

Mechanism, Chemoselectivity and Enantioselectivity for Rhodium-  
Catalyzed Desymmetric Synthesis of Hydrobenzofurans: A  
Theoretical Study

*Supporting Information*

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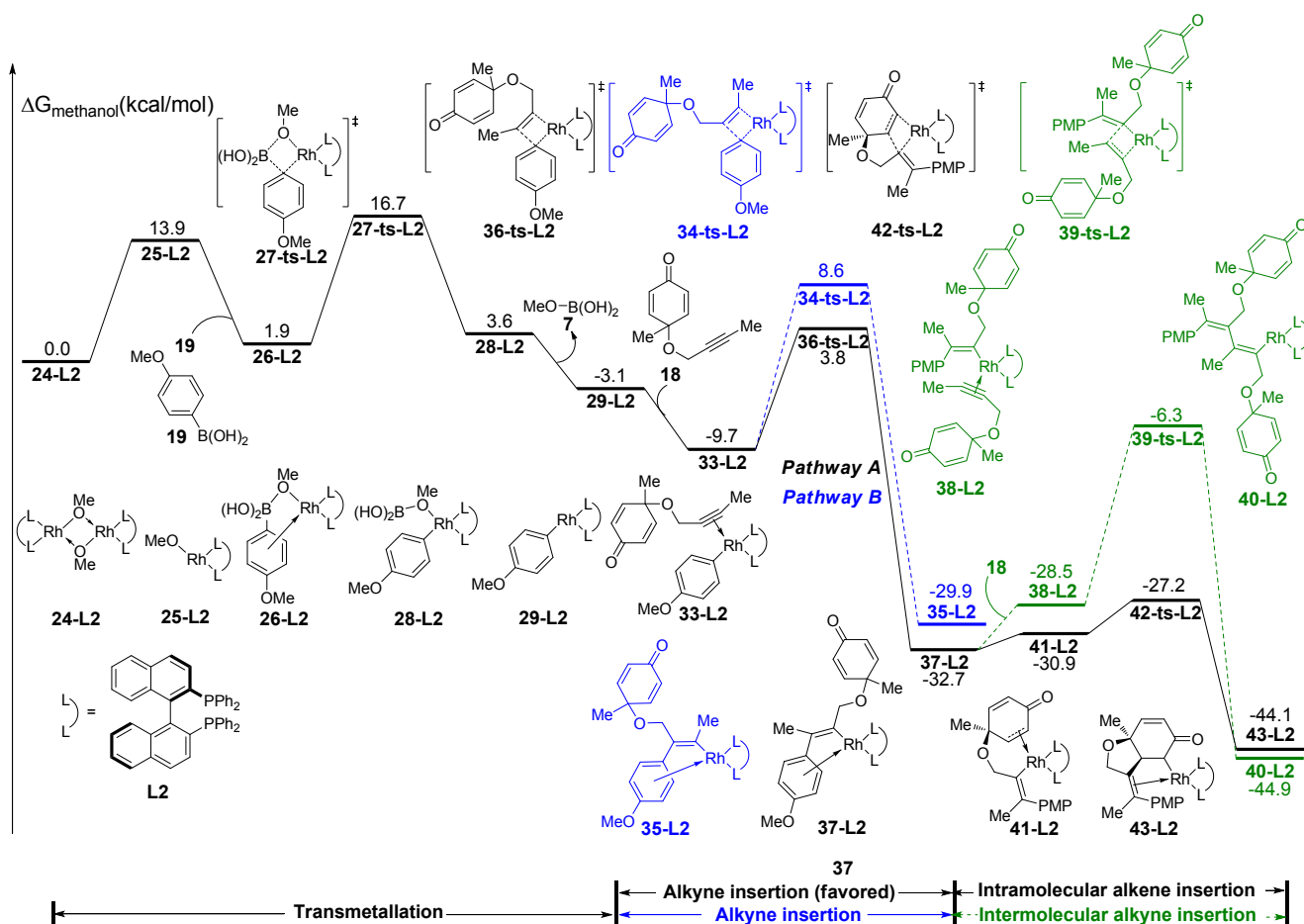
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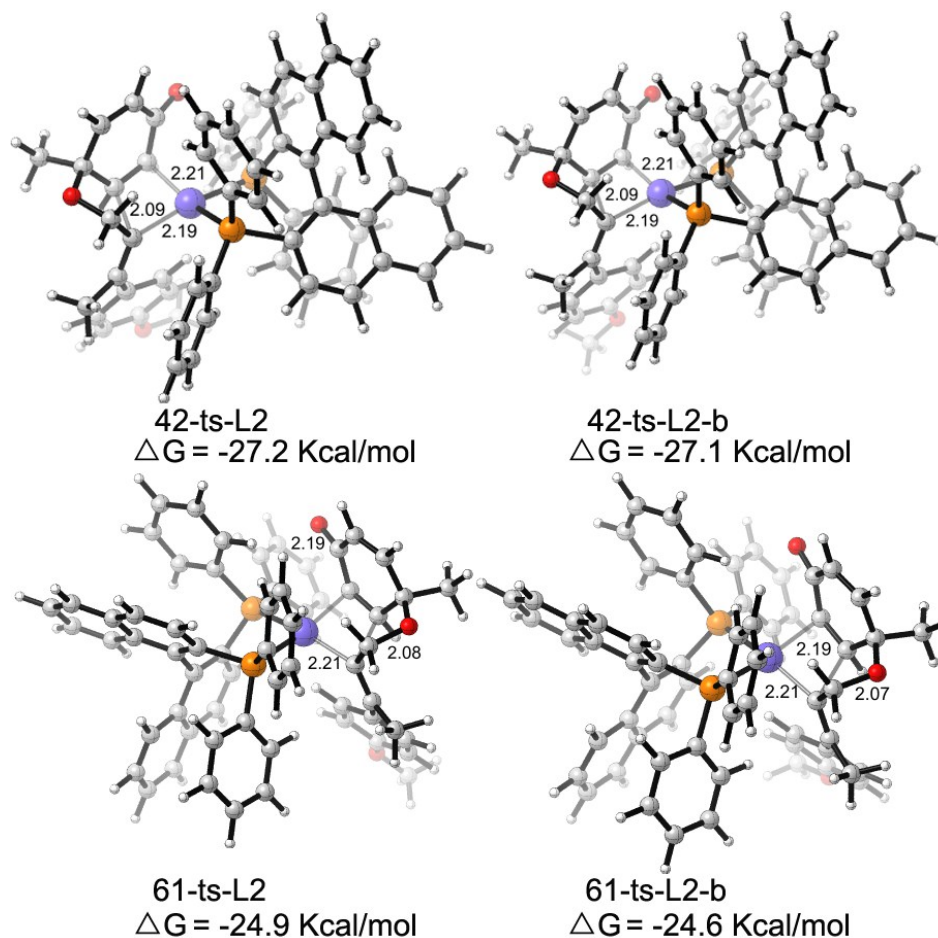
# 1. Free energy profiles for rhodium-catalyzed desymmetric synthesis of hydrobenzofurans with L2, L3, and L4 ligand.

As shown in Figure S1. After dissociation of rhodium complex **24-L2**, the complex **25-L2** undergoes transmetallation with reactant **19** via transition state **27-ts-L2** with an overall energy barrier of 14.8 kcal/mol. There are two insertion modes when intermediate **33-L2** is formed by the coordination of substrate **18**. The relative free energy of transition state **34-ts-L2** is 4.8 kcal/mol higher than **36-ts-L2**. Intermediate **37-L2** could isomerize to **41-L2** then intramolecular alkene insertion takes place in transition state **42-ts-L2** with 5.5 kcal/mol energy barrier. We also considered the competition with intermolecular alkyne insertion. When another molecule **18** coordinates with **37-L2**, the free energy increased 4.2 kcal/mol. The following alkyne insertion would take place via **39-ts-L2** with 26.4 kcal/mol energy barrier.



**Figure S1.** Free energy profile for rhodium-catalyzed synthesis of hydrobenzofurans with **L2** ligand.

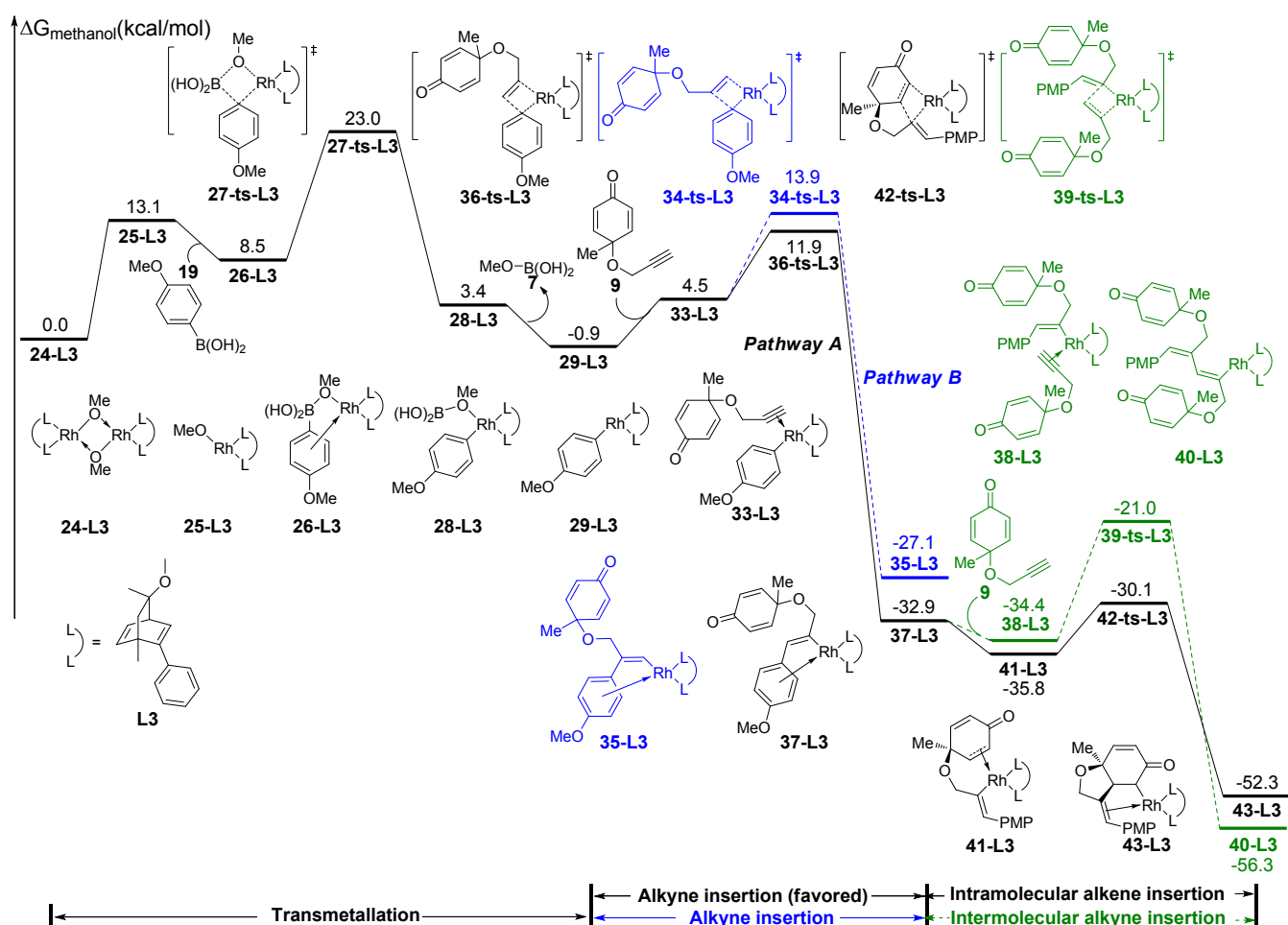
The values given in kcal/mol are the MN12-L calculated relative free energies in methanol solvent.



**Figure S2.** Geometries of **42-ts** and **61-ts** with **L2** ligand. The values of bond lengths are given in angstrom. The values given in kcal/mol are the MN12-L calculated relative free energies in methanol solvent.

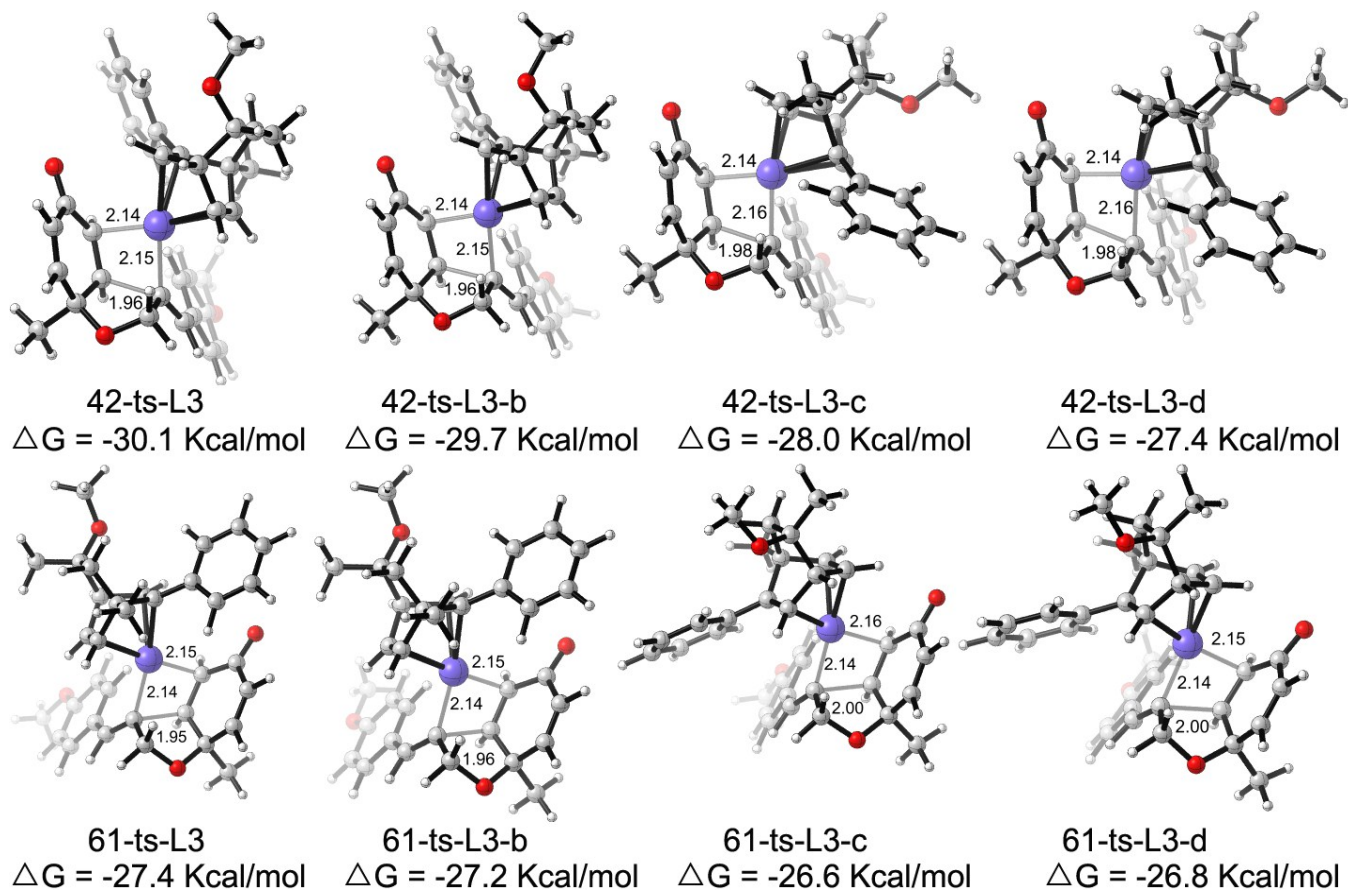
As shown in Figure S3. After dissociation of rhodium complex **24-L3**, the complex **25-L3** undergoes transmetalation with reactant **19** via transition state **27-ts-L3** with an overall energy barrier of 14.5

kcal/mol. There are two insertion modes when intermediate **33-L3** is formed by the coordination of substrate **9**. The relative free energy of transition state **34-ts-L3** is 2.0 kcal/mol higher than **36-ts-L3**. Intermediate **37-L3** could isomerize to **41-L3** then intramolecular alkene insertion takes place in transition state **42-ts-L3** with 5.7 kcal/mol energy barrier. We also considered the competition with intermolecular alkyne insertion. When another molecule **9** coordinates with **37-L3**, the free energy decreased 1.5 kcal/mol. The following alkyne insertion would take place via **39-ts-L3** with 13.4 kcal/mol energy barrier.



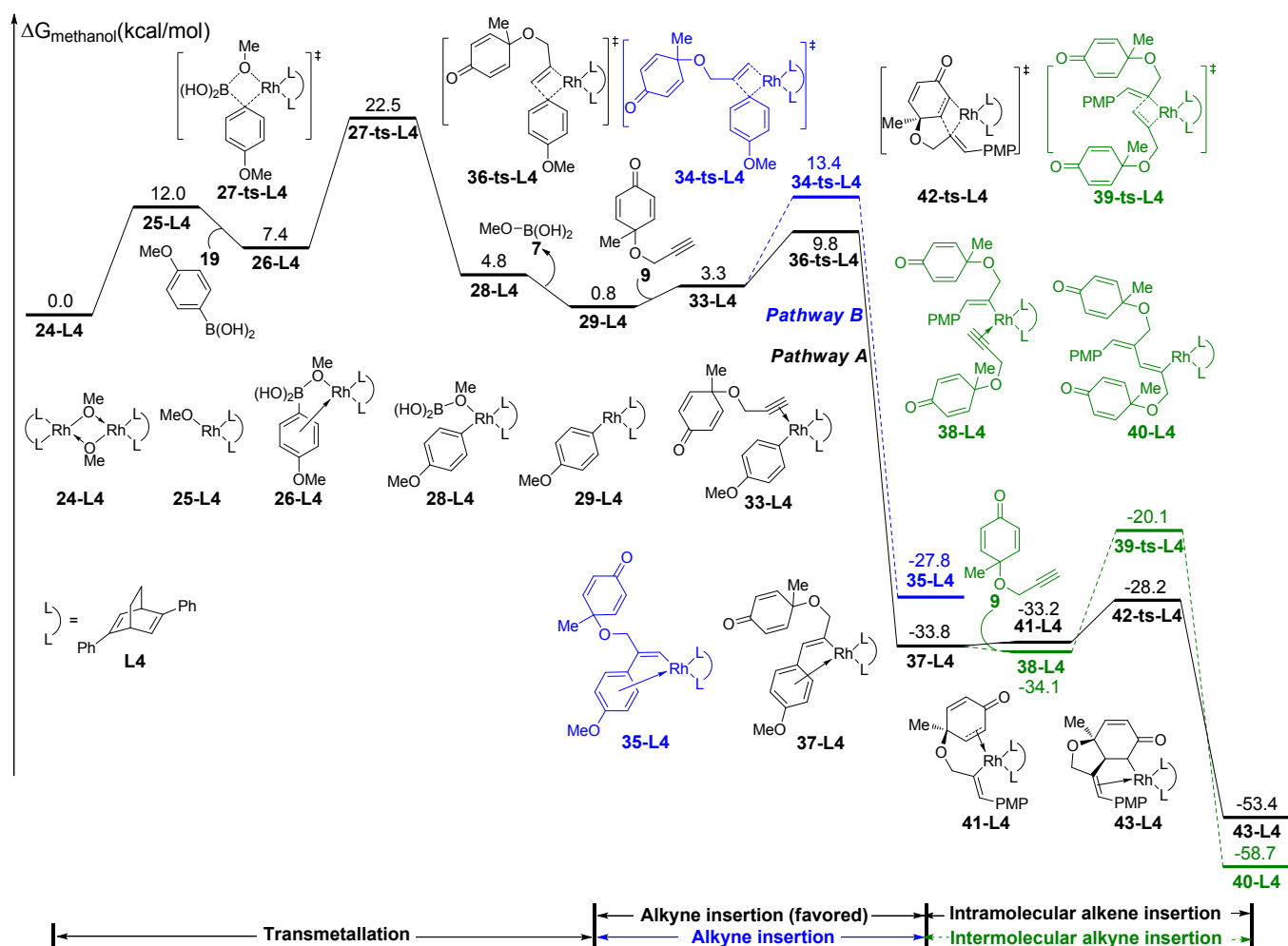
**Figure S3.** Free energy profile for rhodium-catalyzed synthesis of hydrobenzofurans with **L3** ligand.

The values given in kcal/mol are the MN12-L calculated relative free energies in methanol solvent.



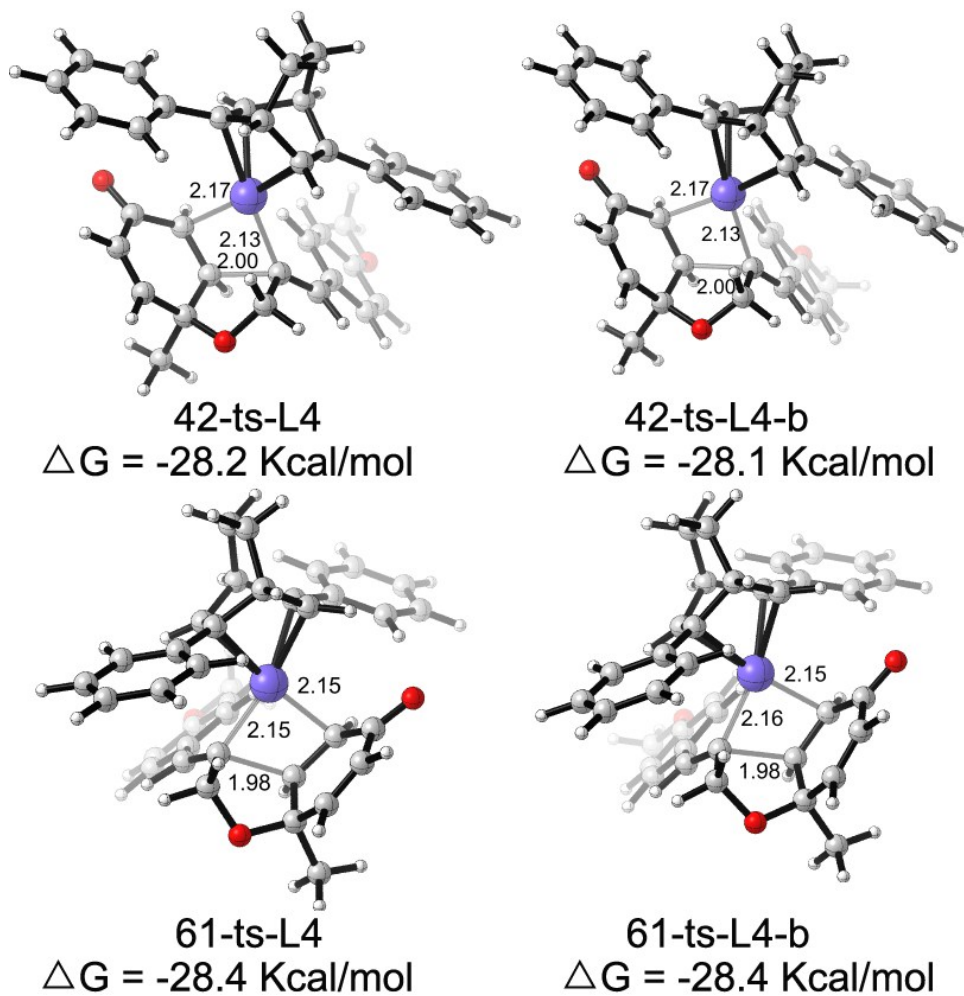
**Figure S4.** Geometries of **42-ts** and **61-ts** with **L3** ligand. The values of bond lengths are given in angstrom. The values given in kcal/mol are the MN12-L calculated relative free energies in methanol solvent.

As shown in Figure S7. After dissociation of rhodium complex **24-L4**, the complex **25-L4** undergoes transmetallation with reactant **19** via transition state **27-ts-L4** with an overall energy barrier of 15.1 kcal/mol. There are two insertion modes when intermediate **33-L4** is formed by the coordination of substrate **9**. The relative free energy of transition state **34-ts-L4** is 3.6 kcal/mol higher than **36-ts-L4**. Intermediate **37-L4** could isomerize to **41-L4** then intramolecular alkene insertion takes place in transition state **42-ts-L4** with 5.6 kcal/mol energy barrier. We also considered the competition with intermolecular alkyne insertion. When another molecule **9** coordinates with **37-L4**, the free energy decreased 0.3 kcal/mol. The following alkyne insertion would take place via **39-ts-L4** with 14.0 kcal/mol energy barrier.



**Figure S5.** Free energy profile for rhodium-catalyzed synthesis of hydrobenzofurans with **L4** ligand.

The values given in kcal/mol are the MN12-L calculated relative free energies in methanol solvent.

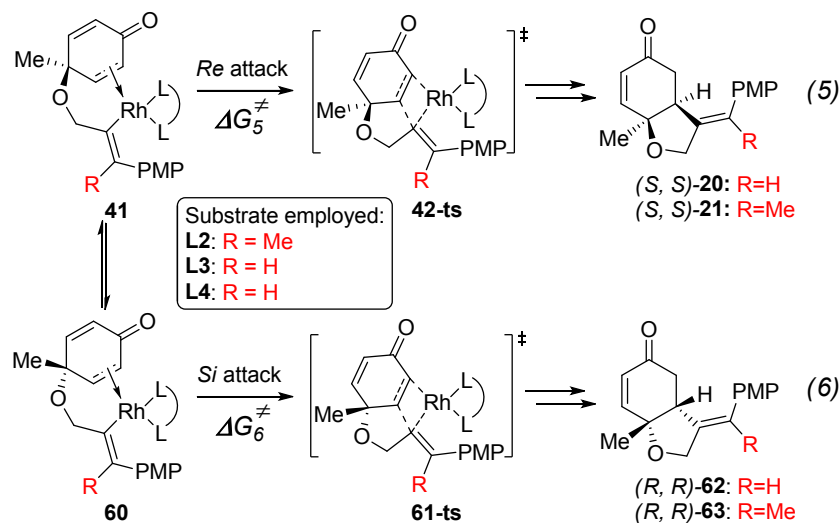


**Figure S6.** Geometries of 42-ts and 61-ts with L5 ligand. The values of bond lengths are given in angstrom. The values given in kcal/mol are the MN12-L calculated relative free energies in methanol solvent.



