500
C	-3.89894500	-0.85780400	4.75381800
C	-2.99768500	-1.87906700	5.47689300
C	-2.75040700	-3.16643500	4.64605200
C	-3.42946100	-3.12917700	3.26307700
H	-4.20203900	-0.06548200	5.44089600
H	-3.47231300	-2.14441100	6.42378200
H	-3.13751100	-4.03020300	5.19080000
H	-3.36579500	-4.10692200	2.78181000
H	-3.31793200	-0.37587500	3.95854600
H	-2.05001400	-1.39852000	5.72873400
H	-1.67991400	-3.33699700	4.51420100
H	-2.88604400	-2.42727500	2.61940400

**DHNap**

C	-2.06353200	0.39951800	0.64972800	H	-6.56597100	-0.42316700	5.25724600
C	-0.84035500	0.70055200	1.25391400	H	-8.58969700	-0.83735300	3.88989900
C	-0.44621500	2.04700600	1.38162600	H	-8.47966600	-2.48986800	2.03030300
C	-1.29016100	3.04880800	0.91900800	C	-4.08552400	-1.53846200	5.00421200
C	-2.51307700	2.73946300	0.32708400	C	-3.22637700	-2.80477700	5.01770600
C	-2.89814100	1.41087600	0.18885200	C	-2.87710800	-3.20037800	3.58660200
H	-2.36325800	-0.63760100	0.54968800	N	-4.05735400	-3.28213700	2.73378400
H	-0.98707800	4.08540500	1.01654700	H	-4.37814200	-1.25609200	6.01806200
H	-3.15887700	3.53391200	-0.02620700	H	-3.78091900	-3.61653000	5.49711400
H	-3.84523300	1.16299600	-0.27427300	H	-2.37409200	-4.16923700	3.56404100
C	0.92083800	2.34161100	1.95067300	H	-4.12176300	-4.11656600	2.10625800
C	1.32761500	1.34309400	3.03772200	H	-3.48822900	-0.70699400	4.60954000
C	1.04271600	-0.07076900	2.61109000	H	-2.30921000	-2.64897100	5.58964600
C	0.03542900	-0.34920000	1.77774900	H	-2.16554700	-2.46409800	3.18640500
H	0.96532500	3.36409600	2.33012900				
H	0.77498800	1.55026200	3.96467800	<b>TSI</b>			
H	1.64082500	-0.87051600	3.03296800	K	0.76124200	0.91661200	-2.16917800
H	1.64821200	2.27764800	1.13092000	O	0.67467400	-1.48638000	-1.47880500
H	2.38514200	1.46631800	3.28044300	C	0.41857000	-2.87097600	-1.38686800
H	-0.19035400	-1.37522000	1.50785600	C	1.32695400	-3.49548400	-0.31709700
				C	-1.05327500	-3.10042700	-1.01152200
<b>M1</b>				C	0.71555000	-3.49406500	-2.75270400
K	-3.72671700	-2.99656200	-0.25531600	H	2.37435800	-3.29135600	-0.55058300
O	-4.09437100	-5.12782900	0.72511200	H	1.10661000	-3.06601600	0.66264000
C	-4.27553700	-6.48845300	0.90307300	H	1.19190800	-4.57830900	-0.25178600
C	-3.48304600	-6.97315900	2.13528700	H	-1.70764000	-2.65998800	-1.76758300
C	-5.77026100	-6.79984400	1.12091800	H	-1.29149500	-4.16462900	-0.93148000
C	-3.78049500	-7.25260300	-0.34051900	H	-1.27499500	-2.62694300	-0.05286700
H	-2.42185300	-6.74638400	2.00277400	H	0.52803000	-4.57104100	-2.75654300
H	-3.83199600	-6.45080600	3.03014100	H	0.08674100	-3.03475700	-3.51958900
H	-3.58546400	-8.04906200	2.30910100	H	1.76056000	-3.32576400	-3.02359500
H	-6.34689800	-6.45875200	0.25698800	C	-1.59992700	0.76126400	-0.18635400
H	-5.96482100	-7.86775400	1.26453400	C	-0.47899700	0.83876700	0.69004800
H	-6.13456000	-6.26436500	2.00092100	C	-0.50140000	1.87756900	1.67149800
H	-3.90419200	-8.33690200	-0.25134200	C	-1.56136200	2.77127600	1.70700700
H	-4.33353500	-6.91752100	-1.22250000	C	-2.62871900	2.70816300	0.80940600
H	-2.72049200	-7.04123200	-0.50635200	C	-2.63843200	1.67896900	-0.12813800
C	-6.40970200	-2.92712900	2.33287300	H	-1.65597700	-0.07479100	-0.87572400
C	-5.24208900	-2.66616200	3.07846100	H	-1.55559500	3.54454200	2.47017500
C	-5.31457800	-1.75293000	4.15410100	H	-3.43926900	3.42335600	0.86250600
C	-6.52097200	-1.11457400	4.42184300	H	-3.47350600	1.57541100	-0.81267400
C	-7.66341400	-1.34886200	3.66192900	C	0.62444700	1.94609800	2.67921600
C	-7.59627700	-2.26951800	2.61848500	C	1.29411500	0.57974900	2.82857200
H	-6.36781100	-3.67387200	1.54752500	C	1.68138800	0.05735000	1.44717700

N	0.54806000	-0.03554500	0.54431300	H	2.16916100	0.71148000	3.59883800
H	0.24276500	2.30059700	3.64060100	H	2.48481400	0.82020300	1.17281200
H	0.59648200	-0.12370700	3.29371200				
H	2.13845700	-0.93342500	1.52696600	<b>TS2</b>			
H	0.58178400	-0.92069700	-0.45895600	K	-3.06456300	-2.88184400	0.69067100
H	1.37858300	2.67658900	2.36050700	O	-4.41302200	-5.17219300	0.87426600
H	2.17494300	0.64544800	3.47219200	C	-4.25467300	-6.59931600	0.83590200
H	2.46771400	0.71969600	1.04122900	C	-3.18294700	-7.01990800	1.84399200
				C	-5.59560100	-7.25811600	1.16598800
<b>M2</b>				C	-3.81953200	-6.93220700	-0.58648300
K	0.79188500	0.96460100	-1.99915000	H	-2.24141100	-6.50719200	1.63700800
O	0.74458100	-1.55128900	-1.43099700	H	-3.49179500	-6.76898300	2.86101700
C	0.43674000	-2.93944000	-1.32038500	H	-3.00414000	-8.09662600	1.80265700
C	1.34270300	-3.57562500	-0.26097200	H	-6.36025100	-6.93376800	0.45762500
C	-1.03523200	-3.10605300	-0.92657600	H	-5.52458900	-8.34750300	1.12510400
C	0.69878900	-3.55706300	-2.69078700	H	-5.91988700	-6.97653600	2.17044500
H	2.39230600	-3.42252000	-0.52041700	H	-3.69912500	-8.00908400	-0.71737600
H	1.16235200	-3.11932800	0.71472800	H	-4.56290600	-6.57919400	-1.30402300
H	1.16054900	-4.64936800	-0.17360900	H	-2.86472100	-6.45311900	-0.81557500
H	-1.68259500	-2.64497000	-1.67571300	C	-6.72902200	-2.96122400	2.66363600
H	-1.30744100	-4.16110200	-0.84208300	C	-5.52477000	-2.78908400	3.35436100
H	-1.22811800	-2.62450100	0.03392400	C	-5.30807000	-1.60654500	4.08912600
H	0.48402000	-4.62790700	-2.68950900	C	-6.30571700	-0.63922500	4.11448200
H	0.06938900	-3.08318300	-3.44773700	C	-7.50593700	-0.81669200	3.42962000
H	1.74320300	-3.41551100	-2.97710600	C	-7.71610500	-1.98434000	2.70404900
C	-1.57123600	0.80311900	-0.09015200	H	-6.87824600	-3.87493400	2.10128400
C	-0.45004400	0.88767300	0.79238300	H	-6.14102700	0.26899300	4.68448400
C	-0.50467400	1.92280500	1.78379700	H	-8.27016700	-0.05038600	3.46707700
C	-1.57712100	2.79975400	1.81543000	H	-8.64613400	-2.13547600	2.16980300
C	-2.63776500	2.72905600	0.90818300	C	-3.99135400	-1.42619800	4.80877200
C	-2.62411500	1.70441000	-0.03451400	C	-3.35692900	-2.77719300	5.13102200
H	-1.61746600	-0.03400600	-0.78035200	C	-3.48348500	-3.72544500	3.97687700
H	-1.58933000	3.56752000	2.58458000	N	-4.55001500	-3.79916900	3.24230900
H	-3.45908000	3.43196500	0.95970800	H	-4.13915400	-0.84398100	5.72071600
H	-3.45347800	1.59089000	-0.72484800	H	-3.88620800	-3.24290600	5.97564500
C	0.60986300	2.00113500	2.80306100	H	-2.77340300	-4.53817900	3.89774100
C	1.29569800	0.64260100	2.94488400	H	-4.57527600	-4.86596000	1.80809300
C	1.70136700	0.14117600	1.55976100	H	-3.30463300	-0.86164600	4.17236700
N	0.58682400	0.03496300	0.63219300	H	-2.31199500	-2.66967800	5.41374700
H	0.21493700	2.34315200	3.76394600	H	-1.82455600	-2.70728600	2.78892200
H	0.60196100	-0.07459700	3.39519300				
H	2.17852300	-0.84145200	1.63906700	<b>TS2<sup>a</sup></b>			
H	0.64367100	-1.06548400	-0.51547600	K	1.17479600	0.64302100	2.67764900
H	1.35780000	2.74379500	2.49732100	O	2.23741600	-0.02113200	0.36348500