## 2. The calculated *ee* values by B97D3 functional, M06-L functional and M11-L functional.

Table S1. Calculated and Experimentally Observed *ee* Values with Different DFT Functional



DFT functional	ligand	$\Delta\Delta G^\ddagger = (\Delta G_5^\ddagger - \Delta G_6^\ddagger)$	ee (calc.)	ee (exp.)
B97D3	L2	0.8	59%	96%
B97D3	L3	1.5	85%	76%
B97D3	L4	-0.5	-40%	-6%
M06-L	L2	1.6	87%	96%
M06-L	L3	2.3	96%	76%
M06-L	L4	-0.7	-53%	-6%
M11-L	L2	0.5	40%	96%
M11-L	L3	2.0	93%	76%
M11-L	L4	0.7	53%	-6%

## 3. B97D3, M06-L and M11-L absolute calculation free energies of 42-ts and 61-ts.

Geometry	$E_{B97D3(\text{Methanol})}$	$E_{M06-L(\text{Methanol})}$	$E_{M11-L(\text{Methanol})}$
<b>42-ts-L2</b>	-3410.547616	-3411.634411	-3411.521496
<b>42-ts-L2-b</b>	-3410.546864	-3411.634167	-3411.521551
<b>61-ts-L2</b>	-3410.543850	-3411.630019	-3411.518885
<b>61-ts-L2-b</b>	-3410.543836	-3411.629216	-3411.517712
<b>42-ts-L3</b>	-1727.910248	-1728.515927	-1728.484339
<b>42-ts-L3-b</b>	-1727.910218	-1728.515816	-1728.484247
<b>42-ts-L3-c</b>	-1727.909532	-1728.513701	-1728.482576
<b>42-ts-L3-d</b>	-1727.910001	-1728.514287	-1728.483175
<b>61-ts-L3</b>	-1727.907048	-1728.512945	-1728.481767
<b>61-ts-L3-b</b>	-1727.907093	-1728.512768	-1728.481411
<b>61-ts-L3-c</b>	-1727.908677	-1728.511982	-1728.480550
<b>61-ts-L3-d</b>	-1727.908838	-1728.512267	-1728.480786
<b>42-ts-L4</b>	-1765.784125	-1766.423371	-1766.401089
<b>42-ts-L4-b</b>	-1765.784008	-1766.423333	-1766.401103
<b>61-ts-L4</b>	-1765.786368	-1766.426032	-1766.401245
<b>61-ts-L4-b</b>	-1765.785559	-1766.425225	-1766.400884

#### 4. B3LYP, MN12-L absolute calculation free energies.

Geometry	E <sub>B3LYP(elec)</sub>	E <sub>MN12-L(Methanol)</sub>	Correction of H <sub>(gas phase)</sub>	Correction of G <sub>(gas phase)</sub>	IF*
<b>L1</b>	-271.472318	-271.271519	0.134833	0.100910	-
<b>L2</b>	-2378.638362	-2377.514983	0.660786	0.546562	-
<b>L3</b>	-735.005039	-734.469628	0.345188	0.285964	-
<b>L4</b>	-772.923685	-772.380833	0.337953	0.278338	-
<b>7</b>	-291.765500	-291.636595	0.083734	0.046495	-
<b>9</b>	-537.395200	-537.051927	0.186277	0.136075	-
<b>12</b>	-115.712204	-115.635456	0.055708	0.028754	-
<b>18</b>	-576.721301	-576.337746	0.216904	0.160821	-
<b>19</b>	-522.773821	-522.490962	0.169162	0.121357	-
<b>20</b>	-884.251081	-883.666832	0.333633	0.268545	-
<b>21</b>	-923.565150	-922.942517	0.363003	0.293742	-
<b>22</b>	-1421.717969	-1420.785707	0.524642	0.428957	-
<b>23</b>	-1500.335733	-1499.328606	0.583819	0.480824	-
<b>24</b>	-992.367464	-990.045609	0.368105	0.297583	-
<b>25</b>	-496.142420	-494.992479	0.182613	0.135520	-
<b>26</b>	-1018.947350	-1017.512887	0.353737	0.281566	-
<b>27-ts</b>	-1018.930525	-1017.485918	0.352217	0.280122	-248.9
<b>28</b>	-1018.965685	-1017.517152	0.354775	0.279408	-
<b>29</b>	-727.166463	-725.866538	0.268118	0.210049	-
<b>30</b>	-1264.582826	-1262.938056	0.456677	0.369237	-
<b>31-ts</b>	-1264.551918	-1262.902012	0.455322	0.371456	-278.5
<b>32</b>	-1264.606847	-1262.957105	0.457803	0.372935	-
<b>33</b>	-1264.592918	-1262.931747	0.457094	0.369020	-
<b>34-ts</b>	-1264.578494	-1262.914741	0.455611	0.369265	-297.5
<b>35</b>	-1264.643203	-1262.983727	0.458721	0.373185	-
<b>36-ts</b>	-1264.580950	-1262.915387	0.455697	0.368334	-264.6
<b>37</b>	-1264.645579	-1262.989320	0.458635	0.372668	-
<b>38</b>	-1802.056578	-1800.065860	0.646987	0.529588	-
<b>39-ts</b>	-1802.049049	-1800.043384	0.646272	0.528843	-269.8
<b>40</b>	-1802.106902	-1800.110221	0.649854	0.535597	-

<b>41</b>	-1264.659833	-1263.003971	0.459756	0.379122	-
<b>42-ts</b>	-1264.644289	-1262.991923	0.457976	0.377782	-301.2
<b>43</b>	-1264.680905	-1263.032341	0.460216	0.379823	-
<b>44</b>	-1264.681954	-1263.026206	0.460331	0.378696	-
<b>45</b>	-1380.411238	-1378.672886	0.518577	0.427259	-
<b>46-ts</b>	-1380.400402	-1378.648197	0.512930	0.421566	-1228.9
<b>47</b>	-1380.418295	-1378.672147	0.517985	0.424174	-
<b>48-ts</b>	-1264.613349	-1262.962652	0.457927	0.378475	-219.1
<b>49</b>	-1264.614002	-1262.965628	0.458995	0.378974	-
<b>50</b>	-1802.054159	-1800.060419	0.646909	0.528913	-
<b>51-ts</b>	-1802.047931	-1800.039964	0.646518	0.530763	-294.8
<b>52</b>	-1802.112851	-1800.112922	0.649958	0.533297	-
<b>53</b>	-1802.124500	-1800.120011	0.650721	0.538806	-
<b>54-ts</b>	-1802.109153	-1800.108340	0.649086	0.539132	-291.6
<b>55</b>	-1802.149604	-1800.154096	0.651077	0.540765	-
<b>56</b>	-1802.149857	-1800.145656	0.651249	0.540357	-
<b>57</b>	-1917.877764	-1915.790174	0.709353	0.589794	-
<b>58-ts</b>	-1917.868257	-1915.768922	0.703987	0.584951	-1251.5
<b>59</b>	-1917.888236	-1915.792191	0.709546	0.589932	-
<b>62</b>	-884.251081	-883.666831	0.333633	0.268543	-
<b>63</b>	-923.565150	-922.942517	0.363003	0.293742	-
<b>24-L2</b>	-5206.685696	-5202.561678	1.422942	1.212443	-
<b>25-L2</b>	-2603.317540	-2601.242062	0.709846	0.589656	-
<b>26-L2</b>	-3126.109750	-3123.777568	0.881194	0.736407	-
<b>27-ts-L2</b>	-3126.096927	-3123.753310	0.879582	0.735672	-246.4
<b>28-L2</b>	-3126.121655	-3123.774450	0.881640	0.735950	-
<b>29-L2</b>	-2834.341408	-2832.120450	0.795045	0.661417	-
<b>33-L2</b>	-3411.077802	-3408.497181	1.014344	0.850713	-
<b>34-ts-L2</b>	-3411.065861	-3408.467585	1.013106	0.850287	-243.4
<b>35-L2</b>	-3411.124317	-3408.530940	1.015663	0.852166	-
<b>36-ts-L2</b>	-3411.069029	-3408.474594	1.013098	0.849665	-248.7

<b>37-L2</b>	-3411.124454	-3408.536462	1.015555	0.853269	-
<b>38-L2</b>	-3987.852734	-3984.897499	1.234726	1.044130	-
<b>39-ts-L2</b>	-3987.823017	-3984.860986	1.233613	1.043004	-219.6
<b>40-L2</b>	-3987.887874	-3984.924657	1.236190	1.045072	-
<b>41-L2</b>	-3411.114812	-3408.541902	1.016463	0.861549	-
<b>42-ts-L2</b>	-3411.109305	-3408.536624	1.015071	0.862192	-200.6
<b>42-ts-L2-b</b>	-3411.108902	-3408.536405	1.015080	0.862175	-203.0
<b>43-L2</b>	-3411.137975	-3408.563703	1.017431	0.862341	-
<b>60-L2</b>	-3411.113676	-3408.540183	1.017090	0.861817	-
<b>61-ts-L2</b>	-3411.110642	-3408.531058	1.015236	0.860385	-233.8
<b>61-ts-L2-b</b>	-3411.110794	-3408.529943	1.015102	0.859647	-234.6
<b>24-L3</b>	-1919.424322	-1916.442368	0.788969	0.668189	-
<b>25 -L3</b>	-959.671393	-958.189213	0.393282	0.323006	-
<b>26-L3</b>	-1482.476382	-1480.710963	0.564218	0.467831	-
<b>27-ts-L3</b>	-1482.460907	-1480.685442	0.562772	0.465468	-244.9
<b>28-L3</b>	-1482.496785	-1480.717971	0.565577	0.466731	-
<b>29-L3</b>	-1190.695967	-1189.063100	0.478493	0.395073	-
<b>33-L3</b>	-1728.122072	-1726.130156	0.667595	0.554917	-
<b>34-ts-L3</b>	-1728.109043	-1726.114771	0.665988	0.554481	-296.3
<b>35-L3</b>	-1728.171188	-1726.183979	0.668917	0.558362	-
<b>36-ts-L3</b>	-1728.112371	-1726.119036	0.666179	0.555533	-275.1
<b>37-L3</b>	-1728.175584	-1726.193855	0.669016	0.558961	-
<b>38-L3</b>	-2265.586016	-2263.269696	0.857592	0.716533	-
<b>39-ts-L3</b>	-2265.578614	-2263.249534	0.857049	0.717829	-284.1
<b>40-L3</b>	-2265.635383	-2263.310182	0.860423	0.722132	-
<b>41-L3</b>	-1728.187744	-1726.204795	0.670387	0.565298	-
<b>42-ts-L3</b>	-1728.172091	-1726.194158	0.668539	0.563667	-296.1
<b>42-ts-L3-b</b>	-1728.172082	-1726.193985	0.668578	0.564190	-297.1
<b>42-ts-L3-c</b>	-1728.173130	-1726.190886	0.668726	0.563818	-298.0
<b>42-ts-L3-d</b>	-1728.173385	-1726.191456	0.669044	0.565360	-295.6
<b>60-L3</b>	-1728.180356	-1726.198076	0.670323	0.565279	-

<b>61-ts-L3</b>	-1728.167911	-1726.190427	0.668591	0.564311	-295.3
<b>61-ts-L3-b</b>	-1728.168045	-1726.190020	0.668538	0.564230	-293.1
<b>61-ts-L3-c</b>	-1728.171529	-1726.189521	0.668735	0.564623	-281.5
<b>61-ts-L3-d</b>	-1728.171659	-1726.189836	0.668762	0.564667	-277.3
<b>24-L4</b>	-1995.244467	-1992.257204	0.773728	0.653676	-
<b>25-L4</b>	-997.582774	-996.096000	0.385560	0.313348	-
<b>26-L4</b>	-1520.385330	-1518.619537	0.556608	0.460038	-
<b>27-ts-L4</b>	-1520.370379	-1518.593618	0.555105	0.458101	-244.6
<b>28-L4</b>	-1520.405993	-1518.621868	0.557667	0.458121	-
<b>29-L4</b>	-1228.607204	-1226.967384	0.470956	0.387319	-
<b>33-L4</b>	-1766.029832	-1764.037381	0.659570	0.545444	-
<b>34-ts-L4</b>	-1766.020545	-1764.022874	0.658523	0.547124	-299.1
<b>35-L4</b>	-1766.084093	-1764.091482	0.661400	0.550071	-
<b>36-ts-L4</b>	-1766.023864	-1764.029862	0.658616	0.548361	-272.5
<b>37-L4</b>	-1766.086953	-1764.102750	0.661481	0.551799	-
<b>38-L4</b>	-2303.503347	-2301.177105	0.850476	0.709717	-
<b>39-ts-L4</b>	-2303.490743	-2301.157802	0.849863	0.712722	-280.8
<b>40-L4</b>	-2303.554088	-2301.220215	0.852718	0.713769	-
<b>41-L4</b>	-1766.084000	-1764.105296	0.662147	0.555229	-
<b>42-ts-L4</b>	-1766.076626	-1764.098379	0.660916	0.556283	-274.3
<b>42-ts-L4-b</b>	-1766.076586	-1764.098457	0.660945	0.556516	-275.5
<b>43-L4</b>	-1766.116254	-1764.141667	0.663061	0.559485	-
<b>60-L4</b>	-1766.103399	-1764.114398	0.663112	0.558075	-
<b>61-ts-L4</b>	-1766.088475	-1764.100177	0.661623	0.557790	-292.7
<b>61-ts-L4-b</b>	-1766.088125	-1764.099698	0.661536	0.557284	-292.3

\* IF: The imaginary frequencies for the transition states.

## 5. B3LYP geometries for all the optimized compounds and transition states.

<b>L1</b>				<b>C</b>	-1.24558100	-0.66804700	-0.52058500
<b>C</b>	-1.24551000	0.66814800	-0.52059800	<b>H</b>	-1.93682300	-1.33862000	-1.01905700
<b>H</b>	-1.93668900	1.33877500	-1.01908700	<b>C</b>	0.00003800	1.12294600	0.27168300

C	1.24557600	0.66807200	-0.52056600
C	1.24551600	-0.66812300	-0.52061500
H	1.93670000	-1.33873900	-1.01911200
C	-0.00003800	-1.12295900	0.27164000
H	1.93681400	1.33865600	-1.01903100
H	0.00006700	2.16035200	0.61265700
H	-0.00006800	-2.16037900	0.61257100
C	-0.00000100	-0.00003000	1.35459300
H	0.89985200	-0.00007400	1.97887300
H	-0.89985500	-0.00001300	1.97887100

**L2**

C	0.52727100	-3.00883100	-3.89851100
C	-0.06114400	-2.08075000	-2.99819200
C	0.36836700	-2.05573500	-1.63043800
C	1.38163200	-2.97329600	-1.23063300
C	1.93276200	-3.86102100	-2.12770500
C	1.50271000	-3.88256600	-3.47593600
H	0.18999500	-3.01420400	-4.93246600
H	1.72290100	-2.96631100	-0.20161100
H	2.70603100	-4.54977400	-1.79860700
H	1.94539400	-4.58846100	-4.17359200
C	-1.06587300	-1.17255500	-3.41781600
H	-1.38870400	-1.18740100	-4.45649100
C	-0.22633200	-1.11731700	-0.71799000
C	-1.62304800	-0.28447400	-2.53092700
C	-1.22311800	-0.24883000	-1.16476800
H	-2.38001900	0.41247600	-2.87590000
P	-1.96009500	0.97979900	0.02424900
C	-2.51029400	2.32244300	-1.13081800
C	-3.84997600	2.62742300	-1.41316300
C	-1.50500200	3.13843100	-1.68288100
C	-4.17581200	3.71312300	-2.23154100
H	-4.64446000	2.01704700	-0.99529000
C	-1.83136300	4.21267300	-2.50892300
H	-0.46020900	2.92506500	-1.46633800
C	-3.17014200	4.50609100	-2.78422100
H	-5.22004700	3.93458300	-2.43827500
H	-1.04010700	4.82653100	-2.93181600
H	-3.42557200	5.34905900	-3.42101800
C	-3.55787600	0.17551700	0.51181400
C	-4.24963900	-0.77202100	-0.26044500
C	-4.09474600	0.54478100	1.75606200
C	-5.44656400	-1.32640700	0.19674900
H	-3.85055600	-1.08147000	-1.22180500
C	-5.29655000	-0.00153000	2.21013100
H	-3.56061600	1.26081500	2.37603100
C	-5.97448600	-0.94062900	1.43115700
H	-5.96810400	-2.05999600	-0.41310300
H	-5.69640100	0.29841200	3.17530800
H	-6.90613600	-1.37405700	1.78556400
C	1.06586300	-1.17213900	3.41795000
C	0.06119000	-2.08041900	2.99839100
C	-0.36826800	-2.05557100	1.63061100
C	0.22643100	-1.11724000	0.71808300
C	1.22317000	-0.24867000	1.16480000
C	1.62303900	-0.28413500	2.53097200
H	1.38864400	-1.18681300	4.45664100

H	2.37995600	0.41288900	2.87591600
C	-0.52722400	-3.00842200	3.89879700
H	-0.18997200	-3.01366600	4.93276000
C	-1.38148700	-2.97322100	1.23088500
H	-1.72271100	-2.96638400	0.20184600
C	-1.50261000	-3.88224300	3.47628900
C	-1.93261000	-3.86086300	2.12803500
H	-1.94530300	-4.58806700	4.17401100
H	-2.70583200	-4.54969200	1.79898400
P	1.96009700	0.97987000	-0.02432500
C	3.55788200	0.17556700	-0.51187900
C	4.09460600	0.54453200	-1.75625500
C	4.24976000	-0.77174200	0.26058000
C	5.29639800	-0.00184700	-2.21030200
H	3.56039300	1.26039100	-2.37635700
C	5.44667000	-1.32617600	-0.19657900
H	3.85078000	-1.08096400	1.22205400
C	5.97445600	-0.94069900	-1.43114800
H	5.69612300	0.29784400	-3.17561000
H	5.96831800	-2.05956500	0.41342200
H	6.90609000	-1.37417500	-1.78553300
C	2.51030900	2.32261000	1.13060500
C	3.84996100	2.62774500	1.41292200
C	1.50493800	3.13852100	1.68264300
C	4.17568300	3.71351700	2.23124200
H	4.64449600	2.01742400	0.99506500
C	1.83118700	4.21284000	2.50863800
H	0.46016200	2.92503600	1.46613300
C	3.16993800	4.50640900	2.78390000
H	5.21989700	3.93510800	2.43794700
H	1.03986600	4.82663000	2.93150600
H	3.42530100	5.34942500	3.42066000

**L3**

C	-1.85909800	-1.79696200	-1.20825800
H	-2.48191000	-2.40394700	-1.85864400
C	-1.12488500	-2.26997900	-0.19985000
H	-1.06953800	-3.31759900	0.08623500
C	-1.78007100	-0.28837700	-1.36425600
C	-0.31984300	0.11818300	-1.41283300
C	0.44139900	-0.35297400	-0.41551400
C	-0.36498900	-1.20993000	0.59189900
H	0.04987200	0.78326200	-2.18638200
H	-2.35171100	0.09039400	-2.21467100
C	-1.47589300	-0.22282500	1.13197800
C	-2.34514100	0.34250600	-0.03095600
H	-2.09390200	-0.75983300	1.86059300
H	-0.98392600	0.59950800	1.66174100
C	0.42503400	-1.79970900	1.76197200
H	-0.25952800	-2.28770200	2.46634500
H	1.14723400	-2.55301500	1.43061700
H	0.97710800	-1.02722600	2.30679800
C	-3.83563000	0.02048000	0.14006400
H	-4.23038500	0.41062400	1.08478500
H	-4.41677200	0.45695200	-0.68065400
H	-3.99095300	-1.06205800	0.14282900
O	-2.14641800	1.75484600	-0.21516200
C	-2.64986100	2.61615500	0.78455400

H	-2.28674000	2.35618100	1.79050000
H	-2.28792600	3.61815600	0.53611100
H	-3.74891400	2.64120400	0.80981800
C	1.86593800	0.02101900	-0.23643900
C	2.88931200	-0.94058100	-0.16145800
C	2.22757300	1.37858400	-0.18002700
C	4.22426000	-0.55796000	-0.03445700
H	2.63910800	-1.99512700	-0.23284000
C	3.56332500	1.76232800	-0.05265400
H	1.44318600	2.12875700	-0.22860700
C	4.56702600	0.79521300	0.02291800
H	4.99975200	-1.31842100	0.01157400
H	3.81887600	2.81812000	-0.00890800
H	5.60766600	1.09196700	0.12395500

**L4**

C	0.65359900	0.29542700	1.23783700
C	1.42284600	0.29116200	0.13496400
C	-0.70990600	0.93288000	1.06012400
C	-1.42284700	0.29117500	-0.13484200
C	-0.65358100	0.29521400	-1.23772800
C	0.70985600	0.93273500	-1.06012900
H	-1.30879600	0.90152000	1.97231600
C	0.44142700	2.42498800	-0.63615800
C	-0.44143900	2.42507200	0.63602400
H	1.39829600	2.92651200	-0.45675300
H	-0.05387200	2.94711400	-1.46134600
H	-1.39828900	2.92659500	0.45651200
H	0.05383100	2.94725500	1.46118900
H	1.30877200	0.90126000	-1.97229300
H	0.96377700	-0.10600400	2.19821900
H	-0.96381800	-0.10638300	-2.19802600
C	2.80746000	-0.21371800	0.04922100
C	3.30660400	-0.77862300	-1.13826200
C	3.66787000	-0.15711900	1.16235200
C	4.60650500	-1.27975000	-1.20647000
H	2.66392300	-0.85008400	-2.01109000
C	4.96571700	-0.65866900	1.09549600
H	3.31549400	0.30633900	2.07952900
C	5.44284600	-1.22309100	-0.09044700
H	4.96467500	-1.71886200	-2.13411200
H	5.61130000	-0.59782700	1.96799900
H	6.45733100	-1.60866900	-0.14496900
C	-2.80750600	-0.21363200	-0.04916800
C	-3.30661900	-0.77866600	1.13828000
C	-3.66784600	-0.15703200	-1.16233200
C	-4.60649300	-1.27983600	1.20643400
H	-2.66391700	-0.85015100	2.01108500
C	-4.96568800	-0.65863700	-1.09551800
H	-3.31544800	0.30648400	-2.07946600
C	-5.44280800	-1.22312800	0.09037900
H	-4.96472300	-1.71903600	2.13401300
H	-5.61125400	-0.59777300	-1.96803200
H	-6.45726300	-1.60879100	0.14488500

**7**

B	0.51021000	-0.03973400	0.00003700
O	0.48526800	1.34221500	-0.00021800

H	1.35590900	1.75954300	0.00178600
O	1.65334200	-0.80659400	-0.00004900
H	2.47206900	-0.29572700	-0.00071100
O	-0.66608400	-0.72251400	0.00026100
C	-1.90565100	-0.03153600	-0.00010400
H	-2.01174000	0.60392300	-0.88746200
H	-2.69905700	-0.78416700	-0.00324200
H	-2.01453300	0.59945600	0.89010800

**9**

C	-0.88907200	1.11917500	-0.88519400
C	-1.92144100	0.27303700	-1.00527300
C	-2.13078300	-0.84156900	-0.04824600
C	-1.10524900	-0.99782900	1.00922300
C	-0.06820900	-0.15543500	1.12153400
C	0.12639500	1.05033700	0.23240400
H	-0.73866800	1.93088900	-1.59534300
H	-2.65308800	0.35914700	-1.80425700
H	-1.23823700	-1.84232600	1.67974100
H	0.68608700	-0.29220900	1.89279900
O	-3.09259800	-1.59722100	-0.13887600
O	1.46264500	1.10019700	-0.31424900
C	0.03767800	2.33234000	1.08514700
H	0.80211800	2.30574300	1.86787900
H	0.22085800	3.20764100	0.45389900
H	-0.94934900	2.42210000	1.54742000
C	1.87371700	-0.01944400	-1.10129900
H	1.02233800	-0.44765700	-1.64819600
H	2.56913600	0.38637500	-1.84519700
C	2.55033600	-1.06541500	-0.32431400
C	3.13856500	-1.92339400	0.28924000
H	3.64680400	-2.68432500	0.83692800

**12**

C	0.66185800	-0.01966500	0.00000100
H	1.07969500	0.99083100	-0.00063300
H	1.03696900	-0.54321100	0.89347100
H	1.03687000	-0.54428200	-0.89287600
O	-0.74856300	0.12248800	0.00000300
H	-1.13617500	-0.76525100	0.00001000

**18**

C	1.72859200	-0.91266700	-0.72689200
C	2.38715600	0.24222200	-0.89659100
C	2.07819000	1.44194200	-0.08019000
C	0.96579000	1.30573200	0.88814200
C	0.30287300	0.15149600	1.04980100
C	0.65588300	-1.12230000	0.31787500
H	1.95562800	-1.78671600	-1.33548600
H	3.17410600	0.35898800	-1.63700400
H	0.71283400	2.20054700	1.45024600
H	-0.52228100	0.07037600	1.75318500
O	2.70165400	2.49029100	-0.21211800
O	-0.50346700	-1.73695300	-0.27970800
C	1.13872500	-2.17560200	1.33703400
H	0.35055800	-2.36253300	2.07313000
H	1.35569200	-3.11512700	0.81889000
H	2.03993100	-1.83201300	1.85251700



C	-1.22472700	-0.95049500	-1.23538800
H	-0.53650900	-0.31227300	-1.80725200
H	-1.65298400	-1.67665200	-1.93627200
C	-2.29774700	-0.14166200	-0.64682400
C	-3.20856100	0.50840400	-0.18644700
C	-4.30222600	1.30049400	0.37001400
H	-3.95916800	2.29234300	0.68854400
H	-5.09870100	1.44628700	-0.36990700
H	-4.74829400	0.80468700	1.24080700

**19**

C	-0.46440400	1.29000200	-0.00001500
C	0.91676800	1.42443100	-0.00002600
C	1.73148800	0.28091100	-0.00002500
C	1.14394600	-0.99120700	-0.00003100
C	-0.24762000	-1.10153700	-0.00001600
C	-1.08578300	0.02415600	-0.00000900
H	-1.08358500	2.18292400	-0.00001600
H	1.39405200	2.39973900	-0.00003100
H	1.75314300	-1.88820200	-0.00005100
H	-0.69418100	-2.09231100	-0.00002400
B	-2.63489700	-0.12010500	-0.00001900
O	-3.39732700	1.02731000	0.00005600
H	-4.35282800	0.87625500	0.00005200
O	-3.17456400	-1.38798200	-0.00000400
H	-4.14156700	-1.41342000	0.00000800
O	3.07561700	0.51325200	-0.00002200
C	3.95198300	-0.60161600	0.00006600
H	3.81417900	-1.22363800	-0.89445200
H	4.96289800	-0.18888000	-0.00003800
H	3.81429900	-1.22343600	0.89474100

**20**

C	3.83963200	0.70472000	-0.36621100
C	3.16692300	1.77369300	-0.81721200
C	1.78447400	2.07040000	-0.38307000
C	1.22450100	1.19065100	0.72664500
C	1.72602100	-0.26683000	0.69020100
C	3.27433600	-0.37030100	0.54187300
H	4.86365300	0.52122900	-0.69033500
H	3.61051900	2.47943300	-1.51539100
H	1.45910700	-0.75030600	1.63998800
O	1.15404500	3.00842600	-0.84661300
O	3.48699700	-1.63537700	-0.10918000
C	4.02682900	-0.41406700	1.87089000
H	3.68543600	-1.27142300	2.46023000
H	5.10334300	-0.52105200	1.70155600
H	3.85863500	0.50389800	2.44431900
C	2.44712100	-1.79461200	-1.07290000
H	2.72963700	-1.32693300	-2.03089800
H	2.31700700	-2.86800900	-1.24193300
C	1.22386500	-1.12467200	-0.46634300
C	-0.01754400	-1.34218000	-0.93284000
H	-0.08437000	-1.96866100	-1.82519600
C	-1.32671200	-0.87971300	-0.44426900
C	-2.38271600	-0.73265500	-1.35732700
C	-1.61338600	-0.63184200	0.91421100
C	-3.65521100	-0.32020200	-0.96178600

H	-2.20246300	-0.93670200	-2.41025400
C	-2.87507500	-0.22768500	1.32642700
H	-0.84359700	-0.78559400	1.66381900
C	-3.90714100	-0.05853400	0.39042000
H	-4.43417500	-0.21107800	-1.70764900
H	-3.09192800	-0.04414300	2.37421100
H	0.13542800	1.25324100	0.69485200
H	1.54031300	1.64738700	1.67724300
O	-5.10709100	0.34597900	0.89592500
C	-6.18385900	0.54413000	-0.00596800
H	-5.95026100	1.31776800	-0.74932800
H	-7.02819400	0.87236500	0.60296300
H	-6.45204200	-0.38544300	-0.52570200

**21**

C	-3.59872700	-1.04571700	-0.38663700
C	-2.80261700	-1.83786200	-1.12062100
C	-1.36452100	-2.00479300	-0.81087900
C	-0.88991200	-1.37634600	0.49112700
C	-1.59117700	-0.04489100	0.81739500
C	-3.13995500	-0.16895700	0.76410000
H	-4.65736300	-0.95201300	-0.62752800
H	-3.17773100	-2.39789800	-1.97393400
H	-1.31862700	0.24893000	1.84010500
O	-0.62324400	-2.65452500	-1.53319600
O	-3.59468600	1.16860200	0.49902100
C	-3.78443700	-0.60864300	2.07783900
H	-3.52652900	0.10099400	2.87078000
H	-4.87495000	-0.63366100	1.98149500
H	-3.44260900	-1.60799800	2.36756500
C	-2.67682900	1.76559500	-0.41594400
H	-2.99863300	1.59212200	-1.45619500
H	-2.69628500	2.84499200	-0.23245400
C	-1.32493400	1.12521800	-0.13083900
C	-0.15647300	1.56347400	-0.63059300
C	1.17129400	1.00443700	-0.23571900
C	2.02402900	0.41299800	-1.17626900
C	1.62968700	1.09892000	1.09122300
C	3.27715700	-0.08973300	-0.81853500
H	1.69770100	0.31356900	-2.20818600
C	2.87564000	0.60941900	1.46331000
H	0.99819100	1.57218200	1.83872900
C	3.70972400	0.00726600	0.50951200
H	3.89657300	-0.55658200	-1.57571500
H	3.22905300	0.68551500	2.48706900
H	0.19513500	-1.27635900	0.45643700
H	-1.11850000	-2.09596200	1.29247300
O	4.91121700	-0.44559000	0.97173500
C	5.78864000	-1.07718900	0.05360300
H	5.33655700	-1.97747500	-0.38330900
H	6.67173200	-1.36037700	0.62944300
H	6.08687400	-0.39616000	-0.75475000
C	-0.09279900	2.71567300	-1.61350000
H	0.44513800	3.56866500	-1.17819400
H	0.46522700	2.42572300	-2.51297700
H	-1.07999600	3.06067300	-1.93277900