C	3.22996900	-0.04993500	-0.67193900	H	-2.85606000	-0.09426900	-3.61956000
C	3.42625200	1.36506600	-1.22131700	H	0.93138400	0.08671000	-3.93076400
C	4.50849400	-0.55889400	-0.01636800	H	-0.55216600	-0.02264500	-4.88669500
C	2.76959300	-0.99762800	-1.78180300	H	-0.02830000	-1.40663500	-3.92151700
H	2.49934800	1.73324000	-1.66685100	H	-1.44631800	2.10394100	-3.65025000
H	3.71431900	2.04768900	-0.41936800	H	0.07217300	2.15023000	-2.73815800
H	4.20282200	1.38545200	-1.98924700	H	-1.47767200	2.09828500	-1.88430800
H	4.34957700	-1.55233900	0.40811500	H	-0.59816800	0.09332400	-0.78681200
H	5.32180100	-0.62168800	-0.74163700	H	2.49929400	1.35096200	0.35963100
H	4.81836800	0.11286200	0.78740800	C	-0.31819800	-1.53459900	1.71164900
H	3.50803900	-1.05292000	-2.58469000	C	0.32509000	-0.26077200	1.55549100
H	2.61516800	-2.00265200	-1.38471400	C	-0.56546600	0.85722000	1.34566800
H	1.82625100	-0.65228400	-2.21049100	C	-1.93596800	0.65745400	1.26000500
C	-1.01432900	-1.40933500	0.05633600	C	-2.52517500	-0.60645300	1.35787700
C	-1.30596100	-0.05884300	-0.16769300	C	-1.68810000	-1.69639300	1.60037400
C	-2.61752500	0.31649500	-0.52290900	H	0.30676400	-2.38535300	1.97148000
C	-3.59759000	-0.66066100	-0.63388300	H	-2.57082200	1.52650100	1.10585600
C	-3.30523300	-2.00299100	-0.39790100	H	-3.59717600	-0.72799400	1.27684500
C	-2.00925500	-2.37372500	-0.05422500	H	-2.11454900	-2.68670600	1.72232600
H	0.00409200	-1.69349100	0.29451000	C	0.03997600	2.23847200	1.24775300
H	-4.60541200	-0.36876500	-0.90888800	C	1.39663400	2.26706100	1.95011000
H	-4.08261100	-2.75153000	-0.48690000	C	2.26210500	1.12321400	1.41798800
H	-1.77029300	-3.41553000	0.12241900	N	1.66313200	-0.19680100	1.54967900
C	-2.85489400	1.77688900	-0.79741100	H	-0.64128900	2.98032300	1.67467900
C	-2.02063900	2.61877200	0.17222700	H	1.25513000	2.13618300	3.02768500
C	-0.58440100	2.13464500	0.15750400	H	0.18304000	2.52077300	0.19671000
N	-0.27775900	0.88928600	-0.09130000	H	1.89614800	3.22834900	1.79877900
H	-3.91455600	2.02280100	-0.71025400	H	3.22727700	1.11931800	1.93708800
H	-2.42542500	2.51742300	1.17793900				
H	-0.17771700	2.61747800	2.17543700	<b>TS3</b>			
H	1.36538000	0.31434100	0.00205500	K	-0.42369600	-0.90611200	-2.83845900
H	-2.55868100	1.99971400	-1.83040300	O	-2.08875200	0.30570700	-4.40854500
H	-2.05055300	3.67998200	-0.08066000	C	-2.83357300	0.76074900	-5.54417000
H	0.20724300	2.86046100	0.04658500	C	-3.94619600	1.70353500	-5.07968700
				C	-3.42337500	-0.49253400	-6.18297500
<b>M3</b>				C	-1.89325900	1.47573600	-6.51806100
K	1.72453600	-1.79215200	-0.59114700	H	-3.52332700	2.58685600	-4.59642400
O	-0.16084700	-0.24145400	-1.59079600	H	-4.59496800	1.19683900	-4.36297600
C	-0.88310700	0.20535600	-2.75830200	H	-4.55648300	2.03700000	-5.92234000
C	-2.28905900	-0.39205900	-2.73494300	H	-2.62661600	-1.17574500	-6.48541000
C	-0.08391600	-0.31572200	-3.94586700	H	-4.01400800	-0.24299100	-7.06685300
C	-0.93589000	1.73262900	-2.75931200	H	-4.06917700	-1.01210300	-5.47240200
H	-2.83317800	-0.05702100	-1.84966000	H	-2.42927300	1.81194300	-7.40892600
H	-2.23836700	-1.48198600	-2.70543400	H	-1.09097200	0.80469400	-6.83225300

H	-1.43969900	2.34710300	-6.04147200	O	0.51629300	0.43918900	-1.96422800
H	-1.64836000	1.07579900	-3.91341300	C	-0.38653000	0.69300000	-3.01944500
H	-0.79572600	1.75665700	-2.91510500	C	-0.84941900	2.15672000	-2.96676900
C	-2.10911100	-1.47598300	0.33476200	C	-1.58760700	-0.23941000	-2.83827700
C	-2.10580400	-0.18424300	-0.21126100	C	0.29825900	0.40842900	-4.36470500
C	-3.34027300	0.43524500	-0.50451300	H	0.00339300	2.82826500	-3.08224900
C	-4.52079100	-0.25038900	-0.24831400	H	-1.31538000	2.36658800	-2.00120500
C	-4.51474200	-1.53521400	0.29128000	H	-1.57266500	2.38081400	-3.75578700
C	-3.30058900	-2.14626000	0.58427200	H	-1.26092700	-1.28203600	-2.85634600
H	-1.15602000	-1.93307100	0.57685200	H	-2.33117900	-0.09956700	-3.62813800
H	-5.46583100	0.23272700	-0.47389900	H	-2.06960800	-0.05022800	-1.87606100
H	-5.44820200	-2.04922300	0.48359200	H	-0.37717200	0.57542900	-5.20846300
H	-3.27987800	-3.14135200	1.01209300	H	0.64009600	-0.62877700	-4.39652700
C	-3.32802600	1.81658500	-1.11400300	H	1.16924300	1.05465900	-4.48879600
C	-2.04638400	2.55732400	-0.74337500	H	1.48334100	1.15191500	-1.97973800
C	-0.84880400	1.65644500	-0.87356000	H	2.41477400	1.64254400	-1.78063100
N	-0.86289900	0.41061000	-0.48366200				
H	-4.20766200	2.37888900	-0.79289500	<b>M5</b>			
H	-2.09147600	2.86915700	0.31028900	K	-0.14579000	0.18780500	-1.90199400
H	-3.38416100	1.72608900	-2.20090500	O	1.76116700	-0.60163600	-0.78617800
H	-1.91283200	3.45288700	-1.34729400	C	3.08334000	-0.77025100	-0.44259500
H	0.12166700	2.12609100	-0.97109900	C	4.00106100	-0.28673400	-1.58788300
<b>M4</b>				C	3.41768400	0.04433300	0.82870700
K	1.94347500	0.17297900	-1.70289600	C	3.38639300	-2.26002100	-0.16730000
O	0.05759900	0.16695000	0.04651200	H	3.77762900	-0.85089400	-2.49766900
C	-1.05405200	-0.13698300	0.89675200	H	3.80953400	0.77105300	-1.79026300
C	-1.49535400	1.13275700	1.62905700	H	5.06703300	-0.40491000	-1.36425500
C	-2.20224000	-0.69637800	0.05146300	H	2.81415300	-0.30983300	1.66819200
C	-0.55538400	-1.18529900	1.88683600	H	4.47242200	-0.02390900	1.11637800
H	-1.80827900	1.89550700	0.91343100	H	4.43135600	-2.44049900	0.10750900
H	-0.66920500	1.53804000	2.21666800	H	2.75212600	-2.62320400	0.64558800
H	-2.33228200	0.92921900	2.30141400	H	3.15786600	-2.85118200	-1.05809900
H	-3.05766400	-0.96727900	0.67527200	C	-3.12335600	0.66012100	-0.35121900
H	-1.87459300	-1.58735200	-0.48857600	C	-2.24329600	0.04372600	0.54298300
H	-2.53158300	0.04275800	-0.68099800	C	-1.31867500	0.82131300	1.26697700
H	-0.17853200	0.88296500	-0.64104600	C	-1.28753700	2.19594200	1.05687000
H	0.02058600	1.73386800	-1.85985900	C	-2.15377200	2.80567400	0.15079200
H	-1.34537200	-1.47204600	2.58413400	C	-3.07661200	2.03617100	-0.55223100
H	-0.22343300	-2.08154700	1.35771700	H	-3.83638600	0.04064200	-0.88163100
H	0.28683600	-0.79498300	2.46197300	H	-0.56837200	2.79593800	1.60269500
<b>TS4</b>				H	-2.11057500	3.87704700	-0.00008800
K	1.97515300	-0.26111200	-0.11962800	H	-3.76069800	2.50480400	-1.24862600
				C	-0.40950100	0.11738700	2.24004900
				C	-0.09575800	-1.29283100	1.73997500

C	-1.32675400	-1.96284000	1.22350000				
N	-2.31016200	-1.36453800	0.66494100	<b>M6</b>			
H	0.62406100	-1.22978400	0.89844700	K	-0.52082200	-0.64643500	-2.20082400
H	-1.38485900	-3.04930300	1.27703000	O	1.48808000	-1.03626300	-0.56938200
H	3.17347800	1.09663000	0.65994700	C	2.87758300	-0.72025500	-0.34963400
H	0.36983700	-1.90159700	2.51636800	C	3.40260200	-0.24190200	-1.69797800
H	0.51117100	0.68506400	2.37859200	C	2.98787700	0.38484300	0.70013100
H	-0.90920400	0.07017100	3.21536200	C	3.60892800	-1.98251100	0.10681200
				H	3.27157600	-1.01674300	-2.45693300
<b>TSS</b>				H	2.87314100	0.65878800	-2.01785800
K	-3.98007800	-2.31714800	1.08431400	H	4.46569600	-0.00373000	-1.63837100
O	-2.19524100	-3.19827300	2.55625600	H	2.60800500	0.03938200	1.66325700
C	-0.80778100	-3.34689600	2.73673200	H	4.02799100	0.68826200	0.83702900
C	-0.10510400	-2.86076600	1.46266500	H	4.67017900	-1.78431100	0.27236000
C	-0.34030600	-2.50290400	3.93354300	H	3.18282700	-2.35170300	1.04235900
C	-0.46792000	-4.82591100	2.98042900	H	3.51627200	-2.76952700	-0.64403500
H	-0.44385500	-3.44322700	0.60170800	C	-2.56833600	0.98112800	-0.54191000
H	-0.33833700	-1.80782200	1.28108300	C	-1.86411800	0.13219600	0.34693500
H	0.98216000	-2.95815400	1.53065100	C	-1.11820500	0.75691800	1.38900200
H	-0.83053300	-2.83848200	4.84950800	C	-1.05405900	2.14210000	1.44882800
H	0.74078800	-2.56958000	4.08326600	C	-1.72751300	2.96199500	0.54232700
H	0.60636300	-4.98421400	3.11035100	C	-2.50240600	2.36457700	-0.44733000
H	-0.97632700	-5.18689300	3.87677600	H	-3.20059800	0.51532900	-1.29303500
H	-0.80731000	-5.43077700	2.13640800	H	-0.46516700	2.59848600	2.23934000
C	-6.83449500	-1.87884800	2.63000500	H	-1.66295100	4.03978800	0.62195100
C	-5.90028400	-2.49903000	3.47598500	H	-3.06379600	2.97666700	-1.14445600
C	-5.01523000	-1.68553000	4.22470000	C	-0.44543500	-0.09786900	2.44738400
C	-5.07206100	-0.30422900	4.07240800	C	-0.31503100	-1.51908100	1.96458200
C	-5.99204500	0.30061800	3.21581900	C	-1.07576000	-1.96574300	0.92865000
C	-6.88322900	-0.49470500	2.50083000	N	-1.87170000	-1.22261500	0.10793200
H	-7.51804900	-2.51342100	2.07758400	H	1.05193500	-1.26739700	0.28194400
H	-4.38142100	0.31245200	4.63797300	H	-1.02596100	-3.02270200	0.66976200
H	-6.01776900	1.37877100	3.11854600	H	2.40711700	1.25788800	0.39817400
H	-7.61527500	-0.03992400	1.84418000	H	0.26062000	-2.22616600	2.55050300
C	-4.04951700	-2.35548000	5.17608300	H	0.52918500	0.33303800	2.70700400
C	-3.70805000	-3.74498300	4.65540400	H	-1.03026100	-0.05419700	3.38147700
C	-4.80539800	-4.43827500	4.06337100				
N	-5.84589900	-3.89888800	3.47734700	<b>TS6</b>			
H	-2.88179200	-3.53984400	3.59016400	K	0.50581300	-2.05823100	-0.83505700
H	-4.74328700	-5.52421800	3.98685700	O	1.79899700	-0.33663300	0.49819000
H	-0.60159800	-1.45411800	3.77470800	C	2.74472400	0.73329100	0.40254600
H	-3.11030400	-4.35344800	5.33226200	C	3.65105000	0.40301200	-0.78151700
H	-3.14950000	-1.74409400	5.28198200	C	2.00253400	2.04954400	0.15702700
H	-4.51108400	-2.39955200	6.17411000	C	3.55908900	0.80768900	1.69658500