**22**

C	-3.23190600	-2.98060200	-1.48659500	H	-4.07013600	7.15874000	0.86526600
C	-4.52833800	-3.14019000	-1.18757300	H	-4.74683700	5.51148500	0.99744700
C	-4.99227800	-3.30956000	0.21105800				
C	-3.94793200	-3.24408000	1.26198200	<b>23</b>			
C	-2.65238800	-3.08204400	0.95909400	C	-4.07796700	-2.61660600	-0.04112100
C	-2.12571200	-3.00768300	-0.45682300	C	-5.33558300	-2.43352900	-0.46658000
H	-2.90395500	-2.84631100	-2.51638400	C	-6.12090500	-1.23394300	-0.08700900
H	-5.30298400	-3.14635100	-1.94962200	C	-5.41992800	-0.22741800	0.74541400
H	-4.29795200	-3.32719500	2.28742400	C	-4.16039300	-0.41314900	1.16503900
H	-1.89353900	-3.02043400	1.73769500	C	-3.35833200	-1.66362600	0.88485400
O	-6.17606700	-3.47792700	0.48397000	H	-3.50976500	-3.49935000	-0.33192900
O	-1.25233100	-1.87551100	-0.61192000	H	-5.84062100	-3.14809900	-1.11108100
C	-1.21320600	-4.22329300	-0.72134700	H	-5.98416200	0.67024100	0.98369800
H	-0.38729100	-4.22616000	-0.00285500	H	-3.64510100	0.34078700	1.75796300
H	-0.79428100	-4.15542300	-1.73047100	O	-7.28053600	-1.07757400	-0.45579700
H	-1.77384900	-5.15744900	-0.62694800	O	-2.05811800	-1.32490000	0.36699900
C	-1.85437500	-0.59610300	-0.46403100	C	-3.05088200	-2.37911800	2.21689200
H	-2.48808800	-0.57384800	0.43650300	H	-2.48426800	-1.70794300	2.86982200
H	-2.52409400	-0.38488300	-1.31347400	H	-2.44063200	-3.26740900	2.02421600
C	-0.80133800	0.48787000	-0.37108800	H	-3.97420900	-2.67950100	2.72033600
C	0.51500200	0.18410200	-0.44615400	C	-2.03960300	-0.65910600	-0.90759000
C	-1.35025400	1.86299600	-0.22673800	H	-2.78775500	0.14177800	-0.92283600
C	-1.02314500	2.87729400	-1.14909200	H	-2.30000100	-1.36744500	-1.70451600
C	-2.24891000	2.18972100	0.79911200	C	-0.65409300	-0.06577900	-1.09152400
C	-1.55621300	4.15441700	-1.04124900	C	0.39802100	-0.83275600	-1.46493800
H	-0.35065000	2.64733700	-1.97049300	C	-0.55929400	1.38844000	-0.75709300
C	-2.79234900	3.47040000	0.92311000	C	-1.23224000	2.34541000	-1.54384800
H	-2.51891100	1.44040000	1.53853600	C	0.12727100	1.84431400	0.37286300
C	-2.44643200	4.46303000	-0.00138300	C	-1.19201000	3.69763900	-1.23199300
H	-1.30586500	4.93122000	-1.75716300	H	-1.78394100	2.02371400	-2.42459200
H	-3.47376900	3.67972800	1.73973100	C	0.16986600	3.20249700	0.70513600
C	3.62457800	-0.50955900	-0.63738000	H	0.60787700	1.13565300	1.03722700
C	3.28322300	-1.68801900	0.29956400	C	-0.48563800	4.13798800	-0.10129300
C	3.82190900	-1.54299600	1.71549800	H	-1.70128300	4.43393100	-1.84618300
C	5.13351600	-0.87377700	1.84227500	H	0.70720300	3.50521900	1.59674300
C	5.73249400	-0.28552900	0.79580600	C	3.09557700	-1.72544900	-0.04888300
C	5.13610700	-0.12609200	-0.59009600	C	2.25558100	-1.52441300	1.22728700
H	3.38739000	-0.81738100	-1.66525900	C	2.70014700	-0.35279000	2.09151700
H	5.58959300	-0.89352000	2.82912000	C	4.14329800	-0.04256700	2.09740900
H	6.70771600	0.18560000	0.91530300	C	5.00406900	-0.65520100	1.27132100
O	3.23745400	-2.00912800	2.68205600	C	4.62804600	-1.67445100	0.21531000
O	5.16476700	1.27992400	-0.89754700	H	2.87726500	-2.72656700	-0.44343000
C	5.99223400	-0.83457400	-1.63851700	H	4.46533600	0.71646000	2.80614200
H	7.03231800	-0.49717800	-1.57985100	H	6.06477300	-0.40747500	1.29774300
H	5.61289300	-0.60524200	-2.63962700	O	1.91205400	0.27504800	2.78753100
H	5.97370000	-1.91968100	-1.48934000	O	5.19187800	-1.23806400	-1.03076600
C	4.02402700	1.87111900	-0.27366800	C	5.24967400	-3.03412800	0.53738600
C	2.93363400	0.82229100	-0.36189100	H	6.33245700	-2.94058500	0.67110100
C	1.61992900	1.11461000	-0.29908200	H	5.06535100	-3.72758100	-0.28965900
H	0.75440600	-0.85932700	-0.61343500	H	4.82479300	-3.45199500	1.45654500
H	4.24997400	2.13722900	0.77273800	C	4.30009100	-0.28335400	-1.60588400
H	3.78961000	2.79223500	-0.81614500	C	2.90249700	-0.70510000	-1.17238800
H	1.35329600	2.15515800	-0.11999000	C	1.76613700	-0.27626300	-1.75510400
H	2.21000200	-1.87343200	0.36402600	H	4.54517800	0.73481200	-1.26032200
H	3.73653600	-2.60258600	-0.11324900	H	4.45383700	-0.31960200	-2.68835300
O	-2.91596300	5.74296800	0.01830700	H	1.19120400	-1.41300200	1.00512700
C	-3.82693600	6.10950700	1.04233400	H	2.35166000	-2.42247200	1.85731800
H	-3.37776700	6.00513700	2.03885300	O	-0.50854800	5.48439900	0.12497800

C	0.17474200	5.98231700	1.26338200
H	1.24979300	5.76251800	1.21832000
H	0.02723500	7.06398500	1.25263000
H	-0.23624500	5.56948400	2.19428000
C	1.80732300	0.71724800	-2.90239900
H	1.45916500	0.24269900	-3.83072500
H	1.14087300	1.56310000	-2.71079100
H	2.80823100	1.11668700	-3.08393900
C	0.25599000	-2.31274100	-1.76598700
H	0.95045500	-2.90855500	-1.16458300
H	-0.74438100	-2.69700400	-1.56471100
H	0.50706300	-2.51396500	-2.81617300

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C	-2.88808800	1.18113500	0.93570300
H	-2.40344600	1.99864400	1.45840700
C	-3.34402400	1.18224100	-0.39730900
H	-3.28034900	1.99867000	-1.10868400
C	-3.60098200	-0.00033000	1.63299700
C	-2.88804100	-1.18155800	0.93528700
C	-3.34397200	-1.18213900	-0.39771000
H	-3.28017800	-1.99826600	-1.10942400
C	-4.33383900	0.00002400	-0.51327900
H	-2.40328900	-1.99919800	1.45767800
H	-3.59729000	-0.00051500	2.72381300
H	-4.99854600	0.00015100	-1.37817100
C	-4.97013400	-0.00021000	0.90230700
H	-5.56496600	-0.89933300	1.10519500
H	-5.56497500	0.89884300	1.10549200
Rh	-1.55897500	0.00007800	-0.25898600
O	0.00008600	-1.29492700	-0.78884800
C	0.00004000	-2.67974500	-0.55910800
H	-0.00100700	-2.93918300	0.51272000
H	-0.88683600	-3.14179900	-1.01849200
H	0.88798100	-3.14159000	-1.01664600
C	2.88781900	-1.18144100	0.93533500
H	2.40297800	-1.99903800	1.45771300
C	3.34399300	-1.18218500	-0.39760200
H	3.28039900	-1.99841200	-1.10921800
C	3.60071300	-0.00021700	1.63308600
C	2.88800800	1.18126200	0.93557500
C	3.34417800	1.18219900	-0.39733700
H	3.28054000	1.99850800	-1.10885400
C	4.33394200	-0.00005400	-0.51306000
H	2.40324700	1.99881200	1.45810200
H	3.59683100	-0.00033000	2.72390100
H	4.99881100	-0.00000500	-1.37782700
C	4.96999000	-0.00026300	0.90263900
H	5.56487200	0.89875000	1.10587200
H	5.56470800	-0.89942900	1.10568500
Rh	1.55902600	0.00006800	-0.25918400
O	-0.00008300	1.29520600	-0.78857100
C	0.00004400	2.68002100	-0.55891800
H	-0.00111000	2.93953500	0.51289500
H	0.88811000	3.14169900	-1.01638100
H	-0.88669800	3.14221800	-1.01843000

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C	-1.44864500	-1.02295400	-0.68594900
H	-1.49072000	-1.89227800	-1.33333000
C	-1.44186600	-1.00717200	0.71455500
H	-1.47842800	-1.86145000	1.38198800
C	-1.79747000	0.41481100	-1.13553300
C	-0.48993800	1.12503800	-0.72935300
C	-0.48321300	1.14204600	0.70086200
H	0.08540400	1.81977200	1.32968700
C	-1.78650800	0.44043600	1.13512700
H	0.07453000	1.78592800	-1.37953700
H	-2.12332100	0.54042600	-2.16859300
H	-2.10259100	0.58925300	2.16814500
C	-2.75669800	0.86328100	-0.00052200
H	-2.96320100	1.94055100	-0.01165600
H	-3.69822700	0.30155900	0.01030000
Rh	0.57379000	-0.53062400	0.00050900
O	2.47124900	-0.16971300	-0.00990500
C	3.18520100	1.02940900	0.00628600
H	2.90665000	1.70026300	-0.82556800
H	3.05394900	1.58833600	0.94958200
H	4.26023000	0.81403100	-0.09752400

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C	-0.08921500	-2.11392400	-0.56246600
H	0.81208100	-2.08488300	-1.16374400
C	-0.17650000	-1.97305500	0.83085700
H	0.64547800	-1.82254900	1.52092100
C	-1.43931600	-2.70949400	-1.02395800
C	-2.36043400	-1.49592100	-0.77540200
C	-2.44841200	-1.35141400	0.62701700
H	-3.19916900	-0.79531100	1.17797700
C	-1.58191200	-2.47950700	1.22914500
H	-3.02498000	-1.06661400	-1.51759500
H	-1.46574700	-3.14812700	-2.02183200
H	-1.74007000	-2.70720700	2.28359800
C	-1.79707200	-3.61089100	0.18819500
H	-2.83032100	-3.97799800	0.16076700
H	-1.10281400	-4.45000000	0.31741800
Rh	-0.84119800	-0.14390900	-0.09672200
O	-1.63059500	1.75969800	-0.35996300
C	-2.94857500	2.20550300	-0.10410900
H	-3.11128000	3.15903500	-0.61994300
H	-3.66093600	1.46802500	-0.49049800
H	-3.11481300	2.34420800	0.97216100
C	1.29176100	1.13973700	-1.26753600
C	0.80937200	1.53751700	0.01129300
C	1.55882800	1.08176800	1.12159100
C	2.71599600	0.30998600	0.98804400
C	3.16370900	-0.04642600	-0.29382600
C	2.44241700	0.36953100	-1.42360100
H	0.77451700	1.50261500	-2.15260500
H	1.23102100	1.38337300	2.11262300
H	3.26483900	0.00644700	1.87330600
H	2.81493700	0.09405100	-2.40622700
B	-0.43617400	2.61748000	0.16174200
O	-0.60487600	2.95387300	1.55836200
H	-1.05262100	3.81039500	1.60466400
O	-0.38685700	3.74977100	-0.73849200

H	0.35115400	4.32015100	-0.48125800
O	4.28116500	-0.78652300	-0.54552200
C	5.07424700	-1.20913800	0.55243300
H	5.91094200	-1.76227600	0.12159600
H	5.45983400	-0.35534500	1.12464100
H	4.51269100	-1.86963400	1.22665700

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C	-1.05120900	-1.99531100	-0.55057500
H	-0.18593200	-2.29894900	-1.12877500
C	-1.10593100	-1.81289300	0.84477400
H	-0.29222900	-1.95602100	1.54623500
C	-2.51578500	-2.15081400	-1.02053700
C	-3.04709100	-0.71775600	-0.78850800
C	-3.10181800	-0.53709300	0.59323600
H	-3.62293900	0.24518100	1.13413900
C	-2.60347000	-1.85748600	1.22523400
H	-3.51143800	-0.10154000	-1.55066500
H	-2.66906300	-2.57165100	-2.01506800
H	-2.83628400	-2.01036100	2.27977700
C	-3.13861500	-2.89030900	0.19527600
H	-4.23424500	-2.93227900	0.15806400
H	-2.72751000	-3.89632800	0.34272500
Rh	-1.11458800	0.09921800	-0.10943500
O	-1.12755000	2.19959100	-0.35165200
C	-2.16008800	3.08299800	0.08378900
H	-2.02546000	4.05810100	-0.39814000
H	-3.11801700	2.65781700	-0.22731600
H	-2.13751400	3.20566500	1.17036700
C	1.65958500	0.24300400	-1.33100000
C	1.03108100	0.49282700	-0.08220800
C	1.78191000	0.13731800	1.05646500
C	3.05850400	-0.42979800	0.98495900
C	3.63212700	-0.67076300	-0.27028100
C	2.92297900	-0.32555100	-1.43350800
H	1.14568400	0.52313500	-2.24816300
H	1.36218700	0.33436700	2.04027600
H	3.59255000	-0.67173900	1.89809400
H	3.39145900	-0.50789200	-2.39687300
B	0.23925400	2.40806500	0.11424100
O	0.29950800	2.69953900	1.49239700
H	1.07744600	3.23994700	1.68352800
O	1.00806900	3.13534700	-0.81243600
H	1.95401000	2.98397200	-0.68542100
O	4.86702600	-1.21698200	-0.46967500
C	5.62313000	-1.60369200	0.66538100
H	5.10071100	-2.36561500	1.25917000
H	6.55323600	-2.02391700	0.27761400
H	5.85526500	-0.74505600	1.30973800

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C	-1.21261500	-2.20034700	-0.31405500
H	-0.37375000	-2.77124300	-0.69700100
C	-1.40268700	-1.79033400	1.03285500
H	-0.73365600	-1.98178600	1.86493700
C	-2.62932500	-2.22832800	-0.94051000
C	-2.99805800	-0.72723300	-0.96943000
C	-3.18250100	-0.33689600	0.33978500

H	-3.58796800	0.60015100	0.70367700
C	-2.92524000	-1.58555900	1.21046400
H	-3.23802900	-0.16849300	-1.86715100
H	-2.73389500	-2.76966400	-1.88194500
H	-3.29312600	-1.54470700	2.23677000
C	-3.47593700	-2.69909200	0.27539700
H	-4.55695700	-2.62333000	0.10525200
H	-3.21737000	-3.71018100	0.61229300
Rh	-0.93158900	-0.12307200	-0.16698500
O	-0.88597900	2.18672800	-0.40534200
C	-1.74173900	2.80405700	-1.37727200
H	-1.59361500	3.88546600	-1.37848200
H	-1.48756300	2.38942700	-2.35546500
H	-2.78842400	2.58055400	-1.14708200
C	1.87493500	-1.11582400	0.67539100
C	1.11592600	-0.19774100	-0.07320100
C	1.85953800	0.64842900	-0.93277000
C	3.24456100	0.57211200	-1.04843400
C	3.96291100	-0.35492200	-0.28126200
C	3.27075900	-1.20075200	0.59138500
H	1.37926600	-1.80586400	1.35590400
H	1.34121200	1.39407300	-1.53282200
H	3.79415100	1.22511600	-1.72118300
H	3.79847700	-1.92635000	1.20197700
B	-0.45475000	2.90217000	0.71409500
O	-0.89295900	4.19064900	0.86565000
H	-0.50135600	4.58121700	1.66026100
O	0.36821900	2.32197600	1.62024400
H	0.64351500	1.42403000	1.33687600
O	5.32188700	-0.35016800	-0.45440400
C	6.09232100	-1.26357400	0.30409100
H	7.13260200	-1.08994000	0.02032500
H	5.97918900	-1.09279400	1.38362400
H	5.82611400	-2.30575200	0.07930800

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C	-3.20872200	-0.77730000	-0.68756500
H	-3.35107500	-1.62196000	-1.35222100
C	-3.20870600	-0.77724400	0.68769400
H	-3.35102700	-1.62184900	1.35242400
C	-3.18914100	0.70182400	-1.13344400
C	-1.76717400	1.14655500	-0.71711000
C	-1.76715500	1.14659900	0.71704400
H	-1.12296900	1.74693200	1.35171000
C	-3.18910800	0.70191500	1.13345000
H	-1.12300800	1.74686400	-1.35182200
H	-3.47603800	0.89897500	-2.16731400
H	-3.47597300	0.89915000	2.16731100
C	-4.03769600	1.34604600	-0.00001300
H	-3.99484300	2.44173200	-0.00006100
H	-5.08193400	1.01111700	0.00001200
Rh	-0.98007200	-0.64569500	0.00000400
C	0.97636700	-0.23768800	-0.00008600
C	1.65175600	0.99093500	-0.00004200
C	1.77369700	-1.40217400	-0.00007000
C	3.04905900	1.07097500	0.00002000
H	1.08759400	1.92268100	-0.00007100
C	3.16518700	-1.34868500	-0.00000500

H	1.30195900	-2.38962700	-0.00009800
C	3.81108300	-0.10441200	0.00002900
H	3.52904500	2.04416800	0.00009900
H	3.77186100	-2.24994600	0.00001400
O	5.18051900	-0.14661100	0.00012300
C	5.88623200	1.08023700	-0.00004300
H	6.94648900	0.81828000	-0.00006300
H	5.66241800	1.67847100	-0.89414900
H	5.66251000	1.67869200	0.89393300

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C	0.85926300	3.07309600	0.73570500
H	1.24692700	3.00286400	1.74543300
C	1.45271600	2.63394300	-0.41470300
H	2.41213500	2.14483900	-0.51750100
C	-0.41222600	3.84542300	0.31179500
C	-1.34527700	2.74332400	-0.25304200
C	-0.72887900	2.28165700	-1.42536900
H	-1.21061400	1.74686100	-2.23566300
C	0.56843100	3.10809700	-1.58575500
H	-2.39263600	2.64214500	0.00645200
H	-0.84771200	4.50320900	1.06473800
H	1.02899800	3.09435100	-2.57473000
C	0.09225200	4.47787800	-1.01752000
H	-0.71133600	4.93419700	-1.60713000
H	0.91117300	5.19318200	-0.87566100
Rh	-0.20158200	0.98591400	0.26729000
C	-1.86853700	-0.17289100	0.21572400
C	-2.44229600	-0.73633000	-0.93101600
C	-2.54786000	-0.37719400	1.43390400
C	-3.63824000	-1.46853300	-0.88538700
H	-1.95650500	-0.61993600	-1.89807000
C	-3.73935900	-1.09775100	1.49869900
H	-2.15195900	0.03994800	2.35962300
C	-4.29392700	-1.64933500	0.33590700
H	-4.03953000	-1.88688400	-1.80270800
H	-4.25767000	-1.24592200	2.44216300
C	0.92651400	-1.08208000	0.02889900
C	1.07435300	-0.53623200	1.29595100
C	2.36337100	0.05138600	1.73603100
C	3.48826900	-0.03147500	0.77100000
C	3.36626500	-0.61632300	-0.43032100
C	2.08545900	-1.23269500	-0.94467700
H	0.08406000	-1.72800700	-0.19286900
H	0.35500400	-0.74567300	2.08841700
H	4.43081000	0.39053300	1.11054300
H	4.22040500	-0.68987800	-1.10037500
O	2.50963600	0.56366900	2.84298500
O	2.27552600	-2.65426600	-1.18927900
C	1.75016700	-0.69388800	-2.34248400
H	2.56999100	-0.92492700	-3.03058400
H	0.84092700	-1.17834300	-2.71108200
H	1.58700300	0.38537200	-2.31502100
C	2.75574000	-3.45558400	-0.10879300
H	2.41401200	-3.06624200	0.85937300
H	2.28948500	-4.43847600	-0.24421300
C	4.21634600	-3.60731400	-0.10395100
C	5.41285300	-3.77171000	-0.10137000

H	6.47067900	-3.90617500	-0.09513300
O	-5.46660800	-2.34109900	0.50213500
C	-6.06883600	-2.91106700	-0.64406700
H	-6.97918900	-3.40297400	-0.29468800
H	-6.33480300	-2.14641800	-1.38741000
H	-5.41625100	-3.65661900	-1.11965000

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C	-2.10226300	-2.81329900	-0.64439700
H	-1.54936100	-3.47858900	-1.29799000
C	-1.96396600	-2.69196800	0.73615500
H	-1.25185800	-3.21654700	1.36348200
C	-3.45033200	-2.14826200	-1.00888000
C	-3.17239500	-0.65381700	-0.72053400
C	-3.04293700	-0.53856100	0.65825500
H	-3.05305900	0.37491100	1.24052100
C	-3.23271700	-1.95940000	1.23603300
H	-3.31783100	0.15129600	-1.43110100
H	-3.85860200	-2.38473600	-1.99255400
H	-3.44030700	-2.02527500	2.30488200
C	-4.29124900	-2.52314500	0.24534100
H	-5.25171700	-1.99575300	0.29349000
H	-4.44683500	-3.60355400	0.35151600
Rh	-1.02076800	-0.93694900	-0.20996500
C	-0.37782000	1.09209000	-0.38305700
C	-0.33464700	1.71508500	0.87775400
C	-0.70296500	1.90299500	-1.49030000
C	-0.66366500	3.06499400	1.04826300
H	-0.04973000	1.13969600	1.75494100
C	-1.01369000	3.24941900	-1.34279400
H	-0.72364800	1.47058200	-2.48880700
C	-1.00296600	3.84079200	-0.06853700
H	-0.63995100	3.49786600	2.04278500
H	-1.26906600	3.86915000	-2.19765100
C	1.24969300	-0.22096900	-0.93163400
C	1.01039700	-1.56955000	-0.50791000
C	1.50201300	-2.02398700	0.80641300
C	2.23833500	-1.01313400	1.61887800
C	2.71969100	0.11979800	1.08397600
C	2.48756800	0.50350100	-0.36062000
H	1.14307200	-0.02801800	-1.99549800
H	0.84774800	-2.34736100	-1.25310400
H	2.44909200	-1.29477300	2.64761800
H	3.34037400	0.79066100	1.67366500
O	1.36367900	-3.17635900	1.22287700
O	3.56513000	0.04056400	-1.24870200
C	2.55665500	2.01703100	-0.57276000
H	3.57398200	2.34370100	-0.33565400
H	2.35862300	2.25604400	-1.62144500
H	1.85064800	2.56292700	0.05094500
C	4.29215200	-1.14894500	-0.96390800
H	3.64414800	-1.95433300	-0.59897900
H	4.68561200	-1.47209000	-1.93507300
C	5.41067900	-0.93851700	-0.03448500
C	6.35326500	-0.77151300	0.70211200
H	7.17840200	-0.62597400	1.36160800
O	-1.32546300	5.16641200	-0.02728000
C	-1.32326200	5.81971100	1.23109600

H	-1.60413100	6.85561900	1.03192500
H	-2.05243000	5.37307300	1.92034500
H	-0.32881500	5.79714200	1.69665100
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C	2.66596000	-0.39712500	0.16722800
H	2.44283900	0.65525300	0.04152800
C	2.53203800	-1.15050300	1.34389700
H	2.20436300	-0.78651600	2.31129200
C	3.58706900	-1.21479900	-0.76678200
C	2.65795600	-2.39829100	-1.11896000
C	2.52368800	-3.15273900	0.05347700
H	2.14717800	-4.16639800	0.13623900
C	3.36884600	-2.43422000	1.13107200
H	2.40725400	-2.71197900	-2.12625600
H	4.03274700	-0.67825200	-1.60544900
H	3.61492900	-3.01216200	2.02275400
C	4.53556900	-1.88351000	0.26585300
H	5.15758100	-2.67486200	-0.17025500
H	5.16405300	-1.16183100	0.80162200
Rh	0.93003100	-1.67792500	-0.00290600
C	-0.51269100	1.73515200	0.56391200
C	0.04709100	1.91151200	-0.70732300
C	-0.06261700	2.58212800	1.58841100
C	1.00555800	2.89699600	-0.96052000
H	-0.26907500	1.27291900	-1.52682300
C	0.90106300	3.56015000	1.36148000
H	-0.47595700	2.47414000	2.58896100
C	1.44026100	3.72962300	0.07976600
H	1.40212200	3.00366800	-1.96416300
H	1.24577100	4.20865000	2.16109100
C	-1.58024900	0.68054300	0.85829500
C	-1.07581200	-0.74805500	0.64627700
C	-1.38001300	-1.43658100	-0.54530700
C	-2.26467700	-0.82104800	-1.54933300
C	-3.01579800	0.24525600	-1.23065700
C	-2.95178100	0.93419000	0.12020800
H	-1.83788400	0.79335900	1.91699200
H	-0.89813200	-1.35953500	1.53417600
H	-2.33961200	-1.31498700	-2.51464400
H	-3.73907500	0.63870500	-1.94170700
O	-0.80915400	-2.57962300	-0.77932600
O	-4.03547600	0.49830500	0.99038900
C	-3.25435800	2.42991900	-0.04322900
H	-4.26450300	2.54258400	-0.44927300
H	-3.21859400	2.93035100	0.92938700
H	-2.54226700	2.91965000	-0.71115800
C	-4.46639600	-0.85903800	0.98794200
H	-3.63379900	-1.55453300	0.83513300
H	-4.85298200	-1.03671500	1.99902900
C	-5.53399400	-1.12899400	0.01378100
C	-6.43202100	-1.35832800	-0.76096300
H	-7.21733800	-1.55928700	-1.45355400
O	2.37113300	4.72110200	-0.05217800
C	2.94572400	4.93517400	-1.32987000
H	3.65070300	5.75977200	-1.20796400
H	3.48605600	4.04717900	-1.68525500
H	2.18769000	5.21467600	-2.07393000

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C	4.41887100	-0.00013700	-0.27442900
C	4.62185200	0.01966300	1.05021400
C	4.18101900	-1.09607200	1.92217400
C	3.45452800	-2.20170400	1.25386400
C	3.25031100	-2.21645100	-0.07102800
C	3.77174100	-1.15266700	-1.00863800
H	4.73469900	0.82892800	-0.90567000
H	5.11137200	0.85123600	1.54984600
H	3.09499400	-2.99519600	1.90339800
H	2.70945900	-3.03117700	-0.54693200
O	4.39598800	-1.09796700	3.12981400
O	2.73667200	-0.66442800	-1.88665500
C	4.79818900	-1.78278400	-1.97265500
H	4.32295800	-2.59023500	-2.53860100
H	5.14845000	-1.02570400	-2.68133800
H	5.65361100	-2.18340000	-1.42141300
C	1.60559200	-0.04663600	-1.26657400
H	1.86762900	0.39881700	-0.30045400
H	1.30134700	0.77614500	-1.92030500
C	0.46965500	-0.98106900	-1.10828200
C	-0.18693300	-2.03853200	-1.21458900
H	-0.35244800	-3.06520700	-1.48211300
C	-3.28592900	-2.25091000	-0.73674300
H	-3.10119300	-2.72488900	-1.69288300
C	-2.76336600	-2.59598500	0.49187500
H	-2.07598900	-3.40197800	0.71738300
C	-4.39907800	-1.21507000	-0.46795400
C	-3.59645000	0.01384700	0.01377200
C	-3.06210400	-0.33799200	1.26457900
H	-2.69939600	0.34323700	2.02420700
C	-3.54068300	-1.77902900	1.54657000
H	-3.72458400	1.01631100	-0.37434100
H	-5.10525900	-1.04584400	-1.28163700
H	-3.46011400	-2.12435800	2.57781600
C	-4.94785400	-1.74662900	0.88641100
H	-5.63481900	-1.04588100	1.37533600
H	-5.41110900	-2.73796800	0.80614200
Rh	-1.58030800	-0.75570300	-0.27166000
C	-0.86163600	1.18596700	-0.07121300
C	-0.25319600	1.63208200	1.11786800
C	-1.07553200	2.14689100	-1.06809200
C	0.10974700	2.96561000	1.30424600
H	-0.05410200	0.92816700	1.92370400
C	-0.71881200	3.49433300	-0.90010400
H	-1.53389500	1.85717200	-2.01216000
C	-0.12257500	3.90861500	0.29439500
H	0.57667900	3.29826400	2.22741000
H	-0.91067800	4.19830300	-1.70352100
O	0.27018100	5.19385600	0.57196200
C	0.04265100	6.18345400	-0.41259800
H	0.41729000	7.11980000	0.00679000
H	0.58306100	5.96444300	-1.34441200
H	-1.02686800	6.29321600	-0.64094700