H	4.14710300	-0.55788300	-0.62645000	H	0.23498400	-0.94990200	-0.92168100
H	3.07091800	0.35096000	-1.70682400	C	-2.00412700	0.53609300	0.20428000
H	4.42158200	1.16620800	-0.91258100	C	-1.00137600	0.08466700	1.09573600
H	1.33268900	2.26592100	0.98999600	C	-0.80514200	0.82674100	2.29738300
H	2.70167100	2.88260700	0.04814900	C	-1.54775300	1.98308700	2.51854100
H	4.30753500	1.60271700	1.64894200	C	-2.51538500	2.42394700	1.61935500
H	2.90144700	1.00235400	2.54541400	C	-2.74661300	1.67695600	0.46394200
H	4.07139300	-0.14004800	1.87507500	H	-2.16971900	-0.03201500	-0.70350300
C	-2.12616000	0.13098400	-1.80983400	H	-1.37666900	2.54163400	3.43396400
C	-2.10566900	-0.40015100	-0.49789900	H	-3.08812100	3.31980700	1.82336900
C	-1.87244800	0.48520200	0.59200700	H	-3.50777700	1.99068100	-0.24147000
C	-1.69274100	1.85642500	0.33660600	C	0.16911100	0.30553500	3.33553800
C	-1.72810300	2.35151900	-0.94748700	C	1.20896700	-0.55259600	2.66426700
C	-1.94098400	1.47743800	-2.02828300	C	0.91757500	-1.16788600	1.49214600
H	-2.31762600	-0.54859600	-2.63250000	N	-0.19371800	-0.96345900	0.71475700
H	-1.50013000	2.51850100	1.17255200	H	2.12965800	-0.78476800	3.18533000
H	-1.58185600	3.40875800	-1.12852600	H	0.62206500	1.14091300	3.88009100
H	-1.96936200	1.86900200	-3.03797700	H	1.63384900	-1.87097100	1.07045400
C	-1.77036600	-0.07797700	1.90868200	H	-0.38002300	-0.27239200	4.09849400
C	-2.20121600	-1.40067400	2.06243000	H	2.57724300	-2.46767400	-1.88388900
C	-2.40162300	-2.18122300	0.93160400				
N	-2.29907400	-1.74941100	-0.32785600	<b>TS<sub>7-7a</sub></b>			
H	1.13078500	-0.17007000	1.29562100	K	1.34870100	1.68391800	-0.67183700
H	-2.65048900	-3.23343200	1.04714900	O	0.92422900	-0.51833300	-1.74232700
H	1.39888100	1.98172000	-0.74969300	C	0.79540600	-1.54626700	-2.69377200
H	-2.28384000	-1.84577300	3.04482500	C	1.51887400	-1.10848700	-3.97153500
H	0.17529600	-0.07590000	2.17983200	C	1.43020700	-2.83688100	-2.15321100
H	-1.73398400	0.58847700	2.75514400	C	-0.69207200	-1.79077200	-2.99383300
				H	1.07757100	-0.18547900	-4.35666800
<b>M7</b>				H	2.57368900	-0.91863700	-3.75755100
K	1.24843600	1.42451200	-0.29055500	H	1.46037100	-1.86848100	-4.75557000
O	0.66623900	-0.62206200	-1.78200600	H	0.92228900	-3.15163500	-1.23883700
C	0.75555300	-1.67304400	-2.74878900	H	1.37035000	-3.65505900	-2.87609400
C	1.44493700	-1.07068600	-3.96818100	H	-0.83692100	-2.57298300	-3.74414000
C	1.58499800	-2.82307500	-2.17019900	H	-1.21414900	-2.09363500	-2.08342700
C	-0.65401200	-2.15343000	-3.10302300	H	-1.15497400	-0.87230000	-3.36270000
H	0.86642700	-0.22819900	-4.35302400	H	0.45791900	-0.77891500	-0.62934000
H	2.44185600	-0.71155800	-3.70226900	C	-1.75298700	0.63303900	0.01799200
H	1.54982300	-1.80799500	-4.76648300	C	-0.81109300	0.18446800	0.96866500
H	1.09966500	-3.23509900	-1.28288800	C	-0.81227500	0.78525900	2.25352200
H	1.70545900	-3.63014800	-2.89655900	C	-1.70675100	1.81776800	2.51718100
H	-0.62501400	-2.94388500	-3.85680500	C	-2.62177300	2.26468500	1.56752200
H	-1.15619500	-2.54509400	-2.21607400	C	-2.64350600	1.65384000	0.31575300
H	-1.24809700	-1.32517500	-3.49444900	H	-1.76562400	0.16066500	-0.95629400

H	-1.69348900	2.27547000	3.50142300	H	0.42656300	1.05683300	4.08394500
H	-3.31234700	3.06381900	1.80530000	H	1.92769100	-1.58768800	1.15318100
H	-3.35880900	1.97257200	-0.43354100	H	-0.48626800	-0.42744700	4.15490700
C	0.12165200	0.26454000	3.32950200	H	2.43412800	-2.67335700	-1.83459400
C	1.27491000	-0.47929100	2.71122900				
C	1.18259100	-0.96814400	1.46098500	<b>TS7</b>			
N	0.12992500	-0.75801100	0.59441000	K	-3.36839900	-0.65138200	1.65015500
H	2.14803400	-0.69874700	3.31255100	O	-3.97051500	-2.91737200	0.40191100
H	0.47137800	1.09446100	3.95304100	C	-3.76523900	-3.80970500	-0.70848100
H	1.98857700	-1.56185600	1.04010600	C	-3.04772100	-2.98527100	-1.77074100
H	-0.43735700	-0.39257700	4.01499000	C	-2.90105600	-4.98640900	-0.25354400
H	2.48230100	-2.66264000	-1.91598800	C	-5.12301800	-4.29505200	-1.21695200
				H	-3.65568200	-2.12643900	-2.06340400
<b>M7a</b>				H	-2.09003000	-2.62146700	-1.39125000
K	1.27013000	1.59480100	-0.93124700	H	-2.85310300	-3.58386300	-2.66217400
O	0.78199200	-0.59702800	-1.78610400	H	-3.41051600	-5.55781000	0.52556400
C	0.75733200	-1.62079400	-2.72108700	H	-2.68817600	-5.66291900	-1.08395500
C	1.53872500	-1.19683000	-3.97951000	H	-5.00663100	-4.95497200	-2.07931500
C	1.40548000	-2.89083800	-2.13375000	H	-5.64867800	-4.84777600	-0.43503700
C	-0.69809700	-1.94047800	-3.11690100	H	-5.74326700	-3.44616300	-1.51067200
H	1.09537800	-0.29095500	-4.40278900	H	-4.42177500	-3.38953300	1.14180400
H	2.57587300	-0.97419000	-3.71310500	C	-6.79317900	-2.00633800	2.32161900
H	1.54397000	-1.96882200	-4.75576800	C	-5.69707600	-2.35944400	3.14431000
H	0.85563000	-3.21204600	-1.24530500	C	-5.29760300	-1.45968700	4.17217800
H	1.42194100	-3.72370700	-2.84364300	C	-6.01182300	-0.26047600	4.35332000
H	-0.76781900	-2.74126500	-3.85997500	C	-7.07812600	0.05973600	3.54288900
H	-1.26353700	-2.24590200	-2.23274500	C	-7.46691700	-0.82274200	2.51648100
H	-1.17364300	-1.04689300	-3.52959200	H	-7.08475100	-2.69468900	1.53807200
H	0.23466600	-0.91308000	-0.27026800	H	-5.68695700	0.42395300	5.12828900
C	-1.81215300	0.62494100	0.15910800	H	-7.61737900	0.98691700	3.69131200
C	-0.88624200	0.17346800	1.11549300	H	-8.30596600	-0.56838200	1.88007600
C	-0.87690400	0.75376200	2.40106600	C	-4.10891600	-1.77060400	4.92160300
C	-1.77259400	1.78295300	2.67466700	C	-3.61865600	-3.07769200	4.79760700
C	-2.68364900	2.23725300	1.72574100	C	-4.07576400	-3.87618500	3.75962300
C	-2.70169000	1.64476800	0.46578500	N	-5.04015200	-3.53861800	2.90045200
H	-1.81306200	0.16278500	-0.82071600	H	-2.81479600	-3.42867000	5.43050900
H	-1.76007800	2.23256700	3.66202200	H	-2.78853500	-0.56288200	4.07637100
H	-3.37480000	3.03381600	1.97003400	H	-3.62128800	-4.84941400	3.59504100
H	-3.41209800	1.97528100	-0.28248200	H	-3.87541500	-1.17635400	5.78948500
C	0.06742600	0.22796100	3.46544200	H	-1.95304300	-4.62744300	0.15160000
C	1.21723400	-0.52092600	2.84619800				
C	1.13239800	-1.00360600	1.60002300	<b>M8</b>			
N	0.04555400	-0.79647100	0.76684900	K	1.08726500	-2.45882300	-0.39522800
H	2.09566400	-0.72891700	3.44250600	O	2.33753500	-0.67624700	0.45393500

C	2.87318600	0.56888800	0.67500700	H	-1.13675000	-4.21342900	-1.25286500
C	2.69121800	1.46118400	-0.57503900	H	-1.15035700	-2.78076200	-0.21030600
C	2.17008400	1.25336900	1.87028500	H	0.67802000	-4.39573500	-3.10851600
C	4.38313700	0.46377300	0.98860300	H	0.20347000	-2.79499900	-3.70365200
H	3.18314200	0.99247900	-1.43211000	H	1.88577800	-3.10515500	-3.24833900
H	1.62706000	1.55413700	-0.80719900	C	-1.64512900	0.59448400	0.08732700
H	3.10548500	2.46853700	-0.45119700	C	-0.50554900	0.88197200	0.85275700
H	2.29978500	0.64685400	2.77029800	C	-0.55744200	1.93938400	1.79554600
H	2.55505500	2.25854500	2.07578000	C	-1.73970600	2.66259300	1.94688300
H	4.85404600	1.43679500	1.16851900	C	-2.86984100	2.36684700	1.19173900
H	4.53014500	-0.15939100	1.87474300	C	-2.81086200	1.33060700	0.26219800
H	4.89730400	-0.01828600	0.15245000	H	-1.60096600	-0.21880900	-0.62705400
C	-1.46033700	-0.14055400	-2.00384100	H	-1.76698900	3.47162300	2.66891200
C	-1.67304400	-0.10522300	-0.60604800	H	-3.78252900	2.93254900	1.32747600
C	-1.97724700	1.14259800	0.01386000	H	-3.68504700	1.08437600	-0.32905900
C	-2.03495600	2.31222900	-0.77987100	C	0.66369800	2.24689600	2.52908000
C	-1.81080300	2.24818700	-2.13051000	C	1.71711000	1.42459000	2.49304800
C	-1.52634500	1.01036500	-2.74655800	C	1.64643000	0.12709100	1.73631600
H	-1.25612500	-1.09524700	-2.47363400	N	0.69058600	0.22542900	0.64007200
H	-2.25478200	3.25831300	-0.29980100	H	1.38172500	-0.68895400	2.43330000
H	-1.85063700	3.14739600	-2.73181300	H	0.65936500	-0.59282300	-0.01411100
H	-1.35747300	0.97391200	-3.81540500	H	2.62121600	-0.13692000	1.32006300
C	-2.19491400	1.14650600	1.40962300	H	0.69499300	3.16277400	3.10965600
C	-2.11019900	-0.02768800	2.10683200	H	2.61856400	1.64206200	3.05352400
C	-1.78538700	-1.20851200	1.40835800				
N	-1.56442900	-1.26105500	0.11251000	<b>TS8</b>			
H	1.63625300	-1.80255900	2.27253900	K	0.70280000	1.12519300	-1.57678900
H	-1.69195000	-2.14137300	1.95600700	O	0.61839800	-1.33501400	-1.22961000
H	1.09850500	1.32743700	1.66879600	C	0.52973300	-2.72852600	-1.41584200
H	-2.26729500	-0.06382900	3.17630900	C	1.51289300	-3.43917000	-0.47277200
H	1.32385000	-2.30856400	2.74053100	C	-0.90242300	-3.19978100	-1.11966600
H	-2.41892000	2.08060000	1.91106600	C	0.88935100	-3.03468100	-2.87204900
				H	2.53069900	-3.08996800	-0.66220000
<b>M9</b>				H	1.26505100	-3.21498100	0.56705900
K	1.36525000	0.75632300	-2.17956200	H	1.49123300	-4.52477500	-0.60127500
O	0.76943600	-1.45403200	-1.48899900	H	-1.60755500	-2.68713000	-1.77822100
C	0.54869900	-2.81773200	-1.56305800	H	-1.01692000	-4.27723600	-1.26677100
C	1.46952400	-3.55787900	-0.57120200	H	-1.16916100	-2.96541200	-0.08691000
C	-0.91906800	-3.14107300	-1.21571800	H	0.85066900	-4.10629400	-3.08554500
C	0.84496400	-3.32003700	-2.99036700	H	0.19333800	-2.52711800	-3.54479400
H	2.51358400	-3.32333600	-0.79505900	H	1.89853900	-2.67763700	-3.09174400
H	1.26112200	-3.22252600	0.44834100	C	-2.00552600	0.41102300	0.38632000
H	1.34543800	-4.64519900	-0.60393700	C	-0.77337400	0.61865000	1.05818900
H	-1.58571300	-2.63247600	-1.91732900	C	-0.58007300	1.89009500	1.69487400

C	-1.60995700	2.83175800	1.70086500	C	1.79363800	1.22620200	2.13160500
C	-2.82789700	2.58554100	1.07801000	C	1.35295800	-0.21191800	2.01884500
C	-3.00428300	1.37161100	0.40788500	N	0.21414200	-0.39693200	1.12546000
H	-2.16218100	-0.53361900	-0.11985800	H	1.11960500	-0.59537800	3.03162300
H	-1.43659800	3.78541200	2.18993500	H	0.45940200	-1.19864500	-0.26276800
H	-3.61996900	3.32258700	1.10378000	H	2.17844700	-0.83482000	1.65893800
H	-3.94349800	1.16628900	-0.09375200	H	1.16653600	3.24791700	2.12750700
C	0.76605600	2.19188500	2.15435400	H	2.82903000	1.44804500	2.36886900
C	1.70793500	1.23983400	2.20452500				
C	1.34023000	-0.19139300	1.90824300	<b>TS9</b>			
N	0.21785500	-0.30222800	0.98670500	K	-3.23322300	-2.83430600	0.46193800
H	1.11989200	-0.71127600	2.85937700	O	-4.39804100	-5.18996800	0.80916500
H	0.38132200	-0.97433500	-0.10452200	C	-4.25140100	-6.61637400	0.86510400
H	2.19035600	-0.72643500	1.47401100	C	-3.07737400	-6.97081900	1.78118900
H	0.99967900	3.22044100	2.41217000	C	-5.54972700	-7.23083900	1.39186000
H	2.72431500	1.47132200	2.50466100	C	-3.97735200	-7.06846600	-0.56465900
				H	-2.16316800	-6.48439000	1.43475900
<b>M10</b>				H	-3.27468500	-6.63991500	2.80302300
K	0.52710500	1.15030800	-1.44847600	H	-2.90660500	-8.04946700	1.80277600
O	0.67232400	-1.40848500	-1.24939200	H	-6.38735300	-6.95460100	0.74848700
C	0.61718900	-2.81217800	-1.50798000	H	-5.48620700	-8.32079400	1.42885600
C	1.61312600	-3.53223800	-0.59428700	H	-5.76035100	-6.86722300	2.40006100
C	-0.80496300	-3.32020100	-1.25195500	H	-3.87322400	-8.15376000	-0.61785300
C	0.99986200	-2.99675600	-2.97332900	H	-4.79581100	-6.76871200	-1.22227300
H	2.61967100	-3.13806900	-0.74921400	H	-3.05429700	-6.61878300	-0.93795700
H	1.34482900	-3.38077700	0.45330900	C	-6.57191200	-2.78682900	2.37237700
H	1.62813500	-4.60687000	-0.79058400	C	-5.42537600	-2.72153100	3.19564500
H	-1.51636200	-2.79323800	-1.89143500	C	-5.33529200	-1.66963400	4.15344100
H	-0.88723300	-4.39058500	-1.45567300	C	-6.37784600	-0.73423900	4.25207900
H	-1.08710800	-3.14713100	-0.21166200	C	-7.48503400	-0.81210200	3.42903000
H	0.98984400	-4.05196400	-3.25393800	C	-7.57833200	-1.84840000	2.48887900
H	0.29763700	-2.46513600	-3.61983000	H	-6.64951200	-3.59821500	1.65819200
H	2.00195600	-2.60250700	-3.15619000	H	-6.30016900	0.05711300	4.98966100
C	-1.97972600	0.34759700	0.48130100	H	-8.28060500	-0.08273100	3.51378700
C	-0.72487000	0.56444000	1.12513100	H	-8.45034800	-1.91592700	1.84926400
C	-0.47852100	1.90392600	1.60698000	C	-4.17940500	-1.65138200	5.00109200
C	-1.46460500	2.88671100	1.49611700	C	-3.18100200	-2.53792600	4.79212200
C	-2.69740500	2.62729300	0.90905600	C	-3.29165400	-3.49344000	3.72318600
C	-2.93260800	1.34696200	0.39191400	N	-4.44499600	-3.66651700	3.06132700
H	-2.18386700	-0.64191300	0.08905500	H	-2.60787700	-4.32863400	3.70666400
H	-1.24262800	3.88404400	1.86483200	H	-4.50665500	-4.81372200	1.73016900
H	-3.45579200	3.39694500	0.84884600	H	-1.98065400	-2.69489000	2.56444700
H	-3.88475300	1.12594100	-0.07849800	H	-4.11590700	-0.91065300	5.79004200
C	0.88655400	2.20611500	2.00039900	H	-2.27562100	-2.52673600	5.38458000