**34-ts**

C	-3.99438900	-1.28987400	1.28641200
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C	-4.83392300	-0.33156300	1.70229600
C	-5.54202200	0.55454000	0.74688500
C	-5.23451900	0.35047000	-0.68914400
C	-4.39288200	-0.60814800	-1.10044100
C	-3.72572500	-1.59542300	-0.16965200
H	-3.47070800	-1.92771200	1.99712500
H	-5.03259200	-0.15109700	2.75536800
H	-5.72386600	1.02943400	-1.38224000
H	-4.16225500	-0.74007700	-2.15656200
O	-6.32665700	1.41817400	1.12557400
O	-2.31161500	-1.66490000	-0.42591800
C	-4.22979000	-3.01791200	-0.49141500
H	-3.99926800	-3.26120600	-1.53338600
H	-3.71949000	-3.74166600	0.15191800
H	-5.30942200	-3.09335300	-0.33370900
C	-1.58541700	-0.45720400	-0.19305200
H	-2.00538800	0.37180600	-0.77908500
H	-1.63953000	-0.16222000	0.86403300
C	-0.17055300	-0.70781200	-0.58541800
C	0.61483900	-1.54841700	-1.14793300
H	0.59525600	-2.50463200	-1.64746400
C	3.79298000	0.90467500	0.17860100
H	3.65685600	1.91964100	-0.17353700
C	3.35780800	0.36530500	1.38525400
H	2.81657900	0.87845200	2.17087700
C	4.82993000	-0.09162900	-0.39174300
C	3.95155200	-1.31379900	-0.74914000
C	3.51878800	-1.84920300	0.45978700
H	3.07812200	-2.82546300	0.62386700
C	4.12474000	-0.96258600	1.57182800
H	3.92482600	-1.78916400	-1.72239100
H	5.47832000	0.28461800	-1.18422700
H	4.12833500	-1.38496600	2.57778900
C	5.48986800	-0.59627400	0.92237300
H	6.14380400	-1.46386900	0.77036400
H	6.02590400	0.19138900	1.46540500
Rh	2.00677900	-0.36534000	-0.24201500
C	0.58816000	1.21254000	-0.24685000
C	0.16707700	1.87512900	0.91930600
C	0.48397300	1.91878600	-1.46346900
C	-0.29142100	3.19473800	0.89234800
H	0.20890700	1.36284800	1.87777800
C	0.04678000	3.23990100	-1.50418300
H	0.74966000	1.42310200	-2.39331100
C	-0.34709500	3.88830100	-0.32534400
H	-0.59588800	3.67044000	1.81843400
H	-0.01768200	3.78420700	-2.44197100
O	-0.77854700	5.17632700	-0.46798000
C	-1.22327600	5.86791200	0.68687000
H	-0.42118800	5.97339700	1.42990100
H	-1.52821000	6.85867500	0.34449400
H	-2.08156700	5.36641400	1.15376100

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C	-4.90806200	1.02092200	-0.46166300
C	-5.51143800	-0.17259500	-0.55068100
C	-5.00948600	-1.35599100	0.18923900
C	-3.76904300	-1.15817000	0.97234800

C	-3.15725000	0.03333900	1.04653600
C	-3.70964700	1.29262000	0.41941000
H	-5.27782700	1.88370300	-1.01363100
H	-6.39129500	-0.33399000	-1.16791500
H	-3.37451400	-2.04104300	1.46842500
H	-2.23501700	0.15826600	1.60869300
O	-5.58307700	-2.44019600	0.13968700
O	-2.71208400	2.02593100	-0.30855000
C	-4.12954900	2.26339900	1.54629600
H	-3.26460700	2.48969000	2.17819500
H	-4.49066400	3.19896700	1.10738800
H	-4.91947300	1.82535300	2.16282800
C	-2.06714300	1.35388400	-1.41744900
H	-2.72748600	0.57961400	-1.82500500
H	-1.95286000	2.13803900	-2.17663600
C	-0.72447600	0.75338200	-1.06906500
C	-0.46824400	-0.57709500	-1.03543300
H	-1.26984200	-1.28335900	-1.27000200
C	0.41772000	1.64696700	-0.74278700
C	1.73075300	1.25537700	-1.11728500
C	0.29173700	2.84400300	-0.01849800
C	2.85254700	1.99693600	-0.74003600
H	1.85535100	0.45494100	-1.86310800
C	1.40695700	3.60049800	0.34410200
H	-0.69685400	3.17247900	0.28364800
C	2.69903600	3.17277700	0.00154000
H	3.85046300	1.69736400	-1.04526200
H	1.25965600	4.51695000	0.90525500
C	0.83058600	-2.84726600	0.66263100
H	-0.18957700	-2.91773400	1.02584500
C	1.26770400	-3.16546800	-0.65431800
H	0.63918400	-3.51477800	-1.46709000
C	2.06787800	-3.03880100	1.57395400
C	2.99534600	-1.88792000	1.12555800
C	3.41650300	-2.19132400	-0.14333000
H	4.16180900	-1.67414400	-0.73621700
C	2.76408700	-3.53958800	-0.52111400
H	3.32666300	-1.07143500	1.75660100
H	1.87493400	-3.11330000	2.64519100
H	3.20790200	-4.07069300	-1.36445900
C	2.76020800	-4.23962400	0.86837400
H	3.76746600	-4.44429800	1.25138000
H	2.15686600	-5.15496000	0.88692100
Rh	1.33891700	-1.08131600	-0.35894800
O	3.85071300	3.83565900	0.31985400
C	3.74760500	5.05242000	1.04005900
H	3.28323400	4.90287400	2.02417000
H	4.77073200	5.40790200	1.17614100
H	3.17410100	5.80556100	0.48306300

**36-ts**

C	4.49070100	-0.00643900	-1.12118600
C	5.31864000	0.82892300	-0.47814400
C	5.73330400	0.58979700	0.92550200
C	5.14473700	-0.59791000	1.59014500
C	4.31584600	-1.42938300	0.94313500
C	3.94254900	-1.27779300	-0.51417500
H	4.18487600	0.18462000	-2.14892800

H	5.72171500	1.72227700	-0.94769500	O	6.89663900	0.87816800	-0.61972800
H	5.42042200	-0.74653900	2.63079700	O	2.43445200	-1.82615800	0.32155700
H	3.87881500	-2.29187600	1.44436900	C	4.20859700	-3.33497000	0.62538300
O	6.50778600	1.34139800	1.50877900	H	3.82065300	-3.56298600	1.62325100
O	2.51669200	-1.35703200	-0.68652500	H	3.73192500	-4.01123300	-0.09141000
C	4.47972900	-2.48993700	-1.30389500	H	5.28988100	-3.49904400	0.61200300
H	4.05187900	-3.41118400	-0.89603000	C	1.83092700	-0.55528000	0.04002500
H	4.17889100	-2.40630500	-2.35297900	H	2.10889100	0.16682600	0.82361100
H	5.57063600	-2.54149000	-1.24433400	H	2.23289600	-0.15461000	-0.90474700
C	1.75647200	-0.31941500	-0.05410000	C	0.34154600	-0.66764600	-0.05920700
H	2.01595400	-0.25600300	1.01409700	C	-0.31047100	-1.84909900	0.02545500
H	1.99910200	0.65901700	-0.49458200	H	0.19466700	-2.79329000	0.23100700
C	0.31477300	-0.59358500	-0.20023600	C	-1.77638300	-1.85305800	-0.11122100
C	-0.53153500	-1.46454800	-0.61001500	C	-2.40946100	-0.92505700	-0.97857900
H	-0.66588500	-2.41804100	-1.08985700	C	-2.61223500	-2.70785900	0.62731600
C	-3.14458600	1.71427800	-0.88627500	C	-3.80176900	-0.82151400	-1.04958700
H	-3.80422200	1.15806400	-1.54103100	H	-1.79905200	-0.40452400	-1.73115400
C	-3.16252800	1.72671000	0.50569300	C	-4.00108800	-2.62580200	0.54718400
H	-3.83420000	1.18250900	1.15766500	H	-2.16344200	-3.43861500	1.29552700
C	-2.29029500	2.92534200	-1.32115200	C	-4.60760000	-1.66554000	-0.28054800
C	-0.87506100	2.50292000	-0.86644500	H	-4.27807300	-0.11804600	-1.72576900
C	-0.88673500	2.51700600	0.52425400	H	-4.60508500	-3.30539400	1.13835400
H	-0.03028400	2.50770300	1.18781500	C	0.06563300	2.31340200	1.05601000
C	-2.31392300	2.94438200	0.93944500	H	0.75442800	1.92335600	1.79833300
H	-0.00728900	2.46996100	-1.51508500	C	0.35758200	2.54311200	-0.31871700
H	-2.38853200	3.24211800	-2.36041400	H	1.30848200	2.36293100	-0.80905900
H	-2.43614200	3.27755900	1.97089000	C	-1.09281800	3.27741500	1.40752800
C	-2.64934900	3.94453200	-0.20279200	C	-2.26656600	2.67805000	0.60269400
H	-2.00458400	4.83206200	-0.20128100	C	-1.98728900	2.89695800	-0.72485700
H	-3.70427400	4.24347600	-0.21756400	H	-2.63898600	2.73215600	-1.57480500
Rh	-1.44829500	0.46337600	-0.14435800	C	-0.63304900	3.63823200	-0.77989100
C	-2.50345100	-1.36721100	0.04885900	H	-3.18340800	2.29064700	1.03129900
C	-2.56799600	-1.89618000	1.34460000	H	-1.27341700	3.45206200	2.46913500
C	-3.47568600	-1.79742800	-0.87902700	H	-0.39573900	4.14326000	-1.71730800
C	-3.59393800	-2.76803200	1.73746200	C	-0.73495400	4.49758600	0.51265100
H	-1.80566000	-1.62991400	2.07172600	H	-1.53248800	5.24936600	0.46896700
C	-4.48734100	-2.67275700	-0.50991700	H	0.21454000	4.97063100	0.79016100
H	-3.44002300	-1.43948900	-1.90507900	Rh	-0.94703600	0.89539600	-0.12483800
C	-4.56001700	-3.15991700	0.80728100	O	-5.95753200	-1.49967600	-0.42082400
H	-3.61313900	-3.14070500	2.75597800	C	-6.81891300	-2.35711900	0.30832800
H	-5.24092300	-2.99659600	-1.22230700	H	-6.68020600	-2.24547800	1.39230100
O	-5.59668500	-4.01311700	1.06608300	H	-7.83473900	-2.05723500	0.04391700
C	-5.72003300	-4.53382100	2.37780900	H	-6.67021200	-3.41031800	0.03399300
H	-5.86026400	-3.73512000	3.11895500				
H	-6.60461100	-5.17373900	2.36617700	<b>38</b>			
H	-4.84356100	-5.13294700	2.66007500	C	-5.82645700	0.74546100	-0.06787000
<b>37</b>				C	-6.56047400	-0.36938200	0.05567900
C	4.35694200	-1.58754600	-1.14002800	C	-6.56285800	-1.16718100	1.30567700
C	5.33482200	-0.71566300	-1.42378600	C	-5.67552100	-0.68750600	2.39215300
C	5.98588400	0.09532300	-0.36735500	C	-4.94133300	0.42657600	2.26265800
C	5.46160500	-0.07695600	1.00893100	C	-4.98511800	1.32588000	1.04702400
C	4.48531500	-0.95198100	1.28778500	H	-5.82252200	1.31725300	-0.99485800
C	3.86538700	-1.87389900	0.26151700	H	-7.18178100	-0.74812600	-0.75160400
H	3.87307600	-2.16726900	-1.92480400	H	-5.65002500	-1.29867900	3.29050500
H	5.69125300	-0.55210400	-2.43736700	H	-4.27981200	0.76162700	3.06028900
H	5.91209000	0.55305000	1.77138300	O	-7.24813300	-2.17785200	1.42741700
H	4.10035600	-1.06219100	2.30066600	O	-3.66237000	1.63253100	0.58786300
				C	-5.56881600	2.69546900	1.45668200



H	-4.94219700	3.14072100	2.23599900	C	4.75152400	5.10509400	-0.63777600
H	-5.56992700	3.36609300	0.59152500	H	4.81011300	4.97160600	0.45119800
H	-6.59052200	2.58901000	1.83222200	H	5.76054500	5.21015100	-1.04127400
C	-2.88375000	0.51881700	0.13125000	H	4.17807900	6.01624100	-0.85582800
H	-2.84142000	-0.25143700	0.91714700				
H	-3.38447600	0.05610400	-0.73307000	<b>39-ts</b>			
C	-1.48944800	0.93562000	-0.24466400	C	-5.62978800	0.69284200	0.37100900
C	-1.07113300	2.21099200	-0.09948500	C	-6.39705700	-0.40247000	0.46389000
H	-1.76105300	2.94173500	0.32240400	C	-6.39415400	-1.25518500	1.67706600
C	0.26934500	2.70625000	-0.42993200	C	-5.46383400	-0.85323800	2.75952700
C	1.09100200	2.08292400	-1.39524800	C	-4.70064000	0.24424100	2.66278800
C	0.80673600	3.82778900	0.22425800	C	-4.74366500	1.19633900	1.48877500
C	2.38931000	2.51311300	-1.64601600	H	-5.62741600	1.30430700	-0.53026000
H	0.66958600	1.29347000	-2.02708600	H	-7.04958100	-0.72461500	-0.34328900
C	2.10381900	4.28238100	-0.02308400	H	-5.43477700	-1.50552500	3.62823800
H	0.19965900	4.34782900	0.96168200	H	-4.01355500	0.52314800	3.46047800
C	2.91038000	3.61678000	-0.95609500	O	-7.10946600	-2.24725500	1.77296000
H	3.00910400	2.03121200	-2.39645200	O	-3.42108700	1.47665500	1.00428000
H	2.47322000	5.14896100	0.51420400	C	-5.26724900	2.56670200	1.96889600
C	-1.62056100	-1.76532100	-1.98445600	H	-4.60779200	2.95745300	2.75027600
H	-2.60473600	-1.82379600	-1.53527400	H	-5.26599600	3.27329600	1.13275700
C	-1.15775200	-0.76135600	-2.86035900	H	-6.28310900	2.47954400	2.36461600
H	-1.72985900	0.09192300	-3.20825900	C	-2.67812400	0.34596300	0.52243300
C	-0.78732500	-3.03240300	-2.30192000	H	-2.40667400	-0.30150700	1.36744700
C	0.64183300	-2.67337700	-1.85685700	H	-3.31684300	-0.25287800	-0.14305700
C	1.09038700	-1.71251500	-2.70303500	C	-1.43469400	0.77841800	-0.22389700
H	2.06650800	-1.24060500	-2.71111500	C	-1.38430300	2.02503300	-0.76282600
C	-0.04273700	-1.43363400	-3.71004400	H	-2.26410200	2.64571600	-0.58617800
H	1.17402600	-3.12589700	-1.02968500	C	-0.31846800	2.72265500	-1.48409700
H	-1.18821700	-3.97341000	-1.92232000	C	0.73737200	2.09582900	-2.18162300
H	0.24409000	-0.90953000	-4.62298500	C	-0.33889400	4.12992000	-1.49962900
C	-0.63034600	-2.86840900	-3.84265300	C	1.73054400	2.83252000	-2.81224000
H	0.06817400	-3.58902300	-4.28480000	H	0.75597100	1.01130900	-2.24345400
H	-1.58640800	-2.89100300	-4.37790800	C	0.64893200	4.88521700	-2.12961800
Rh	-0.22764700	-0.47805000	-0.91386400	H	-1.14567500	4.64913400	-0.98706200
C	3.15390800	-2.50657400	2.12095300	C	1.70062100	4.23470700	-2.78763500
C	3.83290100	-3.16688600	1.17139000	H	2.53481200	2.34315500	-3.35394700
C	5.08884800	-2.63533100	0.59248600	H	0.58927900	5.96749700	-2.10277500
C	5.54153200	-1.31960200	1.10575500	C	-1.65819500	-2.28875200	-1.47893900
C	4.86598100	-0.66689400	2.06195700	H	-2.59464000	-2.25166300	-0.93658900
C	3.62251400	-1.20632300	2.73229800	C	-1.27217500	-1.48477600	-2.55202400
H	2.22688500	-2.90370000	2.52763600	H	-1.84176300	-0.68492500	-3.00906400
H	3.49321200	-4.11999700	0.77424500	C	-0.72292000	-3.51758300	-1.49429200
H	6.44509300	-0.91713600	0.65569200	C	0.63783600	-2.90000200	-1.10714700
H	5.19821000	0.30542400	2.42233400	C	1.02793400	-2.10655700	-2.17559400
O	5.71241700	-3.24189300	-0.27280400	H	2.01156200	-1.69160400	-2.36122800
O	2.58255700	-0.20875300	2.72904900	C	-0.09292300	-2.21932700	-3.23431300
C	3.90980200	-1.42933000	4.23178400	H	1.24806800	-3.22669500	-0.27346900
H	4.21138100	-0.48296300	4.69163900	H	-1.04617600	-4.37907800	-0.90864300
H	3.00119300	-1.78013700	4.73109600	H	0.16247700	-1.89131100	-4.24262600
H	4.70547300	-2.16696500	4.36989600	C	-0.52159600	-3.69934800	-3.02597300
C	2.07697700	0.19072900	1.44881000	H	0.26964000	-4.41631500	-3.27690300
H	1.79988900	1.24467300	1.55052800	H	-1.44760400	-3.95779200	-3.55299300
H	2.86481400	0.13832000	0.68750500	Rh	-0.15204800	-0.80892400	-0.76211500
C	0.88845600	-0.57552600	1.01948200	C	4.95298000	-1.30028200	2.33384400
C	-0.07779700	-1.36456500	1.06234300	C	6.06115400	-1.68663300	1.68628100
H	-0.75908400	-2.08108000	1.48018700	C	6.88926800	-0.72669300	0.91648600
O	4.19226900	3.97007100	-1.27532600	C	6.39616000	0.67057600	0.86400500

C	5.28557900	1.05172400	1.51084600	H	-4.10694900	-0.69777400	-2.35023000
C	4.46744800	0.13058500	2.38717400	C	-4.30797500	-0.53890800	-0.15371200
H	4.34646700	-2.01510200	2.88833000	H	-4.31479300	-1.56114100	0.20345000
H	6.40518400	-2.71750900	1.68774000	C	-4.43285000	1.42637100	-1.42526000
H	6.98358400	1.36066500	0.26431300	C	-3.16889700	1.93978300	-0.69762500
H	4.92509400	2.07783200	1.45396300	C	-3.28388800	1.48115000	0.64585400
O	7.91622700	-1.07372800	0.34224500	H	-2.81621700	1.92447400	1.51815100
O	3.07008100	0.20722000	2.05253500	C	-4.61672500	0.70139300	0.71200100
C	4.52619100	0.63251400	3.84527700	H	-2.60883100	2.80556400	-1.03292100
H	4.13676300	1.65411900	3.89646100	H	-4.66458800	1.89609100	-2.38201100
H	3.90145300	-0.00598400	4.47785200	H	-5.01539700	0.50687100	1.70824600
H	5.55325100	0.61835900	4.22102200	C	-5.48288300	1.52547500	-0.28246700
C	2.73224600	-0.17581300	0.71394800	H	-5.65975000	2.55490600	0.05072900
H	3.27936700	0.44755600	-0.00990200	H	-6.43515200	1.04041200	-0.52854500
H	3.02989600	-1.21785000	0.52444100	Rh	-2.08962600	0.14280800	-0.46472400
C	1.28236400	-0.01306500	0.50489400	C	1.63225700	4.62219000	-0.72382800
C	0.19307400	0.43882000	0.99564600	C	1.02729500	5.77589000	-1.04035000
H	-0.30068900	0.86740800	1.85191100	C	0.25683700	6.55195000	-0.03937300
O	2.71993100	4.86581700	-3.44235300	C	0.15474200	5.95694200	1.31504400
C	2.71910100	6.28273200	-3.47543200	C	0.76269600	4.80369900	1.62693500
H	2.78545600	6.71194400	-2.46644800	C	1.64214900	4.03215500	0.66870300
H	3.60342000	6.57072300	-4.04727000	H	2.18216500	4.05044200	-1.46987500
H	1.82222900	6.67556000	-3.97317400	H	1.06227500	6.19395700	-2.04293000
<b>40</b>				H	-0.44741900	6.50829700	2.03238300
C	-0.43379400	-4.15551900	0.91367500	H	0.67124900	4.37065100	2.62213000
C	-1.14165600	-4.18765400	2.05214200	O	-0.28151700	7.61834700	-0.32022100
C	-2.62281900	-4.24421800	2.05494300	O	1.28076300	2.64495900	0.63605400
C	-3.28169500	-4.20689000	0.72648500	C	3.09041400	4.03026700	1.20423300
C	-2.57248400	-4.16678000	-0.41040900	H	3.11132500	3.57650200	2.20016300
C	-1.06311500	-4.23118000	-0.45770800	H	3.72374600	3.43253400	0.54104100
H	0.65186300	-4.10068500	0.93064100	H	3.48753700	5.04766000	1.26316300
H	-0.66398900	-4.16854100	3.02783500	C	-0.05464500	2.34792100	0.20615300
H	-4.36872800	-4.20735700	0.73319400	H	-0.76313400	2.66885900	0.98395300
H	-3.06232400	-4.12490200	-1.38178800	H	-0.29086100	2.93948300	-0.69298000
O	-3.26988500	-4.30173300	3.09494900	C	-0.23689700	0.88424600	-0.10049200
O	-0.55759000	-3.20965900	-1.34861500	C	0.86402000	0.08955000	-0.19848200
C	-0.64113300	-5.55024500	-1.13930400	H	1.83966200	0.54352100	-0.05152300
H	-1.03965400	-5.58027900	-2.15835800	O	7.41673000	-1.20030500	0.43897900
H	0.45051000	-5.60701900	-1.19362600	C	8.43965500	-1.82169300	-0.32075100
H	-1.01722500	-6.41174400	-0.58054200	H	8.39323000	-1.52830400	-1.37813600
C	-0.52125000	-1.86947200	-0.88555500	H	9.38301400	-1.47729200	0.10729400
H	-0.96055300	-1.25959100	-1.71121300	H	8.38824200	-2.91652500	-0.24956300
H	-1.15044700	-1.77155000	0.03064400	<b>41</b>			
C	0.85816200	-1.31510600	-0.57089400	C	-3.71496400	-1.78542200	0.26492100
C	1.94776100	-2.11281000	-0.72226600	C	-4.21769600	-0.72046000	-0.37568600
H	1.76161300	-3.08750600	-1.16809200	C	-3.46206900	-0.02620900	-1.44429200
C	3.35686600	-1.84570100	-0.41421300	C	-2.04802400	-0.44150600	-1.63433800
C	3.79639600	-1.01976300	0.64441000	C	-1.51239100	-1.51978800	-0.93479600
C	4.34953000	-2.49273600	-1.17098000	C	-2.38127700	-2.42024000	-0.06649100
C	5.14655800	-0.82735800	0.89862400	H	-4.28301600	-2.29727900	1.04013400
H	3.06831300	-0.54764800	1.29492800	H	-5.20929900	-0.32917400	-0.16292400
C	5.71080600	-2.30422400	-0.93212900	H	-1.56437700	-0.05372200	-2.52790600
H	4.04722000	-3.15333200	-1.98053600	H	-0.59077700	-1.97835200	-1.28137400
C	6.11822200	-1.45937300	0.10750300	O	-3.97926200	0.85320700	-2.13168200
H	5.47761700	-0.19896100	1.71984400	O	-1.72588800	-2.86459800	1.12012000
H	6.43599200	-2.81794800	-1.55317500	C	-2.65060800	-3.72715700	-0.84998700
C	-4.19572600	-0.09958000	-1.45063100	H	-1.69903700	-4.22438500	-1.06315900

H	-3.26028600	-4.40065400	-0.23932100	H	-1.10117300	1.36532500	-2.39665900
H	-3.17302800	-3.52258800	-1.78893200	H	0.47284100	1.79454100	-3.11612800
C	-1.15892000	-1.83183500	1.94524700	C	0.62258100	0.83182800	-1.16873000
H	-1.96300100	-1.18138700	2.32259700	C	1.95519600	0.60687700	-1.35115700
H	-0.73489200	-2.38170600	2.79481700	H	2.37979600	0.95570800	-2.29754700
C	-0.09839000	-1.05812200	1.19830600	C	2.94912100	0.03613300	-0.44952900
C	1.18774000	-1.43593300	1.36309700	C	4.31317100	0.18119300	-0.76901600
H	1.37885700	-2.18982400	2.13553200	C	2.64330600	-0.63470100	0.75759700
C	2.40953100	-1.03210100	0.65088700	C	5.32699600	-0.28858800	0.06286200
C	3.66180200	-1.35578500	1.19998100	H	4.58673400	0.68868800	-1.69136200
C	2.41609700	-0.36688300	-0.59474000	C	3.64061700	-1.10200100	1.59906000
C	4.86308500	-1.02312600	0.57159700	H	1.60034600	-0.81171200	1.01539300
H	3.69882600	-1.88267500	2.15115200	C	4.99374000	-0.93288300	1.26211900
C	3.60000700	-0.02949000	-1.23478700	H	6.36187500	-0.14839900	-0.22807900
H	1.46632700	-0.11445200	-1.06046400	H	3.39961900	-1.61999200	2.52250200
C	4.83769100	-0.35124000	-0.65600300	C	-1.24532400	-1.88759700	-1.69392900
H	5.80172600	-1.29326900	1.04250000	H	-1.26149800	-1.38816100	-2.65570100
H	3.59540700	0.47684500	-2.19575400	C	-0.14013700	-2.42431500	-1.04623500
C	-0.67294500	1.85368600	1.73558900	H	0.88612900	-2.42614900	-1.39334500
H	-0.80897900	1.35327800	2.68678000	C	-2.49127100	-2.44621600	-0.97070000
C	0.50362100	1.90022600	0.98091700	C	-2.41337700	-1.74842000	0.40743900
H	1.45116500	1.44134600	1.22778500	C	-1.30635100	-2.29107200	1.05855500
C	-1.56475500	3.00354500	1.21775800	H	-1.09216900	-2.23558300	2.11969600
C	-1.93739000	2.53067600	-0.20270400	C	-0.69176000	-3.32408000	0.08431400
C	-0.78052800	2.57283800	-0.94870300	H	-3.21075700	-1.17523900	0.86570500
H	-0.69040200	2.46906900	-2.02327700	H	-3.43956000	-2.36215600	-1.50315900
C	0.33577700	3.07476400	-0.00661400	H	0.00690000	-4.04278900	0.51466500
H	-2.94343100	2.37955700	-0.57117600	C	-1.98158900	-3.86723200	-0.59475700
H	-2.39500000	3.29921500	1.85994500	H	-2.64619500	-4.39131600	0.10253800
H	1.24714500	3.43528800	-0.48425500	H	-1.77690400	-4.49797400	-1.46839600
C	-0.47879800	4.06413400	0.87626600	Rh	-0.65141100	-0.49650500	-0.03562000
H	-0.87489300	4.91887700	0.31470100	O	5.89487800	-1.43697800	2.15094200
H	0.07661700	4.41286000	1.75509700	C	7.27675600	-1.30981600	1.85540000
Rh	-0.87217700	0.47012900	0.04158700	H	7.57851300	-0.25657800	1.78215400
O	5.94395000	0.02402500	-1.36533500	H	7.80523600	-1.77892600	2.68724000
C	7.21830000	-0.29126800	-0.83209900	H	7.53891200	-1.82540900	0.92199200
H	7.94766800	0.09249800	-1.54821400				
H	7.38029200	0.18968500	0.14218100	<b>43</b>			
H	7.35455000	-1.37574000	-0.72269400	C	3.51354100	-2.25838900	0.27492100
<b>42-ts</b>				C	3.61347500	-1.25579700	1.15540600
C	-2.06264700	2.96681200	-0.22519500	C	2.42924100	-0.60857300	1.78320500
C	-2.79596800	2.22594900	0.61482600	C	1.11617400	-0.87080000	1.18619100
C	-2.16829700	1.31758100	1.60880200	C	0.94779900	-2.01573900	0.17548400
C	-0.72824600	1.05752700	1.44173100	C	2.21286500	-2.84827500	-0.22117000
C	0.07553100	1.77133900	0.46961100	H	4.40654800	-2.72951200	-0.13537900
C	-0.54834900	2.98369700	-0.25694300	H	4.58056300	-0.89933500	1.50385200
H	-2.53084500	3.64923100	-0.93303900	H	0.15958800	-2.71769600	0.47179500
H	-3.88135100	2.28644300	0.64114400	O	2.59583500	0.13866200	2.75622900
H	-0.23367600	0.67070700	2.33189200	O	2.23159600	-2.82232800	-1.66968200
H	1.10186900	1.94284300	0.78605600	C	2.11217600	-4.31960900	0.18309400
O	-2.83983200	0.81173500	2.51144300	H	1.21149000	-4.76476900	-0.25347000
O	-0.11620900	3.03283000	-1.62286000	H	2.98218400	-4.87875200	-0.17772400
C	-0.03645200	4.28355700	0.38623800	H	2.06672600	-4.41579900	1.27303500
H	1.05351800	4.33497800	0.29448600	C	1.75206900	-1.54491900	-2.07578800
H	-0.46628000	5.14802200	-0.13021600	H	2.54512700	-0.78661800	-1.99541700
H	-0.31498900	4.33160400	1.44333200	H	1.43687900	-1.61742300	-3.12125400
C	-0.08110700	1.71296600	-2.17427200	C	0.59745500	-1.28779200	-1.12121200
				C	-0.57623800	-0.65926800	-1.48769900