				H	2.99466300	-0.42398100	6.57513100
<b>M11</b>				H	3.79847300	-0.85221300	5.05494400
K	-0.60278400	-2.18694100	0.91174800	H	4.37401400	0.52680900	6.00126100
O	-0.27812400	0.26580400	1.86147000	H	2.48508700	2.03846600	3.08255800
C	0.76644200	0.97389300	2.57002600	H	4.06546200	2.02362000	3.87799800
C	1.11613500	0.08949600	3.76062500	H	3.49272100	0.59295400	3.00492600
C	1.97059500	1.15168400	1.64675800	H	2.89037600	2.68070100	6.11327900
C	0.22428700	2.32434400	3.03550300	H	1.33812400	2.67100300	5.26355900
H	0.23383600	-0.08823100	4.37832500	H	1.56103800	1.66490300	6.70107700
H	1.50975800	-0.87418200	3.42716500	C	2.46746700	-1.64466400	0.25579800
H	1.87908600	0.56317700	4.38013300	C	1.70161900	-0.46897600	0.43498100
H	1.70820400	1.75749100	0.77866800	C	2.32885100	0.78167100	0.15277700
H	2.79284700	1.64341800	2.17087100	C	3.66922500	0.81362800	-0.25581700
H	2.32360300	0.18557200	1.28146600	C	4.40329800	-0.35021200	-0.39500900
H	0.97820700	2.87367000	3.60300000	C	3.78838800	-1.58421700	-0.14274900
H	-0.06646600	2.93784100	2.18003000	H	1.98567400	-2.60367800	0.41497100
H	-0.65330000	2.18361500	3.66893600	H	4.12835800	1.77498200	-0.46002500
C	0.41576000	-1.68020000	-1.99684500	H	5.43924900	-0.31117300	-0.70667100
C	-0.43900900	-0.59332800	-1.62592400	H	4.35226200	-2.50100800	-0.26943500
C	0.14617400	0.72654000	-1.72950000	C	1.52427900	1.96035300	0.29078600
C	1.44381100	0.89215200	-2.20825800	C	0.26516700	1.86065300	0.76677200
C	2.23179900	-0.18669500	-2.59666500	C	-0.25481000	0.56831100	1.15035800
C	1.69831900	-1.47452700	-2.47367200	N	0.40330700	-0.56765900	0.84656700
H	0.00059200	-2.68456300	-1.97734800	H	0.75044700	0.58524300	3.99917900
H	1.85153300	1.89810000	-2.25528300	H	-0.35982100	2.73313300	0.90899800
H	3.23228100	-0.03473700	-2.97997400	H	1.94447000	2.92079200	0.01331900
H	2.29223400	-2.33112900	-2.77516300	H	-0.28752100	0.81491900	2.92849700
C	-0.60286700	1.80278000	-1.11686800	H	-1.32767000	0.47673500	1.24633000
C	-1.86706000	1.60978500	-0.70430200				
C	-2.55942400	0.30936800	-1.03217400				
N	-1.64999600	-0.83090000	-1.11008400	<b>M1<sub>Nap</sub></b>			
H	-0.57083200	0.79845400	1.09898600	K	0.17274600	0.90332100	-1.78359800
H	-2.41496000	2.39168000	-0.18843200	O	0.60662700	-1.36835400	-1.64632900
H	-0.09858500	2.74907300	-0.94289100	C	0.85980200	-2.71475700	-1.72523800
H	-3.33074800	0.09598600	-0.28405400	C	1.92678800	-3.12888800	-0.68594400
H	-3.11197200	0.43177800	-1.98625300	C	-0.43000200	-3.52188300	-1.45044700
				C	1.37920600	-3.08540800	-3.13381200
<b>TS10</b>				H	2.84077100	-2.55264500	-0.85318200
K	0.34383600	-1.88342700	3.22744000	H	1.56858400	-2.90164300	0.32080000
O	1.39907000	0.07365600	4.57705400	H	2.17819500	-4.19456600	-0.72855200
C	2.52807600	0.89364000	4.92304300	H	-1.19588100	-3.24541300	-2.18007600
C	3.48221900	-0.01861200	5.68612500	H	-0.28081500	-4.60624700	-1.50002400
C	3.18475600	1.41969500	3.64653600	H	-0.81105800	-3.27359100	-0.45624200
C	2.05365900	2.04902100	5.80571600	H	1.59169700	-4.15427900	-3.24971100

H	0.63581400	-2.79977400	-3.88328500	C	-0.83928400	2.88536900	0.74185500
H	2.29704600	-2.52859600	-3.34255600	C	-2.14508900	2.94224100	0.24103400
C	-2.09237500	0.71692400	0.73339500	C	-2.91400700	1.77334300	0.26615600
C	-0.84827100	0.70848900	1.37769400	H	-2.99573300	-0.30837400	0.75732200
C	-0.16226200	1.92208600	1.54426600	H	-0.24049900	3.79094500	0.77127700
C	-0.73302300	3.10015300	1.04592800	H	-2.56263300	3.87660300	-0.11125300
C	-1.96273100	3.09486200	0.40086500	H	-3.94158600	1.79572300	-0.08021600
C	-2.65114800	1.89164200	0.24728300	C	1.12722900	1.64124200	1.74458500
H	-2.61770600	-0.22252300	0.60378000	C	1.22125600	0.62410600	2.88668300
H	-0.20160300	4.03662900	1.17807600	C	0.84105000	-0.77260000	2.38528600
H	-2.38676700	4.01987500	0.02994600	C	-0.42355300	-0.76995400	1.51891600
H	-3.61486500	1.87107400	-0.24649700	H	1.45019100	2.63402000	2.06929400
C	1.19320000	1.97589800	2.21863400	H	0.53911700	0.93213300	3.68582300
C	1.50969700	0.72258600	3.03316100	H	0.71346400	-1.43936200	3.24445600
C	1.21100200	-0.52693400	2.20886100	H	-0.02078600	-1.12569200	0.14386500
C	-0.27494900	-0.60503600	1.86396700	H	1.81929400	1.32891800	0.95039900
H	1.24924800	2.87016100	2.84470700	H	2.23015700	0.61877300	3.30810200
H	0.90195900	0.71276000	3.94450600	H	1.69485900	-1.17454600	1.82442300
H	1.51239100	-1.42965500	2.74416100	H	-1.14070200	-1.55098900	1.77294000
H	-0.43492600	-1.36008900	1.09164500				
H	1.96370000	2.09998900	1.44733200	<b>M2<sub>Nap</sub></b>			
H	2.55537600	0.74202900	3.34857900	K	-0.37822400	1.06759700	-1.83937800
H	1.79355000	-0.50442300	1.28251500	O	0.57315200	-1.19708100	-1.02696000
H	-0.84000600	-0.92403600	2.74732900	C	0.85613600	-2.55006000	-1.41340500
				C	1.97465300	-3.10753300	-0.53157900
<b>TS1<sub>Nap</sub></b>				C	-0.41415500	-3.39232300	-1.27386800
K	-0.56761300	0.96824800	-1.87862100	C	1.30244900	-2.48283400	-2.87035400
O	0.28091400	-1.23050600	-1.00299600	H	2.86273500	-2.47695400	-0.60349100
C	0.58642700	-2.55342100	-1.39361800	H	1.65969100	-3.13660400	0.51285200
C	1.69585300	-3.12548900	-0.49995400	H	2.24518900	-4.12178300	-0.83365500
C	-0.67140300	-3.42891100	-1.28989200	H	-1.21606100	-2.97413000	-1.88611600
C	1.06927100	-2.50770300	-2.84671500	H	-0.24180100	-4.42391900	-1.58960800
H	2.57806600	-2.48320800	-0.54249600	H	-0.75137800	-3.40435500	-0.23582700
H	1.36174400	-3.17545000	0.53754700	H	1.55428500	-3.47506500	-3.24936200
H	1.98640200	-4.13187900	-0.81306500	H	0.50542800	-2.07604500	-3.49839200
H	-1.46700100	-3.01796700	-1.91634700	H	2.18356600	-1.84518200	-2.96882800
H	-0.47949000	-4.45741800	-1.60815800	C	-2.12737200	0.58442800	0.72217100
H	-1.03222100	-3.45110900	-0.26002000	C	-0.79427300	0.47838700	1.25272400
H	1.33726500	-3.50090500	-3.21709300	C	-0.01058900	1.69632000	1.20365500
H	0.28520600	-2.10851400	-3.49686600	C	-0.54376400	2.86285700	0.68639700
H	1.94828400	-1.86392600	-2.92973700	C	-1.84206700	2.92946600	0.14740000
C	-2.38134200	0.58561200	0.74487700	C	-2.62387000	1.76359800	0.19762100
C	-1.04255800	0.49118200	1.21121600	H	-2.76371900	-0.29389100	0.75640600
C	-0.28268500	1.70233400	1.21240400	H	0.07120300	3.75910900	0.69513500

H	-2.24558100	3.86193800	-0.22429300	C	-3.45859400	-3.14952900	5.35016300
H	-3.64375800	1.78637400	-0.17362000	H	-4.72777700	-0.72197200	2.61466200
C	1.39757500	1.62769700	1.74032700	H	-3.70043600	-0.35112400	4.77774400
C	1.48320500	0.66633600	2.93139200	H	-1.74862000	-1.90976100	5.54236300
C	1.04973400	-0.74191400	2.50881100	H	-5.28138300	-5.15239800	2.39409800
C	-0.24411400	-0.71959700	1.71774200	H	-3.59839300	-1.99985100	2.22676400
H	1.74742300	2.62686600	2.01473900	H	-2.38333900	-0.47028600	3.61072300
H	0.82336900	1.02986100	3.72552500	H	-1.28608700	-2.70977600	3.60966300
H	0.93679600	-1.36559200	3.40332400	H	-3.16781600	-3.81501900	6.15793900
H	0.30734300	-1.14981900	-0.05300000				
H	2.08080200	1.25883300	0.96156700	<b>TS3<sub>Nap</sub></b>			
H	2.49941600	0.65151500	3.33521700	K	-0.01371200	-0.19791100	-0.96606900
H	1.87719100	-1.19709400	1.94296100	O	1.22645700	-2.22899300	-0.12647300
H	-0.92211400	-1.55810200	1.85138300	C	2.20252700	-3.21066500	-0.47737600
				C	3.44064600	-3.04068200	0.40989100
<b>TS2<sub>Nap</sub></b>				C	1.60607300	-4.61086300	-0.30308900
K	-2.26261400	-4.92500500	3.26735700	C	2.56327500	-2.96636400	-1.94186300
O	-4.52533700	-5.59807100	1.98229900	H	3.85853600	-2.03872200	0.28963300
C	-4.87589800	-5.95506500	0.62278800	H	3.17340900	-3.17482200	1.45913500
C	-6.08254200	-6.89108500	0.65195100	H	4.21498600	-3.76853500	0.15432900
C	-5.18500800	-4.68375800	-0.16554100	H	0.71053500	-4.71687000	-0.91930200
C	-3.64726100	-6.66156800	0.06382000	H	2.32015500	-5.38562400	-0.59356400
H	-5.85990400	-7.78362400	1.23915100	H	1.32160900	-4.77349000	0.73762200
H	-6.94337900	-6.39149400	1.10254800	H	3.31400300	-3.68026300	-2.28862200
H	-6.36216500	-7.19943900	-0.35737000	H	1.67903900	-3.07302900	-2.57546700
H	-4.33487000	-3.99977400	-0.13830500	H	2.96960600	-1.95997400	-2.07342000
H	-5.40786100	-4.91720200	-1.20853400	C	-1.15068900	2.10325400	1.03049700
H	-6.04889500	-4.16889000	0.25881400	C	-0.32885600	1.17161200	1.70382800
H	-3.83167100	-7.00320600	-0.95560300	C	1.08109100	1.36715700	1.63794600
H	-2.78795100	-5.98686700	0.03597100	C	1.59487600	2.44274900	0.92677700
H	-3.39357000	-7.53119500	0.67352800	C	0.76574800	3.35098600	0.25923000
C	-5.60718300	-4.39970300	5.13675300	C	-0.61366800	3.17233600	0.32106000
C	-4.73340200	-3.37872400	4.71093100	H	-2.22747600	1.98029400	1.08254400
C	-5.12675700	-2.59296700	3.59368200	H	2.67120200	2.57753900	0.88959800
C	-6.34434500	-2.83643700	2.97716100	H	1.19208300	4.18490600	-0.28355900
C	-7.19940500	-3.85505200	3.41043800	H	-1.27557400	3.87135400	-0.17704500
C	-6.81704600	-4.63727900	4.49732600	C	1.99186400	0.34231100	2.28527700
H	-5.32311300	-5.00832300	5.98865300	C	1.32142400	-0.40316600	3.43981000
H	-6.63157600	-2.22582400	2.12746900	C	-0.07169100	-0.84892400	3.07462300
H	-8.14428000	-4.02621500	2.91053500	C	-0.87374300	0.02686200	2.38708100
H	-7.46391500	-5.43241500	4.84882100	H	2.91198600	0.82438100	2.62431200
C	-4.16714300	-1.55333000	3.04927700	H	1.23720100	0.26642700	4.30722300
C	-3.17819500	-1.03620000	4.09497100	H	-0.53126300	-1.59305900	3.70833100
C	-2.60890700	-2.15027200	4.93608500	H	0.92220700	-2.35557900	0.89923900

H	2.28174000	-0.39318800	1.52904700	<b>M1<sub>t</sub></b>			
H	1.93423700	-1.25158200	3.74280800	O	-1.87540500	1.01660300	-1.69342400
H	0.51301100	-2.35441600	2.06621500	C	-2.95759900	0.71526500	-0.91164200
H	-1.94015400	-0.15442800	2.30690200	C	-3.13935900	-0.82000800	-0.76982600
				C	-2.80064700	1.31097300	0.51142400
<b>M3<sub>Nap</sub></b>				C	-4.24346500	1.29697700	-1.54564100
K	-1.10770500	-0.11745600	-1.61562200	H	-3.20925000	-1.26624500	-1.76544300
O	0.50691700	-1.73638000	-1.09788600	H	-2.26796700	-1.24990100	-0.26907200
C	1.42522100	-2.75750600	-1.17979000	H	-4.03313600	-1.10129000	-0.19946400
C	2.27156100	-2.84205000	0.11217900	H	-2.68128500	2.39574100	0.44045800
C	0.70768900	-4.11214700	-1.37844700	H	-3.65405600	1.09899300	1.16775700
C	2.37765500	-2.52665500	-2.37370500	H	-1.89903000	0.90698800	0.97857000
H	2.81765000	-1.90786500	0.26308500	H	-5.14614600	1.10915200	-0.95071000
H	1.61370700	-2.99149100	0.97258600	H	-4.12599500	2.37713400	-1.66762300
H	2.99909400	-3.66053700	0.08964800	H	-4.38680900	0.86518700	-2.54020200
H	0.09499600	-4.07187800	-2.28349100	C	1.09379500	1.77305900	0.01983900
H	1.40141800	-4.95482900	-1.47163700	C	1.30853100	0.44544000	-0.42722700
H	0.04394900	-4.30772900	-0.53246600	C	2.54221300	-0.17750400	-0.08917400
H	3.13661900	-3.31004900	-2.47884600	C	3.48111100	0.52326900	0.65816500
H	1.79965200	-2.48384800	-3.30137100	C	3.26477900	1.83110100	1.08665000
H	2.88884800	-1.56794300	-2.25241100	C	2.05353200	2.44395200	0.75544600
C	-2.04951300	2.47701900	0.72832400	H	0.15295000	2.24325400	-0.23994600
C	-1.14529500	1.58016600	1.30871700	H	4.41210500	0.02470800	0.91465900
C	0.20759800	1.60001400	0.90333900	H	4.01526100	2.35561700	1.66498700
C	0.61309100	2.52602500	-0.05421900	H	1.85575400	3.46087600	1.07789200
C	-0.29523300	3.41886900	-0.62405000	C	2.79179400	-1.60021000	-0.54006400
C	-1.63114200	3.39048600	-0.23515000	C	1.47393300	-2.34188900	-0.77737500
H	-3.08687500	2.45966200	1.04340500	C	0.57417000	-1.50508600	-1.68526300
H	1.65025100	2.54010000	-0.36878300	N	0.34589700	-0.19079700	-1.13701800
H	0.04172700	4.13244600	-1.36551000	H	3.40277700	-2.12606500	0.19974400
H	-2.34147900	4.08182200	-0.67106300	H	0.96370100	-2.50212700	0.17761500
C	1.13447400	0.53176500	1.42593400	H	-0.39526100	-1.99062000	-1.82192500
C	0.79210100	0.08286100	2.84822300	H	-0.59924500	0.32012500	-1.36321300
C	-0.68833600	-0.09282900	3.03325400	H	3.36924100	-1.60317900	-1.47311500
C	-1.57174900	0.60803500	2.31648500	H	1.65677900	-3.32327800	-1.22361600
H	2.17146000	0.86797300	1.36789300	H	1.03893000	-1.44897600	-2.68426300
H	1.14921600	0.81654000	3.58462700				
H	-1.03419200	-0.77679200	3.80014100	<b>TS1<sub>t</sub></b>			
H	-1.40057900	-2.30640800	0.09981800	O	-3.99019700	-5.93381200	2.20076100
H	1.04467200	-0.32914500	0.74753800	C	-4.05566600	-5.99306300	0.81881600
H	1.31528200	-0.84901000	3.07224700	C	-2.88354600	-5.21534600	0.17670700
H	-2.10501900	-2.33624800	0.36723400	C	-3.96825000	-7.46741700	0.38452200
H	-2.63664100	0.49846000	2.49091600	C	-5.38424400	-5.39514500	0.30180800
				H	-2.94787200	-4.15719700	0.43985200



H	-1.93634100	-5.60072100	0.56313000	H	1.50359700	-0.71474200	-1.72276300
H	-2.87165500	-5.29520500	-0.91626300	C	-0.96949000	-1.53889400	-0.07973900
H	-4.78696400	-8.03242100	0.83768700	C	-1.18138000	-0.12434200	-0.14489400
H	-4.01978300	-7.59160700	-0.70318700	C	-2.50605500	0.28943200	-0.53186100
H	-3.02887500	-7.90002500	0.73888800	C	-3.47912500	-0.65391600	-0.82617500
H	-5.46515400	-5.43015100	-0.79071000	C	-3.23636800	-2.02873100	-0.78186300
H	-6.22748600	-5.94517900	0.72727500	C	-1.95906700	-2.44964100	-0.39370800
H	-5.47265900	-4.35426200	0.61951000	H	0.01068500	-1.88128800	0.23072600
C	-6.36409300	-3.74804600	3.58120400	H	-4.47091700	-0.29960600	-1.10032800
C	-5.13061200	-3.03914900	3.62401000	H	-4.01490600	-2.74185400	-1.02333400
C	-5.15778200	-1.73165900	4.20292200	H	-1.73625000	-3.51107100	-0.33355600
C	-6.35083800	-1.21229600	4.68738200	C	-2.81582000	1.76987000	-0.56541800
C	-7.55433100	-1.91393200	4.62096500	C	-1.86916700	2.53157000	0.36310500
C	-7.53623300	-3.19479800	4.06102700	C	-0.42723700	2.12864700	0.04145500
H	-6.35450100	-4.74632700	3.16179000	N	-0.17521900	0.70831300	0.15647500
H	-6.33612500	-0.22168900	5.13555600	H	-3.86066800	1.94365500	-0.28675900
H	-8.47130000	-1.48191900	5.00235600	H	-2.08835600	2.27179800	1.40433500
H	-8.45399400	-3.77126900	4.00118400	H	0.26620200	2.65849000	0.70561200
C	-3.86316900	-0.95567800	4.29772200	H	1.35638300	0.21207600	0.53369800
C	-2.66595100	-1.90803900	4.33003800	H	-2.70029500	2.16522700	-1.58328700
C	-2.76647000	-2.88357000	3.15700300	H	-2.00179000	3.61345800	0.25779700
N	-4.01003400	-3.61823800	3.14763500	H	-0.19885600	2.49728500	-0.97814300
H	-3.87377900	-0.31222700	5.18314100				
H	-2.67235200	-2.47418700	5.26710100	<b>TS<sub>t</sub></b>			
H	-1.94406200	-3.60522800	3.18920700	O	-2.48210500	0.03337300	-4.57146800
H	-4.01670900	-4.76023300	2.65716000	C	-2.75808900	0.86695900	-5.68545300
H	-3.75612200	-0.28709900	3.43355700	C	-3.25258200	2.24505100	-5.21820300
H	-1.72388600	-1.35328900	4.28511000	C	-3.85420600	0.16144100	-6.48373100
H	-2.62944500	-2.30945900	2.22275500	C	-1.49653800	1.02781500	-6.54559000
				H	-2.47810700	2.74336700	-4.63343400
<b>M2<sub>t</sub></b>				H	-4.13675300	2.13134100	-4.58721000
O	2.31683800	-0.06815200	0.75674900	H	-3.51335500	2.88544800	-6.06646900
C	3.10195900	-0.04340500	-0.42008900	H	-3.51455800	-0.82938700	-6.79319000
C	3.15034000	1.38053800	-0.99638800	H	-4.12747800	0.73065400	-7.37670100
C	4.50653900	-0.49022500	-0.01336900	H	-4.74669600	0.03411100	-5.86669000
C	2.52352200	-1.00619900	-1.46836500	H	-1.68437000	1.64683200	-7.42860400
H	2.14945200	1.69990600	-1.28976600	H	-1.14458700	0.04802900	-6.87629300
H	3.52035500	2.07638200	-0.23957500	H	-0.70116800	1.48873400	-5.95755500
H	3.80205400	1.44215300	-1.87353100	H	-1.76840300	0.47172600	-3.98369200
H	4.46840700	-1.49032300	0.42455600	H	-0.83278000	1.10785800	-3.09394400
H	5.18669100	-0.51165300	-0.86949000	C	-1.86990800	-1.15701900	1.16596400
H	4.91548600	0.19058700	0.73708700	C	-2.07018500	-0.17500100	0.18544700
H	3.12319100	-1.01337800	-2.38399600	C	-3.36409200	-0.02137400	-0.36204100
H	2.49231300	-2.02201100	-1.06835800	C	-4.39332300	-0.84352400	0.07872000