H	-0.57926300	-0.25960900	-2.50223600	C	-2.71843800	0.39323500	-0.39866800
C	-1.92478000	-0.65030100	-0.88172000	C	-4.82185900	-0.37484800	1.25214600
C	-2.96691400	-0.06812200	-1.63963300	H	-3.56326900	0.20642800	2.87674000
C	-2.27709700	-1.18470600	0.37071900	C	-3.89498000	-0.10321600	-0.96328200
C	-4.27419400	-0.02244500	-1.18249600	H	-1.91235500	0.66295000	-1.06803500
H	-2.73758600	0.34577100	-2.61910200	C	-4.95892500	-0.48952000	-0.13972700
C	-3.58983300	-1.14871400	0.84315300	H	-5.65025800	-0.68151300	1.88321400
H	-1.52621700	-1.63500100	1.00619000	H	-3.96400900	-0.18960400	-2.04181100
C	-4.60058800	-0.56499700	0.06996600	C	2.17284400	-3.05770700	-0.74997100
H	-5.06457000	0.42245200	-1.77895700	H	2.29579000	-3.36645100	-1.78215700
H	-3.80800200	-1.57525400	1.81556600	C	3.13681900	-2.46767500	0.07136000
C	0.88943100	2.44292600	1.28995300	H	4.15973800	-2.22423900	-0.19333400
H	0.78673100	2.13456200	2.32313700	C	1.03290000	-3.52644900	0.18435600
C	2.04382400	2.31191300	0.50911100	C	0.44339500	-2.16776600	0.63124300
H	2.98551900	1.89097600	0.83851000	C	1.41694600	-1.57531000	1.45376300
C	-0.00461500	3.46848500	0.55057500	H	1.25572700	-0.77180400	2.16235900
C	-0.40992600	2.70001300	-0.73038800	C	2.59783600	-2.57050900	1.51609500
C	0.74086500	2.56879100	-1.49358200	H	-0.60828500	-1.90891200	0.58622000
H	0.81151000	2.27193000	-2.53348600	H	0.33105100	-4.25158000	-0.22945600
C	1.87171200	3.25817500	-0.69785900	H	3.32188900	-2.42112000	2.31809000
H	-1.43209500	2.51240400	-1.03800400	C	1.84199900	-3.92626500	1.44907600
H	-0.82049300	3.90620900	1.12703100	H	1.20759500	-4.10744100	2.32515600
H	2.77693000	3.50285200	-1.25524900	H	2.50695700	-4.78239600	1.28135900
C	1.07980000	4.41964200	-0.03168100	Rh	1.72352700	-0.92246200	-0.57668000
H	0.68070000	5.14052800	-0.75573400	H	0.07927200	0.49401000	-1.69455200
H	1.65317000	4.94077100	0.74438900	O	-6.14795400	-0.98827600	-0.58356300
Rh	0.58850900	0.79266700	-0.09314500	C	-6.34024300	-1.12092300	-1.98260400
H	0.32597600	-0.80590700	1.93920200	H	-5.61123100	-1.81163000	-2.42698100
O	-5.90993600	-0.47643500	0.43500900	H	-7.34533100	-1.52717200	-2.10998200
C	-6.29753800	-1.01544200	1.68950600	H	-6.27388400	-0.15087600	-2.49295100
H	-7.37156300	-0.83955200	1.77157400				
H	-6.10159200	-2.09446900	1.74234800	<b>45</b>			
H	-5.78333900	-0.51430100	2.52014100	C	0.76220400	2.57782100	1.70105100
<b>44</b>				C	-0.09439100	1.60407800	2.03850800
C	2.42387700	3.32773800	-0.42189900	C	-0.02278400	0.25708400	1.42661900
C	2.92603700	2.30943500	-1.13032000	C	1.12727900	-0.11310700	0.80289100
C	2.07803300	1.17509400	-1.52449700	C	2.29709700	0.83650000	0.62317800
C	0.74961700	1.06688200	-1.05136600	C	1.83558500	2.31693200	0.67594400
C	0.09848600	2.15453000	-0.19972700	H	0.68990300	3.57777800	2.12331600
C	0.99869000	3.42223600	0.07870000	H	-0.90467900	1.77139300	2.74478100
H	3.05678400	4.16440600	-0.13119900	H	3.10300100	0.65453900	1.34886200
H	3.96616700	2.27574900	-1.44338300	O	-1.11009300	-0.50158400	1.51792800
H	-0.80229200	2.49702300	-0.72385300	O	1.22123700	2.49450600	-0.65584500
O	2.58087800	0.17433700	-2.18151100	C	3.00194800	3.29698600	0.82648900
O	1.07503100	3.55159200	1.52162500	H	3.79516500	3.09397600	0.09973300
C	0.34645900	4.70927700	-0.43274200	H	2.64850000	4.32327800	0.67913400
H	-0.66340100	4.80254400	-0.01856200	H	3.43560300	3.22261500	1.83005000
H	0.92826100	5.58260100	-0.11838900	C	1.99033000	1.73817500	-1.60737400
H	0.28540000	4.70773500	-1.52673900	H	1.27603000	1.24244900	-2.27725800
C	0.77954000	2.28545300	2.10430300	H	2.61744900	2.40800600	-2.21281900
H	1.68480700	1.65310100	2.12969500	C	2.81874100	0.75633500	-0.79831000
H	0.44508600	2.45468300	3.13229300	C	3.84243000	0.05171800	-1.30887100
C	-0.28361700	1.70736500	1.20584300	H	4.07759200	0.23057300	-2.36043100
C	-1.37347500	1.06941900	1.66933800	C	4.73505800	-0.91920200	-0.65963200
H	-1.41541600	0.94608100	2.75303300	C	5.99255200	-1.17553000	-1.24759100
C	-2.56011600	0.53064400	0.99137700	C	4.41872700	-1.63709700	0.50633300
C	-3.64801500	0.12171700	1.79577400	C	6.89466000	-2.06901000	-0.69064000
				H	6.26501700	-0.65065500	-2.16055700

C	5.31598900	-2.54076000	1.07882700	C	-3.69620300	-1.75684300	-0.88845600
H	3.44573500	-1.51988500	0.97006000	C	-6.08052900	-2.94114200	-0.08063500
C	6.56522800	-2.75848600	0.48610600	H	-5.96808100	-1.65626100	1.62361500
H	7.86173400	-2.25394500	-1.14810000	C	-4.27886100	-2.74767300	-1.68146800
H	5.02258900	-3.07482000	1.97563500	H	-2.74830700	-1.33959300	-1.20681900
C	-3.44871100	-2.11072800	0.37749200	C	-5.48169400	-3.34313500	-1.28417400
H	-2.74302700	-2.86378300	0.71025800	H	-7.00759400	-3.41765200	0.22284900
C	-4.08656500	-1.14344800	1.18382500	H	-3.78029700	-3.05286000	-2.59461500
H	-3.96913100	-1.01723100	2.25424200	C	3.97121600	-0.87065700	-1.37537700
C	-4.24433600	-2.16073300	-0.94722100	H	3.56625600	-1.05873600	-2.36334600
C	-3.85971900	-0.78447500	-1.54096600	C	4.41294600	0.36123000	-0.86612300
C	-4.49707900	0.17919300	-0.73653500	H	4.40980400	1.31552300	-1.38089000
H	-4.69507600	1.21557100	-0.98761200	C	4.53766200	-1.95550300	-0.43052500
C	-5.27136300	-0.60646300	0.34860300	C	3.68283900	-1.68207000	0.82978100
H	-3.45349600	-0.64214800	-2.53669600	C	4.12450200	-0.44176500	1.34187400
H	-4.08196700	-3.03145000	-1.58354400	H	3.96375800	-0.05794400	2.34380400
H	-6.04546000	-0.06071000	0.88950600	C	5.24957800	0.03584800	0.39290500
C	-5.68383200	-1.87776200	-0.44076000	H	3.12353000	-2.44296600	1.36329300
H	-6.39015200	-1.66714300	-1.25305900	H	4.54205800	-2.97943000	-0.80586300
H	-6.07700600	-2.67426900	0.20301900	H	5.90252500	0.82573600	0.76564600
Rh	-2.53627100	-0.22487400	0.06460800	C	5.89073200	-1.31648900	-0.01757400
H	1.19370600	-1.10377800	0.36120300	H	6.37183200	-1.83535300	0.82064600
O	-1.34778800	1.35862500	-1.00222600	H	6.59310300	-1.22167700	-0.85465500
C	-1.92674100	2.56010200	-1.51501500	Rh	2.50610300	-0.11601000	0.00008800
H	-1.21171300	3.06933600	-2.16938000	O	0.85995100	-0.02832600	1.30844900
H	-2.80886900	2.28095600	-2.09441500	H	-0.08845300	0.32939900	0.58492700
H	-2.22247000	3.23933400	-0.70610100	C	0.52045000	-1.03382200	2.23941500
H	-0.45687300	1.58593800	-0.64420600	H	-0.26535900	-0.67117500	2.91677400
O	7.51484000	-3.61701800	0.96020100	H	0.15787300	-1.95198600	1.75076400
C	7.23098600	-4.34148600	2.14544400	H	1.39461700	-1.29197900	2.85116900
H	6.35864900	-4.99678900	2.02014100	H	-0.80778900	-0.45308400	-0.87630900
H	8.11427000	-4.95192700	2.34298500	O	-6.13745300	-4.31771900	-1.97915200
H	7.05616700	-3.67073200	2.99733200	C	-5.57673200	-4.76201500	-3.20316700
<b>46-ts</b>				H	-4.58442700	-5.20892400	-3.05514100
C	-1.13932400	3.43757100	-0.87962000	H	-6.25955800	-5.52191600	-3.58794000
C	-0.02822100	2.83189100	-1.31947300	H	-5.49693200	-3.94417100	-3.93181800
C	0.18232600	1.38341500	-1.16164600	<b>47</b>			
C	-0.82932100	0.59073800	-0.55009600	C	1.98482700	-3.39927600	-1.23036600
C	-2.24044700	1.16398500	-0.38077200	C	0.67493200	-3.13971300	-1.36768400
C	-2.27988700	2.70946300	-0.20954900	C	0.06808500	-1.92687900	-0.80735900
H	-1.24265100	4.51867600	-0.96038200	C	0.93300300	-1.06756100	0.07891700
H	0.78945100	3.38825100	-1.77032500	C	2.41956400	-1.02662600	-0.34586500
H	-2.86447500	0.88061000	-1.23769800	C	2.99083800	-2.43852900	-0.64032000
O	1.33384800	0.91791800	-1.47765100	H	2.38767600	-4.34696800	-1.58468700
O	-2.13844600	2.94488200	1.21597100	H	-0.00278400	-3.83847400	-1.85048900
C	-3.62498100	3.29012100	-0.66976000	H	2.53272600	-0.38195900	-1.22370900
H	-4.45452300	2.74018400	-0.21239600	O	-1.12914400	-1.69312900	-1.01940100
H	-3.69922000	4.34016800	-0.36710800	O	3.37461500	-2.95839100	0.65134300
H	-3.73124900	3.23258600	-1.75974500	C	4.22447900	-2.36951500	-1.55574000
C	-2.46541000	1.75873600	1.94517800	H	4.94472100	-1.64115400	-1.16914100
H	-1.57213500	1.44258800	2.50507700	H	4.71146000	-3.34938600	-1.59626400
H	-3.26167600	1.97274200	2.67093300	H	3.94855800	-2.07314000	-2.57477000
C	-2.88610800	0.72848100	0.92040200	C	3.66117100	-1.87083900	1.54121800
C	-3.74551600	-0.27132200	1.18324200	H	3.04435500	-2.00378200	2.44185000
H	-4.14331200	-0.30499700	2.19949500	H	4.71491900	-1.89880100	1.85082300
C	-4.28765800	-1.32158200	0.30895200	C	3.32284600	-0.59805800	0.78826000
C	-5.48855700	-1.95639400	0.69470100	C	3.86340100	0.59819000	1.07660500

H	4.58132000	0.61048000	1.89911800	H	-2.16786300	1.45117700	2.57004900
C	3.68496100	1.90767200	0.43472100	H	-3.73194600	0.77987900	2.05543000
C	4.69422100	2.87960200	0.60985200	C	-1.93979000	-0.13045500	1.12246100
C	2.57360200	2.27750200	-0.34010000	C	-0.61585200	0.25022000	0.90793500
C	4.61658400	4.13146900	0.02049500	H	-0.33385100	1.04342200	1.60951000
H	5.56218100	2.63500700	1.21775200	C	-2.61981100	-1.21784000	0.42705800
C	2.47855200	3.53455300	-0.93975200	C	-1.87112700	-2.23831500	-0.21078100
H	1.74296400	1.59195200	-0.45991000	C	-4.02481700	-1.32421500	0.36157500
C	3.50598000	4.47010600	-0.76820000	C	-2.48613700	-3.29033600	-0.86631700
H	5.40120400	4.86914600	0.15688100	H	-0.78815400	-2.18124400	-0.17834500
H	1.59612200	3.77504800	-1.52179400	C	-4.65617500	-2.38099100	-0.28961200
C	-2.95304400	1.12497800	-1.37548300	H	-4.65026200	-0.55768900	0.80570300
H	-2.16030200	1.31139800	-2.09185500	C	-3.88802500	-3.37748700	-0.90825100
C	-3.92428500	0.11215200	-1.43629100	H	-1.90520200	-4.06949000	-1.35047000
H	-4.02554700	-0.65146800	-2.19967300	H	-5.73938400	-2.41487700	-0.31576700
C	-3.48683000	2.17671100	-0.37452300	C	2.35482900	-1.22717800	1.48920800
C	-3.35542100	1.38117900	0.94498400	H	2.01099200	-1.06255900	2.50423000
C	-4.33123200	0.36090700	0.87999000	C	1.86893300	-2.18012300	0.58706800
H	-4.71990100	-0.21746500	1.71133200	H	1.08774500	-2.90709800	0.77874800
C	-5.05503100	0.54230400	-0.47331400	C	3.74480900	-0.79798600	0.95922300
H	-2.86325400	1.74867500	1.83886100	C	3.38422200	-0.02978900	-0.33436400
H	-3.01707600	3.16130600	-0.39965300	C	2.90574400	-0.97386300	-1.22735600
H	-6.01490800	0.03626700	-0.58568000	H	2.74197200	-0.84655200	-2.29109700
C	-5.01553100	2.08631500	-0.62960300	C	2.95850200	-2.33694300	-0.50130000
H	-5.60957500	2.61050100	0.12960200	H	3.63888300	1.00281800	-0.54577900
H	-5.30414400	2.42407300	-1.63243900	H	4.39275400	-0.27768000	1.66582800
Rh	-2.48872500	-0.37521800	0.12125500	H	2.89002400	-3.22581800	-1.13046400
O	-1.64404300	-1.27331000	1.68865700	C	4.24165500	-2.14328400	0.35704700
C	-1.86677900	-0.90142400	3.01156400	H	5.15119500	-2.03352200	-0.24596100
H	-1.68620300	-1.76080700	3.68092300	H	4.37963900	-2.92905500	1.10984500
H	-1.19367500	-0.08706700	3.34715500	Rh	1.17539100	-0.17493800	-0.01673100
H	-2.90024800	-0.56167300	3.21460300	O	-4.39692600	-4.45458000	-1.56429500
H	0.49736400	-0.06648400	0.13613300	C	-5.80748000	-4.60241000	-1.63178800
H	0.81294600	-1.48747800	1.08542600	H	-6.27502200	-3.76401100	-2.16433000
O	3.51650100	5.72269500	-1.30545300	H	-5.98481800	-5.52568400	-2.18595900
C	2.41563500	6.11976400	-2.10751500	H	-6.25110300	-4.68779400	-0.63128600
H	1.47810500	6.11816200	-1.53585600				
H	2.63569300	7.13723800	-2.43563200	<b>49</b>			
H	2.30256400	5.47149200	-2.98664300	C	-0.87970100	3.37711100	0.68752700
<b>48-ts</b>				C	0.43271000	3.51430700	0.44085200
C	-0.85204800	3.36072500	0.71146700	C	1.14566600	2.73509200	-0.62159700
C	0.45358400	3.50123600	0.43156100	C	0.45420300	1.54692700	-1.14416500
C	1.13491000	2.72764700	-0.65211000	C	-0.88474800	1.21938100	-0.61181400
C	0.40924300	1.55962100	-1.17498100	C	-1.75949100	2.41555000	-0.08880400
C	-0.90719500	1.26060700	-0.65805300	H	-1.38941000	4.01790300	1.40634000
C	-1.75146800	2.42024800	-0.06809800	H	1.03066600	4.26861200	0.94707100
H	-1.34470400	3.98847200	1.45276200	H	0.68034600	1.29934000	-2.18111900
H	1.06914100	4.24275800	0.93506600	H	-1.47435400	0.61221500	-1.30044400
H	0.67789700	1.22914600	-2.17730700	O	2.23940800	3.13337600	-1.03545800
H	-1.50811600	0.60340000	-1.28437800	O	-2.89840200	1.97987500	0.65974500
O	2.23249500	3.09877400	-1.07928000	C	-2.37973000	3.14611800	-1.29769800
O	-2.89283700	1.98729200	0.66781500	H	-3.07662400	2.47771400	-1.81365600
C	-2.37434600	3.19416400	-1.25643400	H	-2.92963700	4.03192600	-0.96510300
H	-3.07089400	2.54275900	-1.79377600	H	-1.59374700	3.45814600	-1.99083100
H	-2.92790600	4.06096900	-0.88322200	C	-2.72214000	1.01749300	1.74025600
H	-1.59273000	3.53759600	-1.93882700	H	-2.15296300	1.46059000	2.56697300
C	-2.71525300	1.00716300	1.72891900	H	-3.73751500	0.80611000	2.08139600
				C	-1.97033600	-0.11738900	1.10369000

C	-0.66732500	0.32057000	0.80149400	C	-3.71710000	-1.97558500	0.46529900
H	-0.35059000	1.05966800	1.54553100	C	-1.96740200	-2.55842200	-1.06404000
C	-2.65232700	-1.20425200	0.42985000	C	-4.25943100	-3.25704800	0.34490500
C	-1.90202700	-2.20085700	-0.24716200	H	-4.21091800	-1.27167100	1.12906600
C	-4.05788500	-1.34822900	0.42651400	C	-2.48855800	-3.84185600	-1.19023300
C	-2.51702600	-3.25750900	-0.89324100	H	-1.12908400	-2.26691400	-1.70230200
H	-0.81970600	-2.12087200	-0.24550300	C	-3.64046300	-4.20509600	-0.48038200
C	-4.68664000	-2.41167000	-0.21135400	H	-5.15653600	-3.50499300	0.90135200
H	-4.68184600	-0.60314100	0.90770600	H	-2.03606500	-4.57069600	-1.85604500
C	-3.91760800	-3.37860000	-0.87846900	C	1.60974500	-3.96163200	-0.06944000
H	-1.93816800	-4.01787800	-1.40839200	H	1.32796900	-4.47741500	-0.97990700
H	-5.76849400	-2.47602300	-0.19282800	C	2.67708600	-3.14758500	0.12826700
C	2.34288000	-1.30468200	1.48522900	H	3.43089200	-2.85760500	-0.59365100
H	1.96550700	-1.16484300	2.49193600	C	0.87140000	-4.06828900	1.27980200
C	1.87627500	-2.21306800	0.53594800	C	0.29036900	-2.64934000	1.52334800
H	1.07620000	-2.93249200	0.66891300	C	1.39460900	-1.81223700	1.72855800
C	3.74143000	-0.85003800	1.00255600	H	1.39543900	-0.86349700	2.25241700
C	3.39995500	-0.02118400	-0.25890900	C	2.64889800	-2.71671400	1.60710000
C	2.93835900	-0.92879700	-1.20744800	H	-0.72443900	-2.46843800	1.85517400
H	2.82534800	-0.75959300	-2.27207100	H	0.16511000	-4.89337800	1.37588600
C	2.98359100	-2.32224100	-0.53991900	H	3.57664800	-2.30317600	2.00584600
H	3.68502600	1.01103000	-0.43054900	C	2.09163200	-4.02376700	2.24569500
H	4.37566300	-0.36346200	1.74489200	H	1.80196100	-3.90049700	3.29531700
H	2.92706500	-3.18357400	-1.20758600	H	2.76853400	-4.87984300	2.13774300
C	4.25207500	-2.16515000	0.34750400	Rh	0.71624400	-1.60757600	-0.36090700
H	5.17082100	-2.02558600	-0.23507300	C	4.02937300	3.39158700	-0.34744800
H	4.38052800	-2.98465800	1.06532700	C	4.42945100	3.75188500	0.88010700
Rh	1.21396700	-0.16372100	-0.03215700	C	5.57666300	3.09395500	1.55113500
O	-4.42555500	-4.45824300	-1.52578500	C	6.22746000	1.98875200	0.80587700
C	-5.83398000	-4.64768700	-1.53467800	C	5.82335100	1.63162200	-0.42120500
H	-6.34735800	-3.81660200	-2.03484700	C	4.71844600	2.33277500	-1.17783600
H	-6.00675400	-5.56847300	-2.09405700	H	3.17885200	3.87444700	-0.82656800
H	-6.23008300	-4.75996200	-0.51731800	H	3.93332000	4.53641800	1.44513600
<b>50</b>				H	7.04520600	1.48724500	1.31660100
C	-5.69438500	1.64781800	0.15224000	H	6.30306200	0.81277400	-0.95573300
C	-6.17496200	2.41681600	1.13957400	O	5.95764500	3.43431700	2.66600100
C	-5.67213800	3.79233100	1.37068000	O	3.76261800	1.38180100	-1.68570600
C	-4.57673400	4.24806300	0.48178900	C	5.30328400	2.98093400	-2.44971600
C	-4.10156400	3.47561400	-0.50530300	H	5.76704100	2.21041800	-3.07358500
C	-4.65201200	2.10860200	-0.84182100	H	4.49910900	3.45089700	-3.02435400
H	-6.05878700	0.63317400	-0.00226500	H	6.05190900	3.73561300	-2.19255300
H	-6.94722500	2.07187400	1.82217600	C	3.06398400	0.62320500	-0.69395000
H	-4.18132500	5.23979900	0.68480200	H	3.76929400	0.03402000	-0.08888000
H	-3.28895500	3.81689800	-1.14519200	H	2.52805200	1.28696200	0.00087400
O	-6.12673000	4.50744700	2.25833400	C	2.10294400	-0.26568800	-1.36110700
O	-3.59909800	1.14142100	-0.96328300	C	1.42879600	-0.81637500	-2.25999900
C	-5.28363800	2.15048900	-2.25015300	H	1.13228400	-0.98326400	-3.27901900
H	-4.52650800	2.45100700	-2.98128900	O	-4.08331600	-5.48418600	-0.66974200
H	-5.64123600	1.15141200	-2.51851400	C	-5.25955300	-5.89258600	0.00739800
H	-6.11922200	2.85556400	-2.28447600	H	-6.12745700	-5.28648100	-0.28579900
C	-2.79445700	0.92663200	0.20880700	H	-5.43029900	-6.93024600	-0.28588600
H	-2.17989000	1.81182400	0.41792900	H	-5.13840600	-5.84067200	1.09799700
H	-3.45247500	0.77733600	1.07886500	<b>51-ts</b>			
C	-1.90750600	-0.27013500	-0.02890200	C	-5.85931600	-1.90352500	0.32793400
C	-0.56314800	-0.12186600	-0.08861500	C	-7.03544500	-1.26061800	0.32360000
H	-0.15926300	0.89076300	0.00171000	C	-7.45062400	-0.39876400	-0.80913600
C	-2.54902900	-1.59307700	-0.21267900	C	-6.47198800	-0.25070200	-1.91310000

C	-5.29701300	-0.89540700	-1.90343000	H	4.01088000	-3.03972700	-3.39069200
C	-4.87474300	-1.86001600	-0.81817100	H	5.14788000	-4.03471100	-2.44155800
H	-5.56431400	-2.52614200	1.17147600	C	2.90687500	-0.52010600	-0.56788300
H	-7.73858500	-1.33252200	1.14903700	H	3.11521100	-0.81618800	0.47152400
H	-6.76300700	0.41456700	-2.72164100	H	3.62248600	0.27676500	-0.81951700
H	-4.57923500	-0.77008400	-2.71292300	C	1.52684300	-0.01100000	-0.66522700
O	-8.53691900	0.17106700	-0.82560700	C	0.36660300	-0.22024900	-1.16022100
O	-3.54710500	-1.54921400	-0.35687700	H	-0.23356700	-0.82631600	-1.81703200
C	-4.73835900	-3.27277500	-1.42468500	O	0.49693700	-2.38970800	5.10707500
H	-3.98929100	-3.25747100	-2.22272000	C	0.03966300	-3.62711600	5.62448000
H	-4.40383800	-3.97425300	-0.65372700	H	0.14884800	-4.43830900	4.89181700
H	-5.69315500	-3.61594400	-1.83322300	H	0.66655000	-3.84036200	6.49256600
C	-3.39602200	-0.27957500	0.31421300	H	-1.01044400	-3.57046100	5.94157600
H	-3.82709600	0.51444200	-0.30784500				
H	-3.94613700	-0.29971500	1.26470200	<b>52</b>			
C	-1.91984900	-0.01682900	0.54510400	C	6.41875000	0.71504800	0.07723000
C	-1.26733700	0.73803800	-0.38082100	C	7.22076500	0.42406300	1.11157800
H	-1.86880100	1.08573500	-1.22387800	C	7.41100100	-0.96838700	1.58257800
C	-1.30257000	-0.63812500	1.73700800	C	6.62399200	-2.01106200	0.88099200
C	-1.76577900	-1.87422800	2.22307100	C	5.82724700	-1.71583600	-0.15574600
C	-0.24142000	-0.03377000	2.44365800	C	5.68662700	-0.32794400	-0.73699800
C	-1.19596800	-2.49379100	3.33588400	H	6.26509500	1.74262500	-0.24806500
H	-2.56554300	-2.38207200	1.69396500	H	7.76066600	1.19063600	1.66125800
C	0.33853000	-0.63950400	3.55063700	H	6.72903500	-3.02306300	1.26303700
H	0.11296800	0.94287800	2.12421400	H	5.24746400	-2.48925200	-0.65778000
C	-0.13257700	-1.87799100	4.00756800	O	8.16328000	-1.24193800	2.51281300
H	-1.58199600	-3.45336400	3.66184600	O	4.30536300	0.02951000	-0.89810000
H	1.14831900	-0.16077700	4.09344700	C	6.24153800	-0.32261100	-2.17772200
C	2.08583000	3.11941700	0.67945400	H	5.69219900	-1.04977100	-2.78423100
H	2.80801000	2.56411200	1.26589600	H	6.09970600	0.66903400	-2.61875700
C	2.09585500	3.32574600	-0.69228100	H	7.30587700	-0.57449500	-2.18800500
H	2.82213800	2.95770100	-1.40737800	C	3.51396800	0.06698200	0.30088700
C	1.06383600	4.12405900	1.26135800	H	3.22001600	-0.94993100	0.59488200
C	-0.28286400	3.57870300	0.72874400	H	4.11627200	0.48340600	1.12183600
C	-0.26496600	3.78277700	-0.65109600	C	2.29430000	0.91447400	0.04582000
H	-1.11402600	3.75943900	-1.32461600	C	1.06526400	0.33659800	0.07629100
C	1.08599500	4.46011100	-0.97416000	C	2.53425200	2.35171300	-0.24706000
H	-1.14629300	3.36559900	1.34684400	C	1.97880700	2.96796400	-1.37743700
H	1.12233000	4.30296300	2.33569300	C	3.35452100	3.14530400	0.58039000
H	1.16479300	4.94517800	-1.94794600	C	2.20721200	4.31400200	-1.67485300
C	1.28010300	5.32786800	0.30146200	H	1.36789200	2.37581500	-2.05231500
H	0.51719100	6.10769900	0.41075200	C	3.59109200	4.48445900	0.30078100
H	2.28271800	5.76577300	0.37888200	H	3.80029100	2.71198600	1.47185000
Rh	0.54043500	1.75474300	-0.23539400	C	3.01728500	5.08225000	-0.83171700
C	5.45772900	-1.36687500	-1.81415900	H	1.76037800	4.74287100	-2.56481200
C	6.58580500	-1.17554300	-1.11598100	H	4.21279100	5.09412100	0.94948800
C	6.81780700	-1.84138200	0.18882700	C	-0.65146100	-2.74505500	-0.68116900
C	5.71358000	-2.68939900	0.69855100	H	0.17594700	-2.28807900	-1.21237600
C	4.58611500	-2.87604800	-0.00217100	C	-0.85545900	-2.74734800	0.72504500
C	4.34909600	-2.29855300	-1.37926000	H	-0.21113800	-2.29619800	1.47163400
H	5.29330500	-0.86552000	-2.76704300	C	-1.42878600	-3.96749000	-1.22327300
H	7.38134400	-0.52266000	-1.46515200	C	-2.89638200	-3.54814900	-0.98831800
H	5.87128900	-3.14044600	1.67457000	C	-3.09462800	-3.55069700	0.37257400
H	3.77526000	-3.48933200	0.38816900	H	-4.03214100	-3.44702000	0.90679000
O	7.85925900	-1.68585400	0.81814700	C	-1.75532800	-3.97186200	1.01683800
O	3.07173000	-1.63962000	-1.44608000	H	-3.64182700	-3.43151300	-1.76640600
C	4.22444800	-3.45019000	-2.39870800	H	-1.17552700	-4.29500600	-2.23252300
H	3.39549200	-4.10461600	-2.11136800	H	-1.80157100	-4.30421600	2.05485100



C	-1.23675800	-4.97390200	-0.05343300	C	-2.89744000	4.99137800	0.22269700
H	-1.86406500	-5.86891900	-0.14637400	H	-1.77667200	3.53939100	-0.88272400
H	-0.18972000	-5.26153200	0.09885200	C	-4.12006000	4.16370100	2.13865900
Rh	-2.24361300	-1.45846400	-0.19355400	H	-3.92293600	2.07115200	2.53762300
C	-5.29973800	0.76950900	1.35025300	C	-3.75042400	5.22976700	1.31074500
C	-5.90265400	1.82946300	1.90577700	H	-2.62647600	5.82619200	-0.41636700
C	-6.36470600	2.98023200	1.09168400	H	-4.77397600	4.31710400	2.98982700
C	-6.06338800	2.92043100	-0.35969200	C	1.06213500	-1.21786900	2.03150300
C	-5.46156900	1.85897600	-0.91300900	H	0.10983800	-0.71190600	2.11425000
C	-5.09444500	0.61512200	-0.13839000	C	2.30210100	-0.74673300	2.47389800
H	-4.95009100	-0.06456800	1.95694300	H	2.49388100	0.19968400	2.96508100
H	-6.07362400	1.90305900	2.97620800	C	1.22419100	-2.74089500	1.83804900
H	-6.35454700	3.78962200	-0.94291200	C	2.19208500	-2.83231400	0.63837900
H	-5.23778600	1.82680700	-1.97799800	C	3.41247500	-2.37127500	1.08036400
O	-6.94752700	3.93516800	1.59236000	H	4.36055000	-2.44275500	0.56360900
O	-3.71876500	0.26068200	-0.42133100	C	3.22731700	-1.98043300	2.56128600
C	-5.92937100	-0.57166500	-0.65596400	H	1.98540600	-3.34597000	-0.29270300
H	-5.74322900	-0.71882900	-1.72461100	H	0.30145700	-3.31677600	1.76061300
H	-5.65091400	-1.48671500	-0.12357600	H	4.14007600	-1.86077200	3.14575200
H	-6.99529300	-0.38231500	-0.50126200	C	2.20326000	-3.06526800	3.00331400
C	-2.67847700	1.23422400	-0.07755100	H	2.60887100	-4.08317100	2.95634700
C	-1.42834200	0.39066600	-0.06096100	H	1.77197500	-2.87473200	3.99341000
C	-0.21901700	1.00014200	-0.02133000	Rh	2.21506900	-0.53884200	0.28670700
H	1.03128800	-0.73849100	0.23642000	C	2.55673700	0.55121000	-1.71793100
H	-2.91617200	1.66530300	0.90458100	C	3.08791500	-0.73484800	-1.76543500
H	-2.68624500	2.04143700	-0.82391700	C	4.54411800	-0.97580900	-1.59365500
H	-0.18055400	2.09363900	-0.03933600	C	5.36906000	0.19790700	-1.22404600
O	3.31173700	6.40254600	-1.02160900	C	4.86385000	1.43980000	-1.21859200
C	2.75230600	7.05805500	-2.14681400	C	3.45162700	1.78151300	-1.64333600
H	3.10541600	8.09003700	-2.09973600	H	1.56346300	0.73549800	-2.11633300
H	3.08780800	6.60368500	-3.08891600	H	2.52754600	-1.55867400	-2.20136300
H	1.65438900	7.04934700	-2.11597100	H	6.40865600	-0.00753100	-0.98180800
				H	5.48061200	2.29828000	-0.95727700
				O	5.03976000	-2.09198300	-1.74101200
				O	2.91785500	2.82339300	-0.82761900
				C	3.51411800	2.41511700	-3.05388300
				H	4.13962300	3.31295200	-3.02483800
				H	2.50638800	2.70961500	-3.36368400
				H	3.92849100	1.71250900	-3.78259000
				C	2.54177000	2.44492200	0.50932300
				C	1.47398200	1.38014300	0.48720800
				C	0.17826300	1.76010500	0.58153700
				H	-0.76783700	-0.12913100	0.11891300
				H	3.43614200	2.12860300	1.06821200
				H	2.17355000	3.37946600	0.95015900
				H	-0.02773000	2.80930400	0.80586000
				O	-4.16233700	6.52103800	1.47272500
				C	-5.03169700	6.81668900	2.55287100
				H	-4.56543500	6.59030300	3.52121900
				H	-5.23262900	7.88795800	2.49212100
				H	-5.97828300	6.26549800	2.47276400
<b>53</b>				<b>54-ts</b>			
C	-4.19333400	-1.83135200	-1.68149600	C	-4.17023800	-1.74367000	-1.95583000
C	-5.47004100	-1.87120500	-2.08702500	C	-5.48498600	-1.79710500	-2.20988600
C	-6.58092800	-2.13239200	-1.14012100	C	-6.46531400	-2.18721000	-1.16772100
C	-6.20443500	-2.29209800	0.28566800	C	-5.91350800	-2.47023400	0.17986000
C	-4.92616700	-2.25511100	0.68597600	C	-4.59781600	-2.41831500	0.42859900
C	-3.75551300	-2.10465500	-0.25960700				
H	-3.38520600	-1.62316400	-2.38119000				
H	-5.75571200	-1.70505100	-3.12224000				
H	-7.02692300	-2.43355400	0.98166500				
H	-4.66172900	-2.36413600	1.73690100				
O	-7.74784400	-2.19656000	-1.51200000				
O	-2.84925800	-1.09049600	0.20095500				
C	-2.91530000	-3.39940400	-0.23269800				
H	-2.56164800	-3.58557100	0.78669100				
H	-2.04426200	-3.28404000	-0.88580600				
H	-3.50649600	-4.25541600	-0.56970800				
C	-3.38406100	0.22701500	0.29621700				
H	-4.11024700	0.28025400	1.12246600				
H	-3.94679600	0.47740500	-0.61810300				
C	-2.28368200	1.24587500	0.50605600				
C	-0.97936300	0.90286100	0.38460700				
C	-2.77538000	2.62116400	0.79478300				
C	-2.42450600	3.71046200	-0.02787700				
C	-3.63611300	2.88063400	1.87109300				

C	-3.55622400	-2.12274300	-0.62682000	C	2.63871900	2.55471000	0.22992500
H	-3.45938300	-1.44288700	-2.72404900	C	1.59240800	1.47230000	0.15429500
H	-5.89825700	-1.55062700	-3.18418700	C	0.28655200	1.78991900	0.38912200
H	-6.64042600	-2.71554100	0.94947100	H	-0.60390300	-0.09372300	-0.18063000
H	-4.20455600	-2.61899600	1.42422800	H	3.56410900	2.20774100	0.71505600
O	-7.66696700	-2.25702700	-1.40197300	H	2.27932400	3.44470400	0.75835200
O	-2.64737300	-1.10271000	-0.17660400	H	0.06675600	2.78249400	0.78592600
C	-2.66151700	-3.36502600	-0.81878500	O	-4.12790800	6.33747900	1.75965100
H	-2.18260600	-3.62361400	0.13103900	C	-5.02814100	6.52310700	2.84033500
H	-1.87822800	-3.14496300	-1.55113400	H	-4.58067000	6.21821400	3.79568800
H	-3.25038600	-4.21767500	-1.16822600	H	-5.24451600	7.59250300	2.86935600
C	-3.22307600	0.16837800	0.09621500	H	-5.96305300	5.96810400	2.68672700
H	-3.89404700	0.10270200	0.96727800				
H	-3.85381000	0.49550600	-0.74669300	<b>55</b>			
C	-2.15056500	1.20689200	0.34528400	C	4.87306700	-2.24875700	0.52929200
C	-0.83845600	0.91305400	0.15454300	C	6.17402700	-1.98936700	0.33903200
C	-2.66754000	2.53878100	0.75345000	C	6.67754600	-1.41507400	-0.93225300
C	-2.31634600	3.70596300	0.04344600	C	5.65677200	-1.10639400	-1.96322200
C	-3.55629300	2.68447800	1.82944500	C	4.35690200	-1.36833600	-1.76918100
C	-2.81446600	4.95043800	0.40163000	C	3.81316900	-2.04007400	-0.52850900
H	-1.65441900	3.62473600	-0.81354200	H	4.51253800	-2.65902500	1.47150000
C	-4.06387800	3.93008600	2.20494600	H	6.92117300	-2.17788000	1.10522200
H	-3.84506500	1.81365500	2.41185000	H	6.02708000	-0.65203100	-2.87829900
C	-3.69340400	5.07452900	1.48861300	H	3.61377000	-1.12892700	-2.52857500
H	-2.54571700	5.84444600	-0.15245400	O	7.86960600	-1.19304700	-1.11542500
H	-4.73817200	3.99397000	3.05139500	O	2.69952000	-1.29926200	0.00189200
C	1.44186800	-0.92137400	2.45557200	C	3.20494600	-3.40431100	-0.91470600
H	0.54195300	-0.34320100	2.62626300	H	2.40669300	-3.25731300	-1.64916400
C	2.75586800	-0.49062400	2.58348200	H	2.77393800	-3.87877200	-0.02737600
H	3.09570400	0.49342500	2.88492000	H	3.96746600	-4.06312800	-1.33941400
C	1.49527500	-2.46379900	2.36686800	C	2.98232300	0.01548600	0.45967300
C	2.16049800	-2.69270400	0.98938000	H	3.44150600	0.61032200	-0.34566500
C	3.47891700	-2.25706000	1.11306900	H	3.72195400	-0.00986300	1.27697300
H	4.29511900	-2.47948500	0.43556200	C	1.72021300	0.69666300	0.94512500
C	3.63650600	-1.76073200	2.56980500	C	0.54979500	0.01697500	1.00791400
H	1.76081500	-3.32814600	0.20743700	C	1.90610800	2.10940300	1.37133600
H	0.55763000	-2.99125500	2.54755500	C	1.54508800	2.53502700	2.66625400
H	4.65817100	-1.64662800	2.93449000	C	2.48793700	3.06146600	0.52058900
C	2.69812100	-2.75750600	3.30875100	C	1.73582200	3.84669600	3.07793700
H	3.04495700	-3.79639000	3.25217600	H	1.12572700	1.81446800	3.36258900
H	2.50755700	-2.47878600	4.35232400	C	2.68349300	4.38636800	0.91801000
Rh	2.24727200	-0.57281700	0.39943500	H	2.78244000	2.77587700	-0.48605500
C	2.04929600	0.74531100	-1.63003100	C	2.30502700	4.78701500	2.20504300
C	2.44629400	-0.64298500	-1.73416000	H	1.46203300	4.16787200	4.07815900
C	3.85064800	-1.03700200	-1.93706300	H	3.12661600	5.08863100	0.22118900
C	4.86152900	0.04929900	-1.84444300	C	-0.99504300	2.19729500	-1.60541200
C	4.51091000	1.34154700	-1.84524900	H	-0.02016500	2.45032200	-1.20537800
C	3.08517700	1.83895500	-1.96347500	C	-2.23153200	2.52063600	-1.06934800
H	1.06450000	0.96082500	-2.03526800	H	-2.42914400	3.08644800	-0.16637800
H	1.71456900	-1.36444600	-2.09569400	C	-1.25788700	1.69213200	-3.04493600
H	5.90157200	-0.26714100	-1.82006800	C	-1.99178600	0.34837400	-2.80741700
H	5.25892100	2.13184500	-1.80229000	C	-3.23290000	0.68506500	-2.25727400
O	4.19538900	-2.20022500	-2.16001700	H	-4.09781800	0.03609500	-2.20243700
O	2.91207200	2.97717800	-1.11047100	C	-3.27541000	2.22521700	-2.16905700
C	2.84214000	2.35542200	-3.39220600	H	-1.73240000	-0.60785800	-3.24505700
H	3.57033900	3.13646900	-3.63366500	H	-0.39391300	1.66152600	-3.71038600
H	1.83861700	2.78822900	-3.46176600	H	-4.25990000	2.67603000	-2.03651700
H	2.94049000	1.54572600	-4.12148600	C	-2.45848400	2.60005700	-3.43896000

H	-2.94446300	2.28631100	-4.37059400	H	-1.70614200	4.15759600	-0.16332300
H	-2.19946000	3.66487700	-3.48646000	C	-3.60555700	3.34139000	3.11284600
Rh	-1.79485700	0.33224100	-0.63843400	H	-3.29269400	1.28656900	2.61441800
C	-2.01740000	-1.71277200	1.31128700	C	-3.39056800	4.67500300	2.74470100
C	-2.07437600	-1.76762600	-0.22336700	H	-2.54612100	5.99551600	1.27987300
C	-3.29904600	-2.21640200	-0.89193800	H	-4.13435100	3.09168600	4.02560600
C	-4.53870600	-2.29996700	-0.07085300	C	0.60508900	-1.42624100	1.62269400
C	-4.53191700	-2.26205700	1.26688400	H	-0.27466500	-1.04749700	1.11604000
C	-3.29351400	-2.11127400	2.12084600	C	1.64464900	-0.67149700	2.19011800
H	-1.16374500	-2.27854400	1.70372300	H	1.71822800	0.40933700	2.20901300
H	-1.18363400	-2.19674700	-0.69212100	C	0.71795000	-2.84114400	2.23669200
H	-5.45956200	-2.45256900	-0.62995500	C	2.02485000	-3.33973300	1.57870500
H	-5.45938500	-2.36067400	1.83074100	C	3.05867800	-2.58551600	2.14542000
O	-3.35491400	-2.49617200	-2.09666700	H	4.12062000	-2.80179000	2.10448400
O	-3.50871900	-1.00900400	3.03906500	C	2.39249600	-1.62155200	3.15374100
C	-3.09265000	-3.35719600	2.98444000	H	2.12414100	-4.25924800	1.01255900
H	-3.98639800	-3.55972700	3.58447400	H	-0.15484600	-3.48838900	2.13773700
H	-2.24782700	-3.20557000	3.66506200	H	3.04959100	-1.15607500	3.88952300
H	-2.89272600	-4.23097000	2.35530700	C	1.22064900	-2.50257400	3.66701200
C	-3.12414800	0.18958400	2.37090100	H	1.55712900	-3.38516500	4.22481000
C	-1.87918600	-0.22024200	1.60994400	H	0.48868700	-1.93897300	4.25832900
C	-0.74869000	0.55096000	1.41455200	Rh	2.35377800	-1.56149100	0.35609700
H	0.58210800	-1.02598900	0.71288600	C	2.12471600	1.35807800	-1.65519000
H	-3.92887700	0.54305100	1.70873800	C	2.30138700	-0.14697100	-1.45149200
H	-2.93285600	0.95484700	3.13000300	C	3.58242100	-0.74246700	-1.44891100
H	-0.77961300	1.58656400	1.74399000	C	4.79641700	0.08544700	-1.53221300
O	2.44982600	6.04708500	2.70218900	C	4.71529200	1.38468100	-1.84076600
C	3.03195300	7.03771400	1.86916400	C	3.42207400	2.12159000	-2.12392800
H	2.43438800	7.20495300	0.96326600	H	1.37124500	1.48852600	-2.44250300
H	3.05109000	7.95366300	2.46226100	H	1.48811700	-0.77947400	-1.81227700
H	4.05726100	6.77083400	1.58086900	H	5.74432200	-0.41355300	-1.34895600
				H	5.61052100	1.99935000	-1.91742400
<b>56</b>				O	3.68001600	-2.01834900	-1.21917100
C	-4.04145400	-1.08070300	-2.46156600	O	3.44461800	3.35149600	-1.36578200
C	-5.37054300	-1.19234400	-2.59253300	C	3.36870600	2.52153400	-3.60025400
C	-6.20173500	-1.86359800	-1.56415300	H	4.25577900	3.10224100	-3.87559300
C	-5.48579800	-2.36286100	-0.36463700	H	2.48259100	3.13928100	-3.78305300
C	-4.15627900	-2.25218200	-0.23986500	H	3.32406900	1.63237300	-4.23825000
C	-3.26019100	-1.66723900	-1.30746500	C	2.81850700	3.10015100	-0.10995500
H	-3.44127800	-0.57374900	-3.21570900	C	1.67537600	2.17884000	-0.44645700
H	-5.90485400	-0.79101600	-3.44939300	C	0.45648600	2.22775600	0.12321800
H	-6.10517700	-2.81676500	0.40427800	H	-0.46170400	0.56000300	-0.91550900
H	-3.64196900	-2.61446200	0.64923200	H	3.53104200	2.63003300	0.59125000
O	-7.41535600	-1.98588100	-1.69017500	H	2.50415800	4.06023600	0.31044600
O	-2.36862200	-0.68734600	-0.74533200	H	0.29711300	2.94815300	0.92412200
C	-2.31895800	-2.76797900	-1.84057400	O	-3.81388200	5.75729900	3.45740700
H	-1.71256100	-3.16376500	-1.01972300	C	-4.53500100	5.53274200	4.65828000
H	-1.64449900	-2.34450300	-2.59157200	H	-3.93152700	4.98701300	5.39578000
H	-2.89125300	-3.58335400	-2.29168400	H	-4.77651400	6.52170000	5.05192400
C	-2.98149100	0.45703300	-0.15915300	H	-5.46504700	4.97906700	4.47332300
H	-3.57344600	0.16208500	0.71994600				
H	-3.69328700	0.91487200	-0.86552600	<b>57</b>			
C	-1.93282900	1.47443600	0.23816100	C	-3.46864600	-2.38800600	-2.50559800
C	-0.66749100	1.38076800	-0.23612900	C	-4.50297900	-3.22857900	-2.64671900
C	-2.42372500	2.57188200	1.11215200	C	-4.73918500	-4.34232500	-1.69647500
C	-2.22535000	3.92328500	0.76120700	C	-3.79398300	-4.44521400	-0.55782600
C	-3.12895500	2.31306000	2.29726200	C	-2.75840900	-3.60562300	-0.42385300
C	-2.69534600	4.95703800	1.55890900	C	-2.42253000	-2.52077500	-1.42164900

H	-3.31200000	-1.56505600	-3.20133500	C	-0.51531000	3.36033600	-0.27570700
H	-5.22224700	-3.13188100	-3.45548500	C	-1.54942300	2.70019800	0.28246300
H	-3.99656100	-5.23682500	0.15853000	H	-1.42898400	0.87502600	-0.87986500
H	-2.07556700	-3.68587400	0.42100100	H	0.69706700	4.72726500	0.89674400
O	-5.67207400	-5.12601700	-1.83483600	H	-0.89859900	5.38989900	0.45937000
O	-2.21470000	-1.26320700	-0.75291100	H	-2.07870700	3.18309400	1.10252600
C	-1.05801300	-2.83052400	-2.07224300	O	1.52529600	0.33654200	1.35963500
H	-0.28345300	-2.88385800	-1.30037700	H	1.25351700	0.98163000	0.65430100
H	-0.79176600	-2.02983200	-2.76946400	C	0.37305700	-0.29287500	1.93253200
H	-1.09319000	-3.78042000	-2.61303700	H	-0.23590800	0.45290300	2.45346100
C	-3.34221800	-0.72249100	-0.06686300	H	-0.23567900	-0.78673600	1.16765900
H	-3.60481000	-1.35986200	0.79047600	H	0.73653800	-1.02767900	2.65393600
H	-4.22493200	-0.72193500	-0.72676700	O	-6.79818200	2.82412500	4.09864600
C	-3.05220600	0.68879600	0.40144400	C	-7.14484200	2.14079500	5.29238300
C	-2.00908600	1.38131600	-0.11563400	H	-6.27616700	2.01323200	5.95205800
C	-4.01516900	1.22924200	1.39666700	H	-7.88650400	2.76706700	5.79145700
C	-4.67555700	2.45617300	1.17946700	H	-7.58422600	1.15679300	5.08127800
C	-4.33124400	0.53059300	2.57167900				
C	-5.59011500	2.96054400	2.09347300	<b>58-ts</b>			
H	-4.47394800	3.00983300	0.26724300	C	0.87120600	-2.44506900	0.82078400
C	-5.24688800	1.02497900	3.50305800	C	0.81498200	-3.56423200	0.08224400
H	-3.83847500	-0.41415500	2.78677400	C	1.46551400	-4.82533400	0.50673600
C	-5.88461000	2.24845500	3.26619700	C	2.24053500	-4.76870300	1.76991100
H	-6.10046500	3.90232600	1.91689600	C	2.30009000	-3.65199400	2.50858300
H	-5.44930900	0.45325800	4.40165600	C	1.57027500	-2.37477500	2.15937900
C	3.02757300	-2.70083100	1.33073400	H	0.38174400	-1.53045800	0.48803200
H	2.01229800	-3.01535000	1.54880800	H	0.29153400	-3.59895100	-0.87011100
C	3.87391400	-1.93568000	2.15890700	H	2.75760200	-5.68152200	2.05371800
H	3.63917100	-1.53106300	3.13787900	H	2.88135700	-3.61473600	3.42874900
C	3.94946600	-3.40503300	0.30659000	O	1.38041400	-5.85618300	-0.15383400
C	4.38936700	-2.18580900	-0.53608400	O	2.48292300	-1.25777300	2.21199500
C	5.23621000	-1.42360800	0.29185200	C	0.53581600	-2.06266800	3.25923900
H	5.91289700	-0.63769200	-0.02462300	H	1.04565200	-1.94728700	4.22115400
C	5.31220900	-2.17496900	1.64063400	H	0.01818400	-1.12681900	3.02602600
H	4.29506400	-2.10516800	-1.61315600	H	-0.20132800	-2.86701100	3.33693900
H	3.52346400	-4.24878000	-0.23768900	C	3.52845400	-1.23718300	1.24408000
H	6.12693200	-1.89814800	2.31059900	H	4.48542600	-1.25619500	1.78706200
C	5.21893900	-3.64975500	1.16540800	H	3.50940700	-2.14544200	0.62692500
H	6.08540700	-3.96501600	0.57126100	C	3.47802700	-0.01889000	0.33647300
H	5.04994100	-4.35510500	1.98813900	C	2.51970400	0.92292100	0.48844300
Rh	3.23384600	-0.72924700	0.50570600	C	4.55278500	0.02220700	-0.69256100
C	0.35841100	2.94777000	-1.46640900	C	5.90638600	-0.03486400	-0.33011600
C	1.22152300	1.71459400	-1.25450400	C	4.25452700	0.07847900	-2.06838800
C	2.57458600	1.77661000	-1.04652900	C	6.92753700	-0.02032900	-1.28346800
C	3.22036600	3.10745200	-0.95265800	H	6.18071900	-0.06692500	0.72103400
C	2.57815600	4.23423200	-1.27908400	C	5.25698300	0.09256900	-3.02883300
C	1.15082600	4.26469100	-1.78467800	H	3.21550100	0.10002300	-2.38446400
H	-0.30998900	2.75326300	-2.31756500	C	6.60514400	0.04412200	-2.64388200
H	0.76673400	0.74121600	-1.42875600	H	7.95996700	-0.05378700	-0.95426500
H	4.25831400	3.11269800	-0.62848600	H	5.02144100	0.13227000	-4.08791200
H	3.06959900	5.20417900	-1.22398500	C	-4.76939100	-1.05793800	0.42180500
O	3.38276500	0.73974800	-0.92977700	H	-4.92533900	-0.79101600	1.46119500
O	0.43686100	5.31291300	-1.09004000	C	-5.09615400	-0.28475300	-0.70382700
C	1.12745800	4.62971500	-3.26915500	H	-5.55524000	0.69742400	-0.70722100
H	1.65493400	5.57367200	-3.44447300	C	-4.51609000	-2.49260500	-0.09431900
H	0.09140500	4.74444500	-3.60746300	C	-3.18911200	-2.27098700	-0.85899900
H	1.61309900	3.84524700	-3.85901500	C	-3.51723100	-1.49327800	-1.99047200
C	-0.07948900	4.75249000	0.11145000	H	-2.92848900	-1.37994200	-2.89444100

C	-5.04241000	-1.24436800	-1.91476100	H	0.17542200	-1.08742100	-3.00889300
H	-2.29473400	-2.86681300	-0.71259500	H	0.45332900	-2.75401000	-3.57497600
H	-4.52493600	-3.29057100	0.64878800	C	-3.09940100	-1.67105100	-0.90384900
H	-5.52911000	-0.90609400	-2.83015000	H	-4.06128400	-2.00182200	-1.32538800
C	-5.52833400	-2.56931900	-1.26869500	H	-2.76641400	-2.46845400	-0.22477800
H	-5.37210800	-3.44303400	-1.91288000	C	-3.31217400	-0.38753200	-0.11897100
H	-6.57308300	-2.52744100	-0.93740900	C	-2.55213300	0.70129100	-0.37533300
Rh	-2.97371600	-0.19966800	-0.38695800	C	-4.40153200	-0.44998900	0.89003700
C	-1.46304800	4.80184500	0.37292900	C	-4.43593200	-1.47085600	1.86179800
C	-2.35923300	3.81616700	0.23926700	C	-5.45769200	0.47230800	0.88597000
C	-2.06173200	2.44670000	0.69442400	C	-5.46268600	-1.55037200	2.79195900
C	-0.71940700	2.07397400	0.96849300	H	-3.63161500	-2.20012300	1.90559200
C	0.38704900	3.14072600	1.05082300	C	-6.49983000	0.40510600	1.81439800
C	-0.09680300	4.63292100	1.00218000	H	-5.47576900	1.25118000	0.12904400
H	-1.69388900	5.81645800	0.05145200	C	-6.50531900	-0.61130200	2.77654500
H	-3.34900700	3.98594400	-0.17701000	H	-5.47890600	-2.33029500	3.54689300
H	-0.64577800	1.28934500	1.72612600	H	-7.29786200	1.13769200	1.76995600
H	0.90245900	3.00279300	2.00981400	C	4.82139000	-0.11926100	-0.36482700
O	-3.04081300	1.61777900	0.73220600	H	4.91442400	0.42757800	-1.29686800
O	0.86174600	5.33208500	0.18028000	C	5.02300000	0.37944700	0.93004600
C	-0.07685000	5.31518000	2.37252200	H	5.29708900	1.39123100	1.20763000
H	0.93841800	5.28226600	2.78261600	C	4.85876100	-1.66081500	-0.24823800
H	-0.38032900	6.36448900	2.28868800	C	3.53515000	-1.90483200	0.51389700
H	-0.75972900	4.81007200	3.06379900	C	3.74166900	-1.40517100	1.81880200
C	1.36461900	4.41101400	-0.78438700	H	3.15866800	-1.64129500	2.70206800
C	1.44873800	3.09815300	-0.04904100	C	5.18646000	-0.85532100	1.84609500
C	2.38503300	2.15595300	-0.26839200	H	2.76729100	-2.60310300	0.19947700
H	1.80034200	0.75061400	1.28311900	H	4.99971100	-2.22002500	-1.17415300
H	2.33055500	4.78483200	-1.13781800	H	5.62405200	-0.68149700	2.83000200
H	0.68177900	4.34686000	-1.65085200	C	5.89885400	-1.84873900	0.88851300
H	3.11406700	2.33508000	-1.05696500	H	5.92913200	-2.87359800	1.27865500
O	-0.90735500	0.10869500	-0.70453300	H	6.90736700	-1.52357100	0.60553500
H	-0.64506200	1.13293800	-0.06644200	Rh	2.89186900	0.12019600	0.60836200
C	-0.27447100	0.00044600	-1.96763400	C	0.67352400	5.17165600	-0.66352300
H	-0.59248300	-0.92622200	-2.46152000	C	1.64248900	4.38809000	-0.16366100
H	-0.51878500	0.84506800	-2.62849900	C	1.58279300	2.93109400	-0.27336700
H	0.81380300	-0.03841100	-1.83404800	C	0.43626900	2.29751100	-1.02046500
O	7.51520000	0.06273200	-3.66031000	C	-0.84714700	3.15656600	-1.17707300
C	8.89287700	0.00756400	-3.32894200	C	-0.61578700	4.69872000	-1.29581300
H	9.43085600	0.03057900	-4.27848000	H	0.75580600	6.25457000	-0.58105400
H	9.19699100	0.86921600	-2.71963500	H	2.52000800	4.79958500	0.32827500
H	9.14303800	-0.91795200	-2.79326200	H	0.22956500	1.34298000	-0.52314700
<b>59</b>				H	-1.34215700	2.81912300	-2.09546300
C	-0.34023800	-2.72380700	-0.92587900	O	2.51646800	2.26079600	0.19195900
C	-0.10736300	-3.92478400	-0.37308300	O	-1.67280400	5.30944400	-0.52459200
C	-0.71404200	-5.16839200	-0.90206000	C	-0.73871400	5.22932900	-2.72423200
C	-1.65279400	-5.00790000	-2.03958700	H	-1.72634400	4.97626000	-3.12290200
C	-1.88552400	-3.81126500	-2.59597400	H	-0.62902700	6.31878400	-2.74416000
C	-1.19491500	-2.53987800	-2.15922500	H	0.02974000	4.79117700	-3.37070000
H	0.09470500	-1.81157100	-0.51356300	C	-1.97591100	4.42926000	0.56435500
H	0.52550700	-4.04096200	0.50309000	C	-1.84657200	3.05096500	-0.03093200
H	-2.14118100	-5.91492500	-2.38593200	C	-2.60175500	1.98598200	0.29851100
H	-2.58372200	-3.69981400	-3.42441800	H	-1.82304400	0.58810300	-1.16974100
O	-0.47302000	-6.26930100	-0.41580800	H	-2.98419600	4.66866000	0.91400700
O	-2.16004800	-1.48945200	-1.95776700	H	-1.27246800	4.59458200	1.39834100
C	-0.31267000	-2.01890000	-3.31246000	H	-3.30896000	2.09503900	1.11852200
H	-0.93501900	-1.81798600	-4.19062000	O	0.91103300	-0.06736900	0.94376800
				C	0.39993700	-0.85826400	1.97321100