C	-4.18285500	-1.81752300	1.05396800	H	-1.70845500	-0.16581800	-4.08267900
C	-2.91090900	-1.96873000	1.59792600	H	-1.80365200	-0.34405900	-2.31645600
H	-0.87210200	-1.26829400	1.57421500	H	0.34380900	1.01912300	-5.11741200
H	-5.38240700	-0.71973600	-0.35172500	H	1.40812200	-0.09082100	-4.22713200
H	-5.00085600	-2.44854000	1.38050200	H	1.60564300	1.65094200	-4.03777700
H	-2.72832300	-2.72213800	2.35575600	H	1.51289800	1.41605100	-1.59609500
C	-3.56955900	1.01790300	-1.43648000	H	2.27755700	2.07622000	-1.41237600
C	-2.54848300	2.14397500	-1.29230700				
C	-1.17439200	1.59184500	-1.00933300	<b>M1<sub>Li</sub></b>			
N	-0.97043200	0.59070400	-0.21112200	Li	0.39983200	-0.82232200	-0.45600300
H	-4.58933000	1.41064800	-1.39390000	O	0.39055600	-2.17525200	-1.37399000
H	-2.81938800	2.77963100	-0.43455600	C	0.36960400	-3.33556200	-2.11390200
H	-3.44355200	0.55015500	-2.41612800	C	0.17199100	-4.54969300	-1.18393200
H	-2.52423300	2.77397500	-2.17943900	C	-0.78800100	-3.29243900	-3.13169500
H	-0.32428800	2.22206000	-1.23692500	C	1.70039100	-3.50012500	-2.87561500
				H	0.98314000	-4.58790200	-0.45214100
<b>M3<sub>t</sub></b>				H	-0.76904600	-4.44452000	-0.63759100
O	0.67372400	-0.29736200	1.16083300	H	0.15099400	-5.50002600	-1.72689400
C	-0.03675100	-0.01956800	-0.03187600	H	-0.66263200	-2.43391100	-3.79625400
C	-0.76701300	1.32882400	0.08179500	H	-0.84579100	-4.19793700	-3.74401500
C	-1.05222900	-1.15032000	-0.20415700	H	-1.73784900	-3.17277400	-2.60406300
C	0.92647600	0.00577700	-1.22925800	H	1.73263600	-4.41332600	-3.47834300
H	-0.04607600	2.13017000	0.25112000	H	1.85467400	-2.64404600	-3.53737600
H	-1.45363800	1.31018800	0.93195100	H	2.52956100	-3.52828500	-2.16389800
H	-1.34131500	1.55446400	-0.82292000	C	-1.85465100	0.78290400	1.05196500
H	-0.53774900	-2.11213300	-0.26767500	C	-0.55415000	1.21649000	1.32650200
H	-1.64958200	-1.01553700	-1.11071800	C	-0.30555100	2.56796300	1.59250900
H	-1.72785700	-1.18593600	0.65397300	C	-1.38028400	3.45894900	1.54620700
H	0.39838800	0.18851000	-2.17085900	C	-2.66960900	3.03341900	1.26351500
H	1.44906600	-0.95111200	-1.30415700	C	-2.90804700	1.68247300	1.02474500
H	1.67554300	0.78577100	-1.08622700	H	-2.03405300	-0.26893900	0.85541600
H	1.37686200	0.42899900	1.31502800	H	-1.19396500	4.50671200	1.75467900
H	2.41600000	1.49430500	1.54590900	H	-3.48385600	3.74628600	1.23681100
				H	-3.90916400	1.33164500	0.80897300
<b>TS3<sub>t</sub></b>				C	1.08046500	3.04721800	1.95700700
O	0.59754600	0.57969900	-1.78131000	C	1.94748700	1.90193800	2.47365600
C	-0.09356700	0.82687100	-2.95645700	C	1.87636200	0.74240500	1.48990000
C	-0.84596200	2.17650800	-2.88124500	N	0.49804200	0.23755500	1.30524500
C	-1.11896100	-0.30165600	-3.16793800	H	1.00479400	3.84201300	2.70185000
C	0.86753000	0.85765100	-4.16791800	H	1.59196900	1.57078400	3.45431500
H	-0.13553900	2.98898100	-2.71554200	H	2.49338200	-0.09863600	1.80532100
H	-1.53802400	2.16190300	-2.03467800	H	0.29905900	-0.48319000	1.99273800
H	-1.41763900	2.39331500	-3.79166600	H	1.55806400	3.49362400	1.07741800
H	-0.60206000	-1.26311200	-3.22802300	H	2.98364200	2.22435400	2.59253700

H	2.25285200	1.07555100	0.51784900	C	-1.10455300	-2.40950200	-1.66868900
				C	0.93015600	-3.62927500	-2.51377400
<b>TS1<sub>Li</sub></b>				H	1.53609700	-3.69940100	0.17163100
Li	1.33782600	0.44515900	-2.06407500	H	0.09909400	-2.84678600	0.76156700
O	0.90425100	-1.22659100	-1.59200900	H	-0.07168900	-4.41648200	-0.02949500
C	0.35949800	-2.53302500	-1.47286500	H	-1.19183800	-1.89381800	-2.62746700
C	0.83160400	-3.14754900	-0.15186300	H	-1.73251200	-3.30191700	-1.70544000
C	-1.16957000	-2.44550400	-1.50316300	H	-1.49278800	-1.75020500	-0.89018900
C	0.87259000	-3.35100000	-2.65675300	H	0.37764900	-4.56510800	-2.61216500
H	1.92262100	-3.17460200	-0.11788300	H	0.87149000	-3.09760800	-3.46600200
H	0.47823800	-2.55105700	0.69215100	H	1.97706400	-3.86483500	-2.31528900
H	0.45560100	-4.16565200	-0.02857100	C	-1.26296900	1.28798300	-0.67666800
H	-1.50285800	-1.99545100	-2.44083800	C	-0.15171300	1.33365600	0.20532000
H	-1.62827400	-3.43336900	-1.41542100	C	-0.41342900	1.79124700	1.53085600
H	-1.53297600	-1.82486200	-0.68191900	C	-1.70164500	2.16652000	1.89412500
H	0.49106700	-4.37423000	-2.62892000	C	-2.77500600	2.11895700	1.00771200
H	0.55705500	-2.89386300	-3.59751200	C	-2.53577200	1.66932900	-0.29009200
H	1.96397000	-3.38945000	-2.64490600	H	-1.10080400	0.94804300	-1.69614900
C	-1.38626700	1.33485300	-0.66501900	H	-1.87008400	2.50117800	2.91388400
C	-0.29693600	1.36083500	0.23537100	H	-3.76589600	2.42313300	1.31947300
C	-0.50053600	2.00253900	1.48352100	H	-3.34771800	1.61915300	-1.00745100
C	-1.72652000	2.60209000	1.75745000	C	0.71518600	1.83735900	2.53740700
C	-2.77958000	2.59004500	0.84898200	C	1.84288600	0.88959200	2.13460200
C	-2.59693000	1.93796500	-0.36904600	C	2.19445900	1.13369200	0.66716800
H	-1.26867500	0.81487700	-1.61042000	N	1.07321000	0.91285700	-0.24002000
H	-1.85983400	3.08350300	2.72158000	H	0.33742200	1.59093900	3.53377900
H	-3.72144700	3.06662500	1.08883800	H	1.51867300	-0.14968300	2.25621500
H	-3.40409500	1.89607800	-1.09156400	H	3.01980900	0.47598600	0.36981400
C	0.60422700	1.99271100	2.51493500	H	0.93614300	-1.01133400	-0.57137300
C	1.54963300	0.81761700	2.27609400	H	1.11560100	2.85607200	2.60593600
C	1.99971800	0.83382300	0.81753400	H	2.72025900	1.03603600	2.77048300
N	0.88977300	0.75055100	-0.13175400	H	2.57985100	2.16388500	0.57784900
H	0.17378400	1.94855500	3.51873400				
H	1.03113300	-0.12365800	2.48349700	<b>TS2<sub>Li</sub></b>			
H	2.67564700	-0.00477000	0.62114800	Li	-3.60302700	-3.76920000	1.70957800
H	0.76180700	-0.50420600	-0.71280900	O	-4.50129100	-5.37346900	1.21333800
H	1.17601100	2.92734500	2.46593900	C	-4.18123700	-6.74321400	0.85334700
H	2.41499400	0.87060200	2.94140900	C	-3.30680100	-7.35161200	1.94778000
H	2.58472200	1.75235100	0.65287400	C	-5.48768200	-7.51538800	0.69572000
<b>M2<sub>Li</sub></b>				C	-3.42898300	-6.64895500	-0.46634700
Li	1.38846000	0.20050500	-1.97031500	H	-2.38837800	-6.77450600	2.06952600
O	1.14982900	-1.57173900	-1.36068400	H	-3.83745500	-7.36496600	2.90303900
C	0.35022200	-2.78161000	-1.39024100	H	-3.03609300	-8.37972800	1.69993300
C	0.48823800	-3.47960100	-0.03982700	H	-6.11879400	-7.04552400	-0.06019300

H	-5.29451200	-8.54674200	0.39512200	H	0.63191400	2.52221000	0.21272700
H	-6.03907300	-7.53711600	1.63898200	C	0.79980700	-1.66706000	0.87750200
H	-3.16011100	-7.64385600	-0.82429000	C	0.58502000	-0.27330000	1.16449200
H	-4.04567900	-6.16443100	-1.22529700	C	-0.66158100	0.03734400	1.83109600
H	-2.51081800	-6.07069800	-0.34488600	C	-1.61722700	-0.95017100	2.02638000
C	-6.95016600	-2.90794000	3.05389300	C	-1.42432600	-2.28322100	1.62773900
C	-5.64971000	-2.70465500	3.52578000	C	-0.17183200	-2.62828100	1.09195500
C	-5.27686700	-1.43292100	4.00260400	H	1.74497200	-1.93526600	0.42125600
C	-6.21662400	-0.40864000	3.99323300	H	-2.55882200	-0.67063000	2.48994500
C	-7.51092800	-0.61677600	3.52433100	H	-2.18792800	-3.02983900	1.79531900
C	-7.87636600	-1.87368100	3.05390300	H	0.03210500	-3.65824300	0.82181200
H	-7.22145600	-3.89291500	2.69301500	C	-0.90177400	1.46879900	2.25115200
H	-5.92913800	0.56991900	4.36252200	C	0.42592900	2.22043300	2.32693800
H	-8.22726000	0.19524100	3.52894900	C	1.19438000	2.02187500	1.01995900
H	-8.88084000	-2.04903700	2.68882900	N	1.44108400	0.62505000	0.67864500
C	-3.85916400	-1.21679500	4.47910700	H	-1.42579000	1.49210700	3.21089000
C	-3.24444300	-2.52658400	4.96446500	H	1.02291900	1.82935700	3.15699100
C	-3.58083900	-3.65922500	4.03996700	H	-1.55527600	1.97215700	1.52867300
N	-4.75469900	-3.79448600	3.47737700	H	0.25944100	3.28378500	2.51671300
H	-3.83792300	-0.46560500	5.27114500	H	2.15868900	2.53770500	1.07167100
H	-3.66536700	-2.79612900	5.94372500				
H	-2.96422500	-4.54850100	4.09599600	<b>TS3<sub>Li</sub></b>			
H	-4.93713700	-5.32552000	2.08812300	Li	-2.72116200	-0.55834800	-1.55461100
H	-3.25588400	-0.82932100	3.65356800	O	-2.15782900	0.73983600	-2.63028100
H	-2.16563700	-2.44592300	5.08267000	C	-2.23787800	1.05951800	-4.01119300
H	-2.25613900	-3.13254300	2.51534100	C	-2.86819000	2.44826100	-4.17333000
				C	-3.11551700	0.00574400	-4.69214500
<b>M3<sub>Li</sub></b>				C	-0.83035300	1.04135200	-4.61951600
Li	-1.07440700	-1.01778000	-0.30034800	H	-2.25708100	3.20182000	-3.67324400
O	-0.18837600	0.11155700	-1.51201500	H	-3.86285400	2.46438800	-3.72223000
C	0.05817100	0.40666600	-2.90512000	H	-2.96133200	2.72616000	-5.22618400
C	0.30524100	1.90730200	-3.04603200	H	-2.67919700	-0.99011100	-4.57481300
C	-1.19969300	-0.01508500	-3.65307200	H	-3.21610900	0.20219100	-5.76236800
C	1.27339500	-0.39663700	-3.36518700	H	-4.11841800	0.00216200	-4.25637300
H	1.18223200	2.20727300	-2.46878500	H	-0.85299700	1.26846900	-5.68842500
H	-0.55504800	2.47107000	-2.68112600	H	-0.37441200	0.05828500	-4.48367200
H	0.47858500	2.17597500	-4.08984700	H	-0.19506200	1.77782500	-4.12449500
H	-1.38182100	-1.08565000	-3.53204100	H	-1.44215700	1.61047900	-2.01106100
H	-1.10043000	0.19057300	-4.71995700	H	-0.89961700	2.20470700	-1.45074900
H	-2.06884000	0.53032900	-3.27962100	C	-1.63662900	-1.51449900	0.41641300
H	1.48946500	-0.20802000	-4.41865500	C	-1.63266000	-0.10260000	0.46851700
H	1.09481300	-1.46547300	-3.23371200	C	-2.88743900	0.56596400	0.52232000
H	2.15439800	-0.12444300	-2.78036700	C	-4.06315500	-0.18010600	0.47064900
H	0.58954800	0.38381700	-0.94272200	C	-4.05037600	-1.57367500	0.37855500