H	0.82639200	-1.88102500	2.00425700
H	0.56265900	-0.41519800	2.97305600
H	-0.68997800	-0.97416500	1.84724500
H	0.83851900	2.05990800	-2.01787300
O	-7.46751900	-0.77787300	3.72933800
C	-8.54434500	0.14380900	3.76527000
H	-9.12549400	0.12323500	2.83356900
H	-9.18144800	-0.17136700	4.59372900
H	-8.19353100	1.16845400	3.94754200

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C	-3.83947600	0.70502000	-0.36605700
C	-3.16662600	1.77396900	-0.81691100
C	-1.78413700	2.07046100	-0.38274000
C	-1.22423900	1.19044900	0.72679400
C	-1.72597100	-0.26695100	0.69012400
C	-3.27429400	-0.37021800	0.54183200
H	-4.86353300	0.52174100	-0.69018300
H	-3.61015000	2.47987900	-1.51496700
H	-1.45906300	-0.75062500	1.63980400
O	-1.15364000	3.00852400	-0.84611500
O	-3.48712800	-1.63516600	-0.10942700
C	-4.02674300	-0.41412900	1.87087200
H	-3.68539600	-1.27160100	2.46006800
H	-5.10327200	-0.52100100	1.70156100
H	-3.85845400	0.50373500	2.44443500
C	-2.44729200	-1.79437700	-1.07319400
H	-2.72975900	-1.32648200	-2.03110300
H	-2.31733500	-2.86775900	-1.24243900
C	-1.22393800	-1.12470000	-0.46657000
C	0.01744500	-1.34235900	-0.93303200
H	0.08425900	-1.96884100	-1.82538700
C	1.32662700	-0.87985800	-0.44442300
C	2.38247700	-0.73209300	-1.35753700
C	1.61338000	-0.63264000	0.91414200
C	3.65493300	-0.31959300	-0.96191500
H	2.20214000	-0.93560200	-2.41055200
C	2.87504200	-0.22844400	1.32643800
H	0.84367900	-0.78689700	1.66374100
C	3.90697200	-0.05862100	0.39040900
H	4.43377200	-0.20983600	-1.70781800
H	3.09196800	-0.04542000	2.37429700
H	-0.13515600	1.25284400	0.69498100
H	-1.53993700	1.64707600	1.67748300
O	5.10689300	0.34587200	0.89598000
C	6.18370500	0.54412400	-0.00585900
H	5.95031600	1.31821900	-0.74881200
H	7.02817200	0.87176300	0.60321300
H	6.45155200	-0.38527500	-0.52607300

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C	3.59872400	-1.04572200	-0.38663600
C	2.80261200	-1.83786400	-1.12062200
C	1.36451500	-2.00479000	-0.81088100
C	0.88990700	-1.37634500	0.49112600
C	1.59117500	-0.04489100	0.81739400
C	3.13995300	-0.16896100	0.76410200
H	4.65736000	-0.95202100	-0.62752600

H	3.17772500	-2.39790000	-1.97393500
H	1.31862400	0.24893000	1.84010400
O	0.62323600	-2.65451800	-1.53320100
O	3.59468800	1.16859600	0.49902400
C	3.78443300	-0.60865100	2.07784000
H	3.52652400	0.10098500	2.87078200
H	4.87494600	-0.63366900	1.98149700
H	3.44260400	-1.60800600	2.36756400
C	2.67683300	1.76559300	-0.41594100
H	2.99863700	1.59212100	-1.45619200
H	2.69629200	2.84498900	-0.23244800
C	1.32493600	1.12522000	-0.13083800
C	0.15647600	1.56347800	-0.63059200
C	-1.17129200	1.00444000	-0.23572000
C	-2.02402600	0.41299900	-1.17627000
C	-1.62968600	1.09892600	1.09122100
C	-3.27715500	-0.08973200	-0.81853500
H	-1.69769900	0.31356700	-2.20818700
C	-2.87563900	0.60942500	1.46330900
H	-0.99819100	1.57218900	1.83872600
C	-3.70972300	0.00727000	0.50951200
H	-3.89657100	-0.55658100	-1.57571500
H	-3.22905300	0.68552300	2.48706700
H	-0.19513900	-1.27635600	0.45643600
H	1.11849400	-2.09596100	1.29247100
O	-4.91121700	-0.44558300	0.97173400
C	-5.78863200	-1.07720100	0.05360700
H	-5.33653600	-1.97748400	-0.38329900
H	-6.67171900	-1.36039700	0.62944900
H	-6.08687500	-0.39618100	-0.75475100
C	0.09280400	2.71567700	-1.61350100
H	1.08000100	3.06068300	-1.93277000
H	-0.46521200	2.42572200	-2.51298300
H	-0.44514300	3.56866500	-1.17820100

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Rh	-1.67815200	0.06833900	0.40568300
O	0.04639400	1.33688400	0.44128900
C	-0.06607700	2.50390200	1.21097000
H	-0.89038000	3.13362300	0.84094500
H	-0.25013800	2.30227300	2.27949800
H	0.85062700	3.10797300	1.14545500
C	-8.78513600	1.27792400	2.12694500
C	-7.54753100	0.64169700	1.83813900
C	-7.05230600	0.62410700	0.49431300
C	-7.83519200	1.27277100	-0.50485200
C	-9.02962700	1.88443800	-0.19510600
C	-9.51633000	1.88641000	1.13384700
H	-9.14095300	1.27560600	3.15465000
H	-7.48130000	1.28441700	-1.52861800
H	-9.60413300	2.37022800	-0.97945000
H	-10.46186800	2.36968000	1.36488200
C	-6.78299600	0.01809900	2.85263300
H	-7.15676000	0.02204700	3.87405900
C	-5.79845900	-0.02449700	0.20125800
C	-5.58431500	-0.58316400	2.55988100
C	-5.06554200	-0.61590000	1.23369800
H	-5.02314000	-1.04812500	3.36025800

P	-3.36938100	-1.35404100	0.94846200	C	-0.71109200	4.32738800	-3.44967900
C	-2.97431500	-2.06405900	2.62431200	H	-2.11710200	5.88480300	-2.94780600
C	-3.32715200	-3.35814300	3.03410100	H	0.54611800	2.59162100	-3.71170100
C	-2.27205900	-1.24159500	3.52191300	H	-0.16079200	4.93842400	-4.16110400
C	-2.99328600	-3.81490300	4.31140100	Rh	1.67812200	-0.06830800	0.40566900
H	-3.85519100	-4.01945000	2.35515800	O	-0.04642200	-1.33683700	0.44118700
C	-1.94855600	-1.69477600	4.80151300	C	0.06603900	-2.50396700	1.21067400
H	-1.96843400	-0.24964700	3.19409100	H	0.25025400	-2.30252500	2.27921400
C	-2.30767500	-2.98460000	5.19968100	H	-0.85072400	-3.10795100	1.14518600
H	-3.26877700	-4.82323800	4.61002500	H	0.89024000	-3.13370800	0.84045700
H	-1.40727100	-1.04336300	5.48308400	C	8.78505100	-1.27857000	2.12667100
H	-2.04929800	-3.34262200	6.19301700	C	7.54749900	-0.64218000	1.83795300
C	-3.71967900	-2.85998300	-0.06731100	C	7.05225100	-0.62439700	0.49413100
C	-4.90411700	-3.60582800	0.04271700	C	7.83504800	-1.27306700	-0.50511500
C	-2.72366300	-3.29097400	-0.95660200	C	9.02942500	-1.88489900	-0.19544900
C	-5.08491100	-4.76507100	-0.71311300	C	9.51615900	-1.88704400	1.13349600
H	-5.69141600	-3.27856000	0.71649300	H	9.14088900	-1.27639000	3.15437600
C	-2.90507300	-4.45418300	-1.70776200	H	7.48113000	-1.28458000	-1.52888200
H	-1.80793200	-2.71335600	-1.05075400	H	9.60385100	-2.37068600	-0.97985500
C	-4.08360200	-5.19256300	-1.58783700	H	10.46164600	-2.37044900	1.36446900
H	-6.00901400	-5.33023800	-0.62240300	C	6.78302400	-0.01861400	2.85252800
H	-2.11946300	-4.77989100	-2.38371600	H	7.15679800	-0.02268200	3.87395300
H	-4.22503200	-6.09531900	-2.17674900	C	5.79845500	0.02436700	0.20115800
C	-4.64003600	-0.03722600	-3.96973400	C	5.58437900	0.58277500	2.55985600
C	-5.72006800	-0.85195600	-3.55345900	C	5.06558500	0.61570800	1.23367600
C	-6.07534500	-0.86514800	-2.16565500	H	5.02325400	1.04769000	3.36030400
C	-5.33892600	-0.05266100	-1.22996300	P	3.36942300	1.35394700	0.94858100
C	-4.26031800	0.71734200	-1.67634100	C	2.97460300	2.06385800	2.62453600
C	-3.93400200	0.71221800	-3.06273200	C	3.32764400	3.35784700	3.03444900
H	-4.37356100	-0.01107000	-5.02404000	C	2.27236100	1.24133800	3.52210800
H	-3.11000600	1.31921600	-3.41538400	C	2.99396300	3.81446500	4.31185100
C	-6.45503000	-1.64072200	-4.47906100	H	3.85567300	4.01919200	2.35553000
H	-6.16751900	-1.61040100	-5.52753200	C	1.94905200	1.69439100	4.80180200
C	-7.16302900	-1.69834400	-1.77258600	H	1.96859800	0.24946200	3.19418300
H	-7.44859600	-1.73715100	-0.72824800	C	2.30836200	2.98412200	5.20009100
C	-7.50418800	-2.42613000	-4.06230200	H	3.26957500	4.82274000	4.61057000
C	-7.85538400	-2.45469600	-2.69176700	H	1.40778400	1.04295000	5.48335900
H	-8.06078800	-3.02540600	-4.77782000	H	2.05015500	3.34203900	6.19350800
H	-8.67967100	-3.08093600	-2.36070100	C	3.71974100	2.85994600	-0.06712400
P	-3.08784300	1.58463400	-0.49939900	C	4.90435400	3.60555900	0.04272700
C	-4.15639500	2.74782700	0.46895400	C	2.72363100	3.29120500	-0.95618300
C	-3.82709100	2.97418800	1.81297800	C	5.08522500	4.76483400	-0.71304100
C	-5.23852600	3.44645900	-0.08907700	H	5.69174900	3.27805600	0.71628900
C	-4.55260900	3.88938900	2.57834300	C	2.90512400	4.45445300	-1.70726200
H	-3.00091600	2.42207000	2.25206900	H	1.80778500	2.71375300	-1.05021600
C	-5.96413700	4.36107200	0.67515000	C	4.08381400	5.19259800	-1.58751400
H	-5.52231200	3.26783900	-1.12253600	H	6.00946700	5.32980100	-0.62247700
C	-5.61998300	4.58657400	2.00998600	H	2.11944300	4.78037600	-2.38302400
H	-4.28520600	4.05417800	3.61898300	H	4.22530200	6.09537300	-2.17638000
H	-6.80431100	4.88842500	0.23136200	C	4.63985300	0.03781100	-3.96979000
H	-6.18706700	5.29733800	2.60557200	C	5.71992700	0.85244500	-3.55343100
C	-2.15786000	2.73588400	-1.62986900	C	6.07527100	0.86540200	-2.16564200
C	-2.53059200	4.06656300	-1.87347700	C	5.33889200	0.05274600	-1.23005000
C	-1.02656800	2.22503800	-2.29055600	C	4.26022100	-0.71712700	-1.67650500
C	-1.81126200	4.85626700	-2.77367200	C	3.93382600	-0.71175700	-3.06288100
H	-3.38141400	4.49851500	-1.35894300	H	4.37331100	0.01185700	-5.02408300
C	-0.31863300	3.00935700	-3.20262000	H	3.10977300	-1.31864800	-3.41558800
H	-0.70136800	1.21312000	-2.07562300	C	6.45484200	1.64136300	-4.47893800

H	6.16728200	1.61120300	-5.52739800	C	3.37635800	4.71707300	1.33312700
C	7.16295100	1.69856900	-1.77247400	H	3.66662900	3.01249900	0.05920700
H	7.44855800	1.73722500	-0.72813400	C	1.17871200	4.96617300	2.30330000
C	7.50400900	2.42671700	-4.06210100	H	-0.25577500	3.44117700	1.77594600
C	7.85525700	2.45508200	-2.69157100	C	2.48615700	5.42827400	2.14042800
H	8.06056900	3.02612200	-4.77754600	H	4.39297500	5.07628500	1.19552000
H	8.67954500	3.08128800	-2.36043600	H	0.47658400	5.51756900	2.92296200
P	3.08774500	-1.58451600	-0.49962100	H	2.80799400	6.34157700	2.63389500
C	4.15631600	-2.74781100	0.46860700	C	2.13508200	1.32068700	-1.41269300
C	3.82694100	-2.97443500	1.81257000	C	3.43269700	0.80139900	-1.28554600
C	5.23858700	-3.44621400	-0.08946500	C	1.68733200	1.73176200	-2.67714400
C	4.55249800	-3.88970500	2.57782700	C	4.26895300	0.70692000	-2.39883800
H	3.00068300	-2.42246000	2.25169700	H	3.78824300	0.46015700	-0.31710600
C	5.96423800	-4.36088700	0.67466000	C	2.52509300	1.63827300	-3.78975800
H	5.52246700	-3.26734000	-1.12285900	H	0.67422600	2.11363800	-2.77994400
C	5.61998900	-4.58667600	2.00942300	C	3.81722200	1.12785500	-3.65175100
H	4.28502800	-4.05471000	3.61841600	H	5.26929800	0.29667100	-2.28916400
H	6.80451500	-4.88806200	0.23084800	H	2.16546600	1.95879300	-4.76391300
H	6.18709600	-5.29749500	2.60492500	H	4.46870100	1.05101200	-4.51834800
C	2.15770900	-2.73563500	-1.63023300	C	0.06891200	-2.41478600	-3.15689900
C	2.53026700	-4.06636600	-1.87385700	C	1.35142500	-2.73150900	-2.64775000
C	1.02650900	-2.22462300	-2.29095600	C	1.69412100	-2.30247200	-1.32419500
C	1.81085000	-4.85595400	-2.77409200	C	0.72944800	-1.57828100	-0.53143000
H	3.38099700	-4.49846200	-1.35928500	C	-0.52870900	-1.28879500	-1.07199700
C	0.31848400	-3.00883300	-3.20304400	C	-0.83221300	-1.71241300	-2.39937200
H	0.70145200	-1.21266000	-2.07601700	H	-0.19320700	-2.73167500	-4.16360700
C	0.71076200	-4.32691600	-3.45011400	H	-1.80024900	-1.47178400	-2.82145800
H	2.11655600	-5.88453100	-2.94823100	C	2.29608600	-3.45458300	-3.42427600
H	-0.54618900	-2.59096400	-3.71214400	H	2.00905400	-3.77175400	-4.42404200
H	0.16039700	-4.93786800	-4.16156100	C	3.00329300	-2.61160900	-0.85221300

## 25-L2

Rh	-1.20437200	1.98699600	-0.43813800	C	3.29935500	-2.28845700	0.13825700
O	-2.82120800	3.03417900	-0.90939100	C	3.54556100	-3.74507600	-2.92848200
C	-3.88552800	3.34336300	-0.05869100	C	3.89960500	-3.31202500	-1.62897200
H	-3.57872700	3.56408700	0.97996700	H	4.26086700	-4.29942500	-3.52993900
H	-4.41053700	4.23736500	-0.43622600	H	4.88977000	-3.53297400	-1.23921200
H	-4.63087500	2.52714800	-0.01822700	P	-1.77078900	-0.14514200	-0.27968000
C	1.90757800	-2.84534200	4.16172900	C	-2.09298700	-0.77218200	1.43053100
C	1.74645100	-1.83563900	3.17444000	C	-2.48313200	0.16263200	2.40148100
C	1.30255300	-2.19198800	1.85932200	C	-2.05525700	-2.13082100	1.77650700
C	1.03341500	-3.56836000	1.60347600	C	-2.84026700	-0.25392000	3.68466800
C	1.19500400	-4.52406200	2.58165800	H	-2.49831400	1.21693100	2.13808100
C	1.63925700	-4.16354700	3.87653600	C	-2.40606200	-2.54650200	3.06162700
H	2.24633500	-2.55114000	5.15232400	H	-1.72977200	-2.86956800	1.05087000
H	0.69479600	-3.86575300	0.61793000	C	-2.80380600	-1.60943800	4.01707000
H	0.98138600	-5.56562300	2.35664400	H	-3.14266000	0.48194200	4.42523100
H	1.76549200	-4.92751100	4.63884200	H	-2.35754500	-3.60148100	3.31722500
C	2.01576400	-0.47537900	3.45999000	H	-3.07719900	-1.93399400	5.01769900
H	2.36193600	-0.20291700	4.45429000	C	-3.35890600	-0.57729600	-1.14477600
C	1.13405500	-1.16832500	0.86014100	C	-3.93545900	-1.85565000	-1.04076100
C	1.84010400	0.49100500	2.50113300	C	-3.99961600	0.39711700	-1.92444100
C	1.39365700	0.16537300	1.18994200	C	-5.11939200	-2.15633000	-1.71181900
H	2.04706700	1.52558000	2.74823200	H	-3.46533800	-2.62248600	-0.43414500
P	0.98755700	1.55130500	0.01557900	C	-5.18972100	0.09004400	-2.59280700
C	1.65639700	3.06809800	0.85321400	H	-3.58121500	1.40119200	-1.97107000
C	2.96609400	3.54608200	0.69289400	C	-5.74913700	-1.18295000	-2.49311300
C	0.76633900	3.79769200	1.66130200	H	-5.55179900	-3.14966800	-1.62243300
				H	-5.67921900	0.85635600	-3.18829300
				H	-6.67405700	-1.41771400	-3.01390100



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Rh	-1.65662700	0.27095500	-0.43068100
O	-3.19898500	1.71052800	-0.65043400
C	-3.23468000	2.91696100	-1.38896300
H	-3.75229600	2.76722800	-2.34613700
H	-3.75509500	3.69414700	-0.81531300
H	-2.21433000	3.25680100	-1.58584500
C	5.28696800	0.09869400	-2.84834500
C	4.03656500	-0.29511300	-2.29963200
C	3.70165900	0.07071200	-0.95574200
C	4.65361600	0.83975900	-0.22462100
C	5.85621900	1.21039500	-0.78405000
C	6.18283200	0.83488000	-2.10911800
H	5.51935100	-0.19384600	-3.86956800
H	4.42490300	1.13915600	0.79107800
H	6.56202600	1.79654000	-0.20153600
H	7.13672200	1.13077800	-2.53717800
C	3.10296300	-1.04476200	-3.05398600
H	3.35554100	-1.33300800	-4.07172100
C	2.43213900	-0.32724300	-0.40150200
C	1.89241200	-1.40480200	-2.51673700
C	1.53061600	-1.05131800	-1.18572400
H	1.20027400	-1.97538800	-3.12258400
P	-0.19190000	-1.46719000	-0.58678500
C	-0.80697600	-2.60930700	-1.91778700
C	-0.67094800	-4.00432700	-1.87579900
C	-1.45614600	-2.02940700	-3.02131700
C	-1.16896900	-4.79782000	-2.91301700
H	-0.18541600	-4.47981500	-1.03048300
C	-1.95161200	-2.82153600	-4.05755200
H	-1.58019900	-0.94942400	-3.05494200
C	-1.81004100	-4.21041000	-4.00506600
H	-1.05591500	-5.87786800	-2.86378800
H	-2.45450900	-2.35425500	-4.89993500
H	-2.19971700	-4.83003000	-4.80833400
C	0.09287900	-2.57326100	0.85906400
C	1.13493300	-3.51384600	0.90877900
C	-0.80219500	-2.48627600	1.93343400
C	1.26804600	-4.36033500	2.00948600
H	1.84964100	-3.57870500	0.09271200
C	-0.66774700	-3.33604700	3.03323900
H	-1.60534400	-1.75688700	1.89930600
C	0.36484500	-4.27368400	3.07221200
H	2.08121600	-5.08060700	2.04152400
H	-1.37349000	-3.26393800	3.85590800
H	0.47078700	-4.93300500	3.92976400
C	1.69345600	0.77224300	3.72199100
C	2.66271100	-0.21964100	3.43676100
C	2.88479000	-0.59462000	2.07203100
C	2.13026700	0.04457700	1.02318500
C	1.17091800	1.00777300	1.34935000
C	0.96966500	1.35909400	2.71515500
H	1.52567700	1.06534900	4.75566400
H	0.22992500	2.10904100	2.96623700
C	3.41346800	-0.84123500	4.47065700
H	3.22911800	-0.53761400	5.49841700
C	3.85568200	-1.60565300	1.81507400

H	4.03521900	-1.91897900	0.79375200
C	4.35010900	-1.80605900	4.18213600
C	4.56710500	-2.19189600	2.83812500
H	4.91976000	-2.27481400	4.97991000
H	5.30150700	-2.96004500	2.61083200
P	-0.02228400	1.72061700	0.10464700
C	1.00563700	2.43934200	-1.25254000
C	0.50049600	2.38852900	-2.55992200
C	2.22969200	3.08676100	-1.02326700
C	1.19443900	2.98712300	-3.61302100
H	-0.43663300	1.86838900	-2.74077000
C	2.92500500	3.68175100	-2.07654200
H	2.64908400	3.11506600	-0.02183000
C	2.40634300	3.63685500	-3.37244600
H	0.79023100	2.94040800	-4.62078000
H	3.87643600	4.17041700	-1.88559900
H	2.94937600	4.10002100	-4.19204700
C	-0.69853700	3.21863000	0.96550800
C	-0.08507700	4.48081900	0.89777800
C	-1.87633500	3.07890300	1.71763700
C	-0.63042400	5.57079200	1.57742400
H	0.81025500	4.62682400	0.30474800
C	-2.42234700	4.17310400	2.39001400
H	-2.39941400	2.13165000	1.74701800
C	-1.79938000	5.41973200	2.32658900
H	-0.14430100	6.54085400	1.51137900
H	-3.35319900	4.04162000	2.93263300
H	-2.22854100	6.27356400	2.84487100
C	-3.95109900	-1.34430100	-0.64765800
C	-3.89726500	-2.72118900	-0.34664600
C	-4.10617500	-3.14090000	0.96470000
C	-4.34130700	-2.18368900	1.97100600
C	-4.37367700	-0.83473300	1.65449500
C	-4.20769900	-0.36375500	0.32944900
H	-3.90685700	-1.04643700	-1.69346200
H	-3.71767400	-3.43395300	-1.14316900
H	-4.50386800	-2.53668000	2.98637000
H	-4.57441400	-0.10617200	2.43671000
B	-4.52548600	1.19137800	-0.06899400
O	-5.57460700	1.19984100	-1.07217400
H	-5.92658800	2.10031600	-1.13256600
O	-4.81470100	2.06240700	1.07477500
H	-5.72945400	1.89376000	1.34165100
O	-4.10194300	-4.44508000	1.38343500
C	-3.92932100	-5.45378000	0.40490600
H	-2.96013700	-5.36560900	-0.10367100
H	-3.97120900	-6.40466700	0.94085200
H	-4.72869800	-5.42673100	-0.34846200

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Rh	1.58697500	0.66034400	0.11253500
O	2.94366700	2.37784800	0.22358600
C	2.68022300	3.55478000	0.99007700
H	2.60381000	3.32208300	2.05669800
H	3.49269400	4.27439500	0.83213500
H	1.74527500	3.98841700	0.63327000
C	-4.97436500	-0.63734100	3.15211300
C	-3.70973600	-0.81802400	2.52945100

C	-3.54637400	-0.50525300	1.14148900	H	0.02511000	2.19651300	2.52063400
C	-4.68343000	-0.00399300	0.44236900	C	-3.60143600	3.38191700	1.82981100
C	-5.89668000	0.16324600	1.07235900	H	-3.26180100	2.74174300	-0.19512300
C	-6.05022100	-0.15882700	2.44185800	C	-3.06407900	3.50341700	3.11375800
H	-5.07218800	-0.88515700	4.20653200	H	-1.33782600	3.16359800	4.36208200
H	-4.58998100	0.25190600	-0.60586900	H	-4.62245000	3.69800400	1.63359500
H	-6.74496700	0.54663700	0.51140600	H	-3.66531700	3.92073000	3.91730700
H	-7.01373500	-0.02519900	2.92633000	C	-0.02673000	3.29389200	-1.28831100
C	-2.59431200	-1.30403000	3.25099400	C	-0.69986900	4.51612000	-1.13478700
H	-2.71196200	-1.55068000	4.30377700	C	1.02604700	3.22316800	-2.21892900
C	-2.26289900	-0.69247700	0.50968200	C	-0.33699600	5.63013500	-1.89603500
C	-1.37658500	-1.46403200	2.63877200	H	-1.50330200	4.60971900	-0.41282100
C	-1.17990100	-1.16129400	1.26043400	C	1.38093500	4.33300600	-2.98520200
H	-0.54568900	-1.83492200	3.22407000	H	1.57390500	2.29247100	-2.32933600
P	0.55858400	-1.30489800	0.55900400	C	0.70055000	5.54211800	-2.82458100
C	1.45265700	-2.14905900	1.95795600	H	-0.86789900	6.56860100	-1.75798400
C	1.58172600	-3.53971800	2.08057100	H	2.19856600	4.25505900	-3.69674700
C	2.03330700	-1.32926300	2.94144500	H	0.98279000	6.41081400	-3.41359400
C	2.26051600	-4.09834300	3.16699200	C	4.22864200	-1.28660100	0.28198000
H	1.16263900	-4.19566900	1.32568700	C	5.08132000	-2.16828400	-0.39666600
C	2.70102000	-1.88888800	4.03128100	C	5.27865800	-2.01157900	-1.77242900
H	1.99234100	-0.24969200	2.82563400	C	4.63973300	-0.95467900	-2.44396800
C	2.81562200	-3.27648300	4.14858600	C	3.80905500	-0.09278200	-1.74072600
H	2.35484600	-5.17880400	3.24217000	C	3.55469000	-0.22289300	-0.34705500
H	3.14483800	-1.23764500	4.77982700	H	4.10935400	-1.42702300	1.35184600
H	3.34194400	-3.71301000	4.99369500	H	5.57293300	-2.96567300	0.15141500
C	0.37844600	-2.65527400	-0.69549600	H	4.82273600	-0.83244800	-3.50826300
C	-0.50753200	-3.73073700	-0.51658500	H	3.35985200	0.73435500	-2.28582400
C	1.18360900	-2.62600400	-1.84259100	B	4.06653200	1.56737400	0.64402100
C	-0.57816100	-4.75762000	-1.45837200	O	4.10095600	1.27526600	2.02554000
H	-1.14810700	-3.76490700	0.36015200	H	5.02133100	1.21628900	2.31549200
C	1.11044100	-3.65385100	-2.78550100	O	5.26135800	1.89910800	-0.02202700
H	1.86911300	-1.79950000	-1.99297400	H	5.87948400	1.15580400	-0.02572100
C	0.23201800	-4.72119300	-2.59558600	O	6.07592200	-2.80999600	-2.54309200
H	-1.27141300	-5.58111400	-1.30791700	C	6.72491300	-3.90475300	-1.92125200
H	1.74248300	-3.61559000	-3.66882500	H	7.28030300	-4.41390000	-2.71199100
H	0.17362600	-5.51903000	-3.33157700	H	7.42659700	-3.57322900	-1.14321000
C	-2.15434900	0.27077800	-3.71049900	H	6.00389400	-4.60378500	-1.47601000
C	-2.82736300	-0.90221100	-3.29181100				
C	-2.83273100	-1.23289500	-1.89759900	<b>28-L2</b>			
C	-2.15949900	-0.37493800	-0.95695900	Rh	-1.62670400	0.37311000	-0.18553600
C	-1.48983800	0.76355800	-1.41370700	O	-3.06827600	2.24737900	-0.01592700
C	-1.50649200	1.07194300	-2.80340900	C	-3.36232500	2.92137800	-1.24262300
H	-2.15865000	0.53424000	-4.76577400	H	-3.79870300	2.23382800	-1.97476800
H	-1.00082600	1.96226900	-3.15623600	H	-4.05506300	3.75110200	-1.06595100
C	-3.50289200	-1.74147000	-4.21864400	H	-2.42046400	3.31301600	-1.63132100
H	-3.48556000	-1.46948900	-5.27150100	C	4.15855900	-0.53076700	4.08023500
C	-3.52375800	-2.41457100	-1.50195900	C	3.31195400	0.03128400	3.08680300
H	-3.53899500	-2.69061100	-0.45451600	C	3.17489900	-0.61800700	1.81731400
C	-4.16466700	-2.87094700	-3.79731500	C	3.90788400	-1.82296200	1.61131500
C	-4.17036800	-3.20810300	-2.42274500	C	4.72186900	-2.34398500	2.59239200
H	-4.68011300	-3.50508300	-4.51356500	C	4.85309700	-1.69375700	3.84242800
H	-4.68960700	-4.10331600	-2.09095300	H	4.24640800	-0.01846800	5.03559300
P	-0.39658500	1.76996500	-0.28501700	H	3.82002500	-2.33864900	0.66251900
C	-1.51520900	2.42041100	1.03618600	H	5.26863500	-3.26436900	2.40460400
C	-0.98879800	2.53933200	2.33052600	H	5.49993900	-2.11418700	4.60779200
C	-2.83273900	2.84234400	0.79796100	C	2.60407400	1.23593100	3.31406200
C	-1.75794600	3.07947100	3.36320000	H	2.71821300	1.74419100	4.26892800