C	-2.82147800	-2.23829400	0.36689200	C	2.91067600	1.58827100	-1.62701200
H	-0.67821900	-2.01626700	0.37170100	C	1.45772500	1.38061700	-1.92428900
H	-5.01279600	0.34428800	0.48328100	H	4.28141800	1.23706300	0.01726600
H	-4.97849800	-2.12688400	0.32530400	H	3.47652000	0.90644500	-2.27651500
H	-2.78836300	-3.31881500	0.30311200	H	2.82845300	2.11685600	0.45990900
C	-2.93462300	2.07782700	0.54204600	H	3.20698100	2.60047800	-1.90416300
C	-1.55598400	2.68535200	0.79562400	H	0.98853300	1.98040500	-2.70097600
C	-0.45831500	1.84674400	0.18396300	N	0.72390800	0.51250200	-1.33689900
N	-0.42047800	0.54144400	0.31518900				
H	-3.64424800	2.41296600	1.30223300	<b>TS4<sub>Li</sub></b>			
H	-1.35031500	2.71105400	1.87325900	O	-1.81630200	0.50446300	-0.51289800
H	-3.31693300	2.42634600	-0.42017600	C	-2.84154200	0.31697800	0.44880400
H	-1.50527200	3.71153200	0.43215000	C	-3.14739800	1.65088200	1.14295100
H	0.50058000	2.33748300	0.04240300	C	-4.09645000	-0.21345600	-0.25405100
				H	-3.47708500	2.39209700	0.41247400
<b>M4<sub>Li</sub></b>				H	-2.25006200	2.03438000	1.63421100
O	-2.72237600	-0.21484800	-0.81612400	H	-3.93138300	1.54133800	1.89668800
C	-3.44543000	0.08366500	0.40268200	H	-4.90660700	-0.39845100	0.45610200
C	-3.38528700	1.58800600	0.66952200	H	-3.86993900	-1.14740600	-0.77254700
C	-4.88894100	-0.38672000	0.23798000	H	-4.44935800	0.50702800	-0.99500300
H	-3.83943000	2.14450000	-0.15259400	H	-2.03249900	1.32776700	-1.33546500
H	-2.34932500	1.91759700	0.77329700	H	-1.76832900	2.06909200	-2.10059400
H	-3.91747100	1.84105000	1.58898800	C	-2.33569300	-0.70381400	1.46978800
H	-5.46251300	-0.21041000	1.15036200	H	-3.09081900	-0.91073900	2.23243200
H	-4.91639400	-1.45393400	0.01178100	H	-2.08415700	-1.64315300	0.97264600
H	-5.37864800	0.14917500	-0.57849100	H	-1.44021300	-0.32879800	1.96966000
H	-3.12480100	0.24992400	-1.59040700	Li	-0.33110000	1.27083100	-1.22408600
H	-2.35169800	1.05017500	-3.01498500	C	1.42923500	-0.64830500	0.51560800
C	-2.73753300	-0.69415800	1.50415300	C	2.25308300	0.24537200	-0.16683700
H	-3.22905100	-0.52750800	2.46441700	C	3.61972300	0.33015100	0.13911700
H	-2.75528400	-1.76421400	1.29049000	C	4.13308900	-0.49220400	1.13422900
H	-1.69695900	-0.37847900	1.59225800	C	3.31340700	-1.38989100	1.81338200
Li	-1.22089100	0.44370200	-1.84220000	C	1.96034400	-1.46854200	1.50222300
C	0.62047400	-1.46739200	0.04126100	H	0.37531700	-0.69483800	0.26906400
C	1.30667800	-0.31600000	-0.34045900	H	5.18748400	-0.43164500	1.37867800
C	2.52884200	0.01498100	0.26527300	H	3.73249500	-2.02584100	2.58297200
C	3.03647800	-0.82406200	1.24975200	H	1.31691200	-2.16297000	2.02707900
C	2.35358200	-1.97710000	1.62778100	C	4.45198800	1.34474900	-0.60023400
C	1.14509800	-2.29985700	1.02095200	C	3.91455300	1.53670800	-2.01825700
H	-0.32545600	-1.70298000	-0.42965000	C	2.42239900	1.66384300	-2.00393300
H	3.97836400	-0.57433900	1.72474200	H	5.49956600	1.04334500	-0.62284600
H	2.76596300	-2.62106100	2.39427500	H	4.16072100	0.66584500	-2.64120500
H	0.60843500	-3.19389100	1.31112600	H	4.40807200	2.30055000	-0.06478300
C	3.20652100	1.29280000	-0.15677100	H	4.35925200	2.40463800	-2.50583200

H	1.94045900	2.27141400	-2.76686100	C	-0.24053100	0.40307000	-3.24140400
N	1.66279600	1.07438900	-1.16005600	C	-0.27888900	1.93251400	-3.04212100
				C	-1.56305700	-0.05067000	-3.89098700
<b>M4a<sub>Li</sub></b>				C	0.92747300	0.05204800	-4.18501600
O	0.21377500	0.35277600	-1.14941700	H	0.65097500	2.26707700	-2.57570700
C	-0.45216900	0.09276000	0.13578800	H	-1.10379900	2.19557100	-2.37455100
C	-0.77975900	1.43431000	0.78025200	H	-0.40835700	2.47805000	-3.98219400
C	-1.70770000	-0.72628000	-0.13686900	H	-1.54819400	-1.13387100	-4.03675300
H	-1.46636200	2.01021900	0.15460200	H	-1.74375200	0.42466500	-4.86046300
H	0.12799700	2.02111100	0.92685900	H	-2.39980600	0.18764300	-3.22894600
H	-1.25697800	1.28670100	1.75038200	H	0.83476000	0.52924100	-5.16576200
H	-2.22196400	-0.95775800	0.79726700	H	0.96962600	-1.03022300	-4.33067500
H	-1.45566400	-1.66374300	-0.63442100	H	1.87273400	0.36771700	-3.73697400
H	-2.40437900	-0.17388500	-0.77285800	H	2.14039900	0.58913800	-1.12869100
H	-0.39454700	0.83580100	-1.72359800	H	2.70436900	0.72762700	-0.65580900
H	3.53534100	-0.17022300	-2.21903400	C	1.04733000	-1.63164600	1.71832900
C	0.55901400	-0.69197600	0.95753400	C	0.75101500	-0.27426000	1.87558100
H	0.13656900	-0.93863700	1.93185700	C	-0.57259000	0.17909300	1.71225000
H	0.82572600	-1.62682800	0.46041000	C	-1.56968600	-0.74364500	1.40483700
H	1.46713800	-0.10876800	1.12575000	C	-1.27385700	-2.10028200	1.26206500
Li	1.98752700	0.02267100	-1.67072500	C	0.03902700	-2.54442100	1.41861800
				H	2.07517800	-1.95104800	1.83090900
<b>TS4a<sub>Li</sub></b>				H	-2.58635600	-0.39711600	1.26322600
O	-1.74309100	0.58070700	-0.45517200	H	-2.06138300	-2.80140800	1.01921700
C	-2.78644900	0.53266700	0.50802400	H	0.27743400	-3.59330800	1.30013100
C	-3.12851400	1.95982700	0.94755700	C	-0.82684700	1.65853600	1.81774200
C	-4.01320000	-0.14234400	-0.11396700	C	0.15180700	2.29587300	2.80400000
H	-3.47661300	2.54710400	0.09538400	C	1.54316200	1.77295200	2.57935900
H	-2.24385200	2.45000200	1.35888900	N	1.82035900	0.60304900	2.15628600
H	-3.91205800	1.96323700	1.70908300	H	-1.85950700	1.85255300	2.10854100
H	-4.83495600	-0.21217700	0.60257600	H	-0.13014800	2.05591600	3.83798100
H	-3.75909500	-1.15052000	-0.44760000	H	-0.68601700	2.10253600	0.82565800
H	-4.36083700	0.42453300	-0.97992500	H	0.14360000	3.38336100	2.72434900
H	-1.97093400	1.16050500	-1.45858900	H	2.38345700	2.42549900	2.81051700
H	-1.69624500	1.50771000	-2.47391800				
C	-2.27433200	-0.28296700	1.69514300				
H	-3.02959500	-0.35470100	2.48153900				
H	-2.01424500	-1.29472300	1.37616800				
H	-1.38166700	0.18266100	2.11839700				
Li	-0.44328300	0.50492700	-1.63275300				
<b>M5<sub>Li</sub></b>							
Li	0.02260000	-0.94827700	-0.56451400				
O	-0.07164900	-0.22343600	-2.02738400				