C	2.31991100	-0.04587200	0.80729900
C	1.78690100	1.76387300	2.34615900
C	1.62144200	1.13380600	1.08013100
H	1.25976600	2.68729800	2.55175700
P	0.30662300	1.77766800	-0.07832500
C	-0.06351900	3.47717500	0.57894000
C	0.42351200	4.66643100	0.01473200
C	-0.93925500	3.56720900	1.67596800
C	0.06064900	5.90792800	0.54412300
H	1.08422600	4.63322600	-0.84428000
C	-1.29113600	4.80631300	2.21067600
H	-1.36526000	2.66453500	2.10037800
C	-0.79176800	5.98237500	1.64606300
H	0.44844100	6.81698900	0.09111800
H	-1.97112000	4.84801700	3.05727200
H	-1.07216900	6.94914400	2.05647400
C	1.19229500	2.14212000	-1.66009000
C	2.46862500	2.72333300	-1.71941500
C	0.52282600	1.85769500	-2.85951000
C	3.05484200	3.02483400	-2.94915800
H	3.00865100	2.93672100	-0.80116400
C	1.10911000	2.15880000	-4.09066500
H	-0.45352300	1.38021700	-2.81203900
C	2.37457800	2.74598500	-4.13706300
H	4.04668900	3.46779400	-2.97988400
H	0.58021500	1.92861400	-5.01205900
H	2.83405200	2.97833900	-5.09429500
C	2.48839100	-2.01235100	-3.04957100
C	3.58526900	-1.23279500	-2.61375700
C	3.49424500	-0.57313500	-1.34638900
C	2.29944600	-0.70687300	-0.54550100
C	1.22290800	-1.46222800	-1.02616000
C	1.35357800	-2.11587900	-2.28640100
H	2.55422600	-2.53381600	-4.00192200
H	0.53855000	-2.72448500	-2.65461600
C	4.76188500	-1.10288700	-3.39955400
H	4.80410800	-1.61806800	-4.35644600
C	4.61317100	0.20852500	-0.93366800
H	4.57423500	0.72972400	0.01499800
C	5.82287800	-0.34408700	-2.96399300
C	5.74051000	0.31977000	-1.71726600
H	6.71933700	-0.25106800	-3.57115700
H	6.57572700	0.92424600	-1.37320000
P	-0.45594500	-1.52692700	-0.17790300
C	-0.06977600	-2.16255600	1.51748300
C	-0.71357700	-1.56973800	2.61367000
C	0.81923400	-3.22456700	1.74807900
C	-0.48638300	-2.03787700	3.90938200
H	-1.38027700	-0.72972800	2.43328100
C	1.04226200	-3.69563300	3.04249000
H	1.34526100	-3.68194800	0.91456500
C	0.38796500	-3.10420900	4.12550100
H	-0.98974300	-1.56581700	4.74916400
H	1.73663700	-4.51535100	3.20616800
H	0.56653700	-3.46879600	5.13378000
C	-1.26773700	-2.98472600	-1.00849300
C	-1.36337700	-4.26288500	-0.44287400
C	-1.85664200	-2.76924700	-2.26702600

C	-2.00863000	-5.29980200	-1.12398500
H	-0.95025600	-4.45989100	0.53931400
C	-2.48341000	-3.80620300	-2.95481000
H	-1.82988900	-1.77373800	-2.69959800
C	-2.56229600	-5.07907800	-2.38364200
H	-2.07774400	-6.28102000	-0.66124800
H	-2.92626800	-3.61587400	-3.92906800
H	-3.06252300	-5.88646400	-2.91209700
C	-4.22128700	-0.51031000	-1.44501300
C	-5.54254700	-0.98410800	-1.53524500
C	-6.10611000	-1.65894700	-0.44653000
C	-5.33477100	-1.84796500	0.70651700
C	-4.02994800	-1.35986800	0.77055400
C	-3.42173200	-0.65642700	-0.29399900
H	-3.80996500	-0.01861100	-2.32648800
H	-6.10015800	-0.84474700	-2.45671700
H	-5.77889200	-2.38290400	1.54227100
H	-3.47252800	-1.53542300	1.68815200
B	-4.10539800	1.97752300	0.87964400
O	-5.41630500	1.84434300	0.50984800
H	-5.50919100	1.40394500	-0.35125700
O	-3.76417500	1.96051000	2.20514300
H	-4.51923200	1.63946100	2.72004100
O	-7.37997000	-2.16992600	-0.41227100
C	-8.18719900	-2.01341200	-1.56190400
H	-7.74840800	-2.50833400	-2.43997300
H	-9.14471600	-2.48376800	-1.32708100
H	-8.35651900	-0.95366500	-1.80121900

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Rh	-1.74012200	0.89799000	-0.24492600
C	4.27468900	-1.68620200	-3.28236800
C	3.05591500	-1.60386500	-2.55666900
C	3.04268400	-1.03430100	-1.24236000
C	4.28108500	-0.55205600	-0.72526700
C	5.44721400	-0.64255200	-1.45243600
C	5.45082000	-1.21920300	-2.74447400
H	4.25591800	-2.12625900	-4.27670100
H	4.30472300	-0.10423600	0.26052200
H	6.37445100	-0.26582300	-1.02876400
H	6.37835900	-1.28731500	-3.30648700
C	1.83957100	-2.07644200	-3.10261500
H	1.84059600	-2.51416900	-4.09830200
C	1.80709100	-0.96207800	-0.49791600
C	0.66975300	-1.98514100	-2.39281200
C	0.62108100	-1.43062400	-1.07990600
H	-0.24239600	-2.35027100	-2.84662800
P	-1.08174200	-1.20478200	-0.32354700
C	-2.14502000	-2.31007500	-1.38069700
C	-2.32249500	-3.68066400	-1.13922500
C	-2.79968900	-1.73107000	-2.48040800
C	-3.12475800	-4.45325600	-1.98253300
H	-1.84673100	-4.15213000	-0.28625800
C	-3.58995600	-2.50558300	-3.32980100
H	-2.69701100	-0.66308500	-2.64998300
C	-3.75589700	-3.87009600	-3.08210800
H	-3.25721000	-5.51210300	-1.77516900
H	-4.08840600	-2.03868600	-4.17523500

H	-4.38079700	-4.47260400	-3.73633300	H	-5.93140700	3.25375200	-0.27877500
C	-1.02516100	-2.11424000	1.28566300	H	-6.74086900	-0.90576800	0.45955400
C	-0.25785100	-3.27391100	1.47669300	H	-4.36838500	-1.43094800	0.23431400
C	-1.82816300	-1.65139700	2.33914200	O	-7.80355200	1.61245800	0.20674600
C	-0.29817300	-3.95993800	2.69152300	C	-8.77653800	0.62215900	0.47431800
H	0.38216200	-3.63831600	0.67852800	H	-8.59910800	0.12495200	1.43845100
C	-1.86997800	-2.34041700	3.55248900	H	-9.73638800	1.14254800	0.51121700
H	-2.41460900	-0.74849000	2.19468900	H	-8.81043800	-0.14088600	-0.31608800
C	-1.10641200	-3.49559500	3.73100700				
H	0.31016200	-4.84996400	2.82801100	<b>33-L2</b>			
H	-2.49687700	-1.97044200	4.35961500	C	6.42020000	0.79520700	-0.08073500
H	-1.13502900	-4.02851000	4.67790500	C	6.73145500	-0.02337800	0.93451700
C	2.25633300	0.66071700	3.49796300	C	6.78467200	-1.49285000	0.75914300
C	2.71091900	-0.65328600	3.23127000	C	6.52557800	-2.00327000	-0.60765700
C	2.53582700	-1.19221700	1.91458000	C	6.21350100	-1.18111200	-1.61965400
C	1.88972600	-0.40146800	0.89887200	C	6.12923000	0.32287600	-1.48819900
C	1.44423200	0.88706600	1.20882300	H	6.34653600	1.87120700	0.06848600
C	1.64484800	1.40393700	2.51913100	H	6.93025800	0.34593700	1.93693300
H	2.40329700	1.07868600	4.49125000	H	6.57750700	-3.08184200	-0.73089900
H	1.30717900	2.40738200	2.75001600	H	5.99381100	-1.57272500	-2.61194900
C	3.34799900	-1.43378700	4.23379100	O	7.00653900	-2.25149800	1.70063300
H	3.46752100	-1.00431300	5.22575300	O	4.83765600	0.79750900	-1.91118300
C	3.02729600	-2.50770600	1.66954500	C	7.11794500	0.98276300	-2.46781300
H	2.91470900	-2.93685900	0.68092400	H	6.88277500	0.67333900	-3.49115200
C	3.80745400	-2.70042400	3.95923300	H	7.02094700	2.07131300	-2.40719200
C	3.64401400	-3.23861900	2.66022900	H	8.14898000	0.70008100	-2.23434200
H	4.29609800	-3.28755000	4.73208700	C	3.72350200	0.25337100	-1.17809500
H	4.01023300	-4.23846100	2.44228100	H	3.57359700	-0.79943000	-1.46007000
P	0.40940200	1.84969500	-0.00207200	H	3.94551000	0.25949000	-0.10120500
C	1.55381300	2.26709600	-1.38881600	C	2.49951700	1.03603300	-1.42030700
C	1.02423300	2.25480900	-2.68725300	C	1.93410700	2.03895500	-2.00029300
C	2.90052800	2.61972900	-1.20678500	Rh	0.60261500	1.19866400	-0.65135500
C	1.81934700	2.60079200	-3.78150900	C	1.01576600	2.76783700	0.56325800
H	-0.01267100	1.95990600	-2.83008700	C	0.41309500	4.02803600	0.45643000
C	3.69511300	2.96487000	-2.30050600	C	2.05113000	2.63250200	1.50595700
H	3.33011600	2.62045100	-0.20844800	C	0.77804800	5.09915000	1.28664200
C	3.15484400	2.95813100	-3.58916000	H	-0.36085400	4.20468100	-0.28362500
H	1.39703800	2.58508500	-4.78282200	C	2.42435700	3.68725500	2.33771300
H	4.73737300	3.23255500	-2.14792500	H	2.58049900	1.69102500	1.60033000
H	3.77626400	3.22423000	-4.44024200	C	1.78574900	4.92961500	2.23933300
C	0.12585800	3.48611500	0.82824700	H	0.26885800	6.05032500	1.17008800
C	0.81576500	4.66699800	0.51606600	H	3.21942500	3.56612900	3.06855800
C	-0.91336000	3.54669200	1.77676300	C	-2.88558800	-3.46120200	-3.92871500
C	0.48167600	5.87145400	1.14052100	C	-2.71461900	-2.29846200	-3.13042200
H	1.61057200	4.65377200	-0.22186800	C	-2.58450400	-2.42053900	-1.70892500
C	-1.24067000	4.74839400	2.40500800	C	-2.61306800	-3.73458900	-1.15722700
H	-1.46433400	2.63976500	2.02041100	C	-2.77004000	-4.84472200	-1.95688300
C	-0.54293700	5.91605000	2.08701600	C	-2.91594500	-4.71200600	-3.35774500
H	1.02469000	6.77718300	0.88279200	H	-2.98824900	-3.33986800	-5.00460100
H	-2.04482600	4.77240200	3.13565700	H	-2.49578700	-3.86245400	-0.08830200
H	-0.80058500	6.85512600	2.56961100	H	-2.78001000	-5.83343600	-1.50619100
C	-4.21770300	1.91793500	-0.28130000	H	-3.04534900	-5.59594700	-3.97641500
C	-5.56857700	2.23615200	-0.16271600	C	-2.67331400	-1.00644400	-3.70801100
C	-6.49225200	1.21617200	0.10685000	H	-2.78723100	-0.90352100	-4.78475800
C	-6.04303800	-0.10103000	0.25135300	C	-2.42715700	-1.23974100	-0.89091800
C	-4.67753500	-0.39419000	0.12502100	C	-2.48616400	0.10384400	-2.92567200
C	-3.72985100	0.60298300	-0.13519100	C	-2.35544200	0.01723600	-1.50776700
H	-3.51990800	2.73997500	-0.49580800	H	-2.44592800	1.07710400	-3.39966000

P	-1.78167100	1.56770600	-0.64189000	C	3.35391100	-0.67430200	4.25134900
C	-2.40828700	2.95088600	-1.72945100	H	4.57229500	-2.03571300	3.10056200
C	-3.65402900	3.58009500	-1.58007800	H	1.93434800	0.69350900	5.13194900
C	-1.55029700	3.40650000	-2.74443200	H	4.07404900	-0.57995200	5.05969300
C	-4.03490000	4.61885400	-2.43232400	O	2.22219700	5.90260400	3.10506200
H	-4.32998900	3.27534300	-0.78969700	C	1.62034500	7.17913400	3.01963900
C	-1.93401300	4.43825800	-3.60231800	H	0.54152400	7.13694500	3.22689200
H	-0.57167100	2.94756300	-2.84329900	H	2.10683600	7.79570700	3.77896200
C	-3.18023100	5.04816800	-3.44884200	H	1.77248600	7.63700400	2.03196400
H	-5.00272600	5.09485200	-2.29650800	C	2.14315600	3.21635800	-2.88147500
H	-1.25326600	4.77223600	-4.38118900	H	3.19461000	3.29648400	-3.18460300
H	-3.47891300	5.85823900	-4.10907100	H	1.53269700	3.15798000	-3.79240200
C	-2.83854600	1.75839500	0.86396500	H	1.86083900	4.13939300	-2.36058400
C	-4.21143900	1.46230200	0.87178000				
C	-2.25359700	2.27457500	2.03074400	<b>34-ts-L2</b>			
C	-4.98236100	1.68365800	2.01329100	C	6.37809200	0.24411800	2.03610900
H	-4.67972600	1.04165600	-0.01288200	C	7.31265500	-0.70025900	1.86081100
C	-3.02741900	2.49974400	3.17171700	C	8.24071500	-0.67472900	0.70456600
H	-1.19415900	2.50776900	2.04048000	C	8.03134300	0.41391400	-0.27944100
C	-4.39186200	2.20723200	3.16548900	C	7.09192500	1.35349200	-0.10167200
H	-6.04018900	1.43550700	2.00409800	C	6.20791500	1.43687500	1.12265100
H	-2.55952100	2.90383800	4.06566000	H	5.69615400	0.21067000	2.88473800
H	-4.99223200	2.37992900	4.05494900	H	7.43466300	-1.53170300	2.54984100
C	-2.64022300	-2.10678300	3.35397900	H	8.67700100	0.39665300	-1.15336100
C	-3.82281200	-2.11640600	2.57595100	H	6.93614100	2.14118100	-0.83747700
C	-3.73329000	-1.79733900	1.18247400	O	9.12291800	-1.51577700	0.56403800
C	-2.45725700	-1.45115200	0.60357000	O	4.83134600	1.61205300	0.75359700
C	-1.31935500	-1.42227800	1.41582100	C	6.55042000	2.72383300	1.90401500
C	-1.43503600	-1.76957100	2.79228100	H	6.39126200	3.59533200	1.26101300
H	-2.69729800	-2.37423500	4.40671200	H	5.88919300	2.81207100	2.77188900
H	-0.54773800	-1.77595400	3.41310500	H	7.59051700	2.71033100	2.24203600
C	-5.08163500	-2.44434900	3.14758600	C	4.24522300	0.52961100	0.01446300
H	-5.12176300	-2.68402300	4.20761400	H	4.87390900	0.27857100	-0.85204900
C	-4.93935100	-1.82669700	0.42291400	H	4.18156300	-0.37172700	0.63823600
H	-4.90463700	-1.58992400	-0.63387600	C	2.89348900	0.97238100	-0.42246100
C	-6.22437900	-2.45881100	2.38231000	C	2.17175100	2.01897800	-0.62176700
C	-6.14693700	-2.14440000	1.00467500	Rh	0.80510500	0.44957300	-0.51373100
H	-7.18234400	-2.71153000	2.82864800	C	2.26187200	-0.72356000	-1.52387700
H	-7.04884100	-2.15658800	0.39835200	C	2.78656200	-1.97210700	-1.13089500
P	0.32957700	-0.90065000	0.70932200	C	2.38048600	-0.39224800	-2.88485900
C	0.79696000	-2.44143200	-0.21590400	C	3.32140200	-2.86474200	-2.05471300
C	1.17445900	-2.35709300	-1.56263000	H	2.76496600	-2.26653700	-0.08814100
C	0.75809200	-3.70640600	0.39595200	C	2.89952000	-1.28462700	-3.83085000
C	1.51386400	-3.50682500	-2.28157900	H	2.06886800	0.59141800	-3.22133700
H	1.20083900	-1.38702700	-2.05161600	C	3.37000400	-2.53545500	-3.41638200
C	1.10462700	-4.85248700	-0.31818800	H	3.70345400	-3.83217400	-1.74112300
H	0.46009500	-3.79458200	1.43712500	H	2.95110000	-0.98304200	-4.87179700
C	1.48298400	-4.75471900	-1.66043200	C	-4.64625300	0.55369900	4.34288200
H	1.79888100	-3.42296800	-3.32695700	C	-3.67835800	0.07347100	3.41990400
H	1.07638000	-5.82253700	0.17140700	C	-3.90869600	0.20129700	2.01211400
H	1.74835700	-5.64917700	-2.21789700	C	-5.12469000	0.82107500	1.59948900
C	1.48388200	-0.91979100	2.15496900	C	-6.04612700	1.27543100	2.51674400
C	2.69899000	-1.62419600	2.12351300	C	-5.80979300	1.14175000	3.90559300
C	1.23615000	-0.06796400	3.24729600	H	-4.44626700	0.44378900	5.40622200
C	3.63000300	-1.49722900	3.15857100	H	-5.32787400	0.93545500	0.54168800
H	2.92818100	-2.27563400	1.28709800	H	-6.96489100	1.74094500	2.16964600
C	2.15240900	0.03741600	4.29341300	H	-6.54567900	1.50282900	4.61901500
H	0.32549700	0.52319900	3.27678900	C	-2.48334000	-0.54433000	3.85732400

H	-2.30625200	-0.65743600	4.92455500	C	-0.30144000	2.66139500	-3.18278400
C	-2.92589800	-0.28793000	1.07569000	C	-1.23208300	5.27324400	-2.94461200
C	-1.55793400	-1.00336500	2.95408600	H	-1.94889200	4.69180200	-1.00789700
C	-1.75043400	-0.88249100	1.54728500	C	-0.11042300	3.56598400	-4.22652800
H	-0.65894100	-1.47569900	3.32779400	H	0.08216000	1.64848200	-3.26468000
P	-0.35346800	-1.39459600	0.40283500	C	-0.57305700	4.87971000	-4.10864100
C	0.78803900	-2.29107300	1.57584900	H	-1.58916800	6.29444800	-2.83857400
C	0.83640800	-3.68416200	1.72346000	H	0.40991900	3.24853800	-5.12658600
C	1.69179000	-1.50927300	2.31969500	H	-0.41467000	5.59031200	-4.91558600
C	1.75501900	-4.27901200	2.59399800	O	3.90739400	-3.48416500	-4.24430900
H	0.16820300	-4.31659000	1.14983400	C	4.00413700	-3.18578700	-5.62447800
C	2.59769900	-2.10208200	3.19890900	H	4.45061200	-4.06534400	-6.09309600
H	1.68728100	-0.43003500	2.18702200	H	3.01726400	-3.00035200	-6.07106600
C	2.63421000	-3.49250200	3.33771400	H	4.64704400	-2.31375200	-5.80780700
H	1.78172100	-5.36185300	2.68545000	C	2.26675900	3.50012700	-0.70602000
H	3.28143000	-1.47816900	3.76927600	H	3.28163600	3.83988300	-0.46443400
H	3.34690500	-3.95727700	4.01390100	H	2.01196800	3.85359500	-1.71310400
C	-1.08950400	-2.77794100	-0.58314400	H	1.56539900	3.98691800	-0.01823600
C	-1.98046000	-3.71795200	-0.03940000				
C	-0.70835700	-2.90497700	-1.92702100	<b>35-L2</b>			
C	-2.46871900	-4.76726900	-0.81827400	C	-7.80664200	-0.55015700	0.39618300
H	-2.29617600	-3.62791900	0.99654700	C	-8.52034600	-0.09768900	1.43704100
C	-1.19895000	-3.95525800	-2.70613100	C	-8.64236000	1.35022400	1.72967300
H	-0.02591300	-2.17871200	-2.35726000	C	-7.88544800	2.26394700	0.84181300
C	-2.07683500	-4.88862900	-2.15369100	C	-7.16902000	1.80611300	-0.19508500
H	-3.16007800	-5.48546100	-0.38508100	C	-7.10432100	0.34916900	-0.59479400
H	-0.89333800	-4.04144800	-3.74548300	H	-7.71596500	-1.61724300	0.19791600
H	-2.45977400	-5.70483700	-2.76086400	H	-9.03765900	-0.76587600	2.12052500
C	-4.07690700	0.11350700	-3.08043900	H	-7.93775300	3.32078200	1.09043900
C	-4.69793100	-0.87825900	-2.28455000	H	-6.59446500	2.48120100	-0.82749200
C	-4.28602900	-1.02126100	-0.91978700	O	-9.31742100	1.76767700	2.66641500
C	-3.25336900	-0.16741100	-0.38862000	O	-5.74428700	-0.06168800	-0.79609500
C	-2.65071800	0.78794700	-1.21404400	C	-7.75693800	0.17922500	-1.98375400
C	-3.08933700	0.91387600	-2.56342800	H	-7.22429800	0.79652700	-2.71404900
H	-4.39614700	0.23949300	-4.11254400	H	-7.68008800	-0.86662800	-2.29761600
H	-2.63900900	1.66405700	-3.20086100	H	-8.81034500	0.47335600	-1.96090800
C	-5.72237700	-1.71414700	-2.80517500	C	-4.89714100	-0.05069700	0.37259200
H	-6.01710900	-1.58585900	-3.84413500	H	-5.11278100	0.85252500	0.96175700
C	-4.93704100	-2.01831600	-0.13640400	H	-5.12477700	-0.91484000	1.00658100
H	-4.64276100	-2.15244900	0.89747700	C	-3.46116800	-0.05959400	-0.07980600
C	-6.33015500	-2.66230000	-2.01610400	C	-2.57885700	-1.08530200	0.03141200
C	-5.92825600	-2.81283700	-0.66753100	Rh	-0.79422500	-0.14886300	-0.19642800
H	-7.11446500	-3.29509700	-2.42259200	C	-2.96363900	1.18766900	-0.74917300
H	-6.40580500	-3.56470100	-0.04480600	C	-3.14306400	2.47640500	-0.20371000
P	-1.15415500	1.76459200	-0.66668500	C	-2.37914100	1.11556200	-2.03829200
C	-1.71877800	2.76767900	0.77834700	C	-2.76476100	3.62966700	-0.88425700
C	-0.80084800	2.98548200	1.81640200	H	-3.57943900	2.57960500	0.78559400
C	-2.99367800	3.34858800	0.86643800	C	-1.99808800	2.26767600	-2.73085200
C	-1.14415500	3.77990300	2.91217000	H	-2.33018700	0.15302200	-2.53437300
H	0.17805000	2.51641900	1.75868900	C	-2.18237600	3.52905000	-2.15890500
C	-3.33695000	4.14057600	1.96267600	H	-2.90925800	4.59430300	-0.41162500
H	-3.72352100	3.17453200	0.08080200	H	-1.58115100	2.20604600	-3.73174600
C	-2.41156200	4.36002600	2.98589300	C	4.95404700	-1.26276300	4.16559000
H	-0.42332700	3.93942900	3.70985500	C	4.06196200	-0.62573300	3.26120500
H	-4.33016100	4.57732400	2.02243800	C	4.02085900	-1.04073400	1.89043400
H	-2.68175700	4.97456700	3.84066400	C	4.89448800	-2.09523600	1.49447500
C	-0.97720100	3.04139200	-2.00951300	C	5.75023700	-2.69253000	2.39304900
C	-1.43781300	4.36107700	-1.90497400	C	5.78495600	-2.27460400	3.74481600

H	4.96659600	-0.93000100	5.20091400	H	-0.06735600	-2.88069300	4.56696700
H	4.88327400	-2.43217000	0.46472800	H	3.01158700	-5.19809500	2.65334600
H	6.40596500	-3.49301400	2.06055000	H	1.69523600	-4.63286200	4.68518300
H	6.46599800	-2.75312500	4.44344700	C	-0.16175900	-3.32705600	-1.32210300
C	3.21283500	0.42663700	3.67947700	C	-0.05578600	-4.69193500	-1.01997800
H	3.25130500	0.75665000	4.71522100	C	-0.86475300	-2.95543900	-2.48209200
C	3.11650800	-0.39395300	0.97373800	C	-0.62518500	-5.65546800	-1.85795600
C	2.35468300	1.03106100	2.79462200	H	0.45454200	-5.01610400	-0.12054000
C	2.28256700	0.63039600	1.43063200	C	-1.42039700	-3.91595900	-3.32602700
H	1.72001500	1.83514500	3.14596200	H	-0.98514100	-1.89963000	-2.70732100
P	0.99010500	1.38602200	0.31027400	C	-1.30348100	-5.27323000	-3.01470700
C	0.21120400	2.68337000	1.39118000	H	-0.53911600	-6.70757500	-1.59849100
C	0.46283500	4.05812200	1.27696100	H	-1.95722300	-3.60360300	-4.21802600
C	-0.73428700	2.25375600	2.34058500	H	-1.74671400	-6.02411700	-3.66348100
C	-0.20298200	4.97553700	2.09541400	O	-1.78009100	4.59569300	-2.91309900
H	1.17852200	4.42080000	0.54737000	C	-1.93132500	5.89540700	-2.36880500
C	-1.38923100	3.16781700	3.16557500	H	-1.35870400	6.01300400	-1.43923000
H	-0.95745400	1.19245300	2.42204700	H	-1.54196500	6.58362100	-3.12177900
C	-1.12621200	4.53498700	3.04415000	H	-2.98584000	6.13343400	-2.17324800
H	0.00766900	6.03721500	1.99196500	C	-2.94198600	-2.47442700	0.47836600
H	-2.10941600	2.81286900	3.89846400	H	-4.00780800	-2.59385500	0.71475400
H	-1.63849400	5.24950500	3.68325500	H	-2.70461000	-3.19760300	-0.31044100
C	2.01192200	2.39328700	-0.86139400	H	-2.36617800	-2.78279000	1.35931000
C	3.16508500	3.08984600	-0.46329900				
C	1.59450300	2.48303400	-2.19595100	<b>36-ts-L2</b>			
C	3.87458800	3.86804100	-1.37813600	C	-6.65951700	0.81482700	-0.40007700
H	3.50881900	3.02386600	0.56550800	C	-7.08577600	-0.21765800	-1.14104700
C	2.30514200	3.26182600	-3.11233900	C	-7.07257400	-1.60555300	-0.62306100
H	0.70733400	1.94249300	-2.50986800	C	-6.58608800	-1.78363500	0.76538800
C	3.44443300	3.95643500	-2.70484100	C	-6.16351300	-0.74765700	1.50363900
H	4.76600900	4.40099200	-1.05725200	C	-6.17492100	0.68721200	1.02681100
H	1.96715700	3.32364800	-4.14334700	H	-6.64359000	1.82661400	-0.80248800
H	3.99981500	4.56055200	-3.41762100	H	-7.43681500	-0.09316100	-2.16190600
C	3.45860200	-1.66303800	-3.15562800	H	-6.57365300	-2.80435900	1.13835900
C	4.47526300	-0.85806700	-2.58924900	H	-5.78459200	-0.89740000	2.51371500
C	4.32840200	-0.42107700	-1.23295100	O	-7.42632700	-2.55852800	-1.31272600
C	3.16510700	-0.80983700	-0.47271100	O	-4.87486200	1.28432700	1.16952800
C	2.17095900	-1.58872800	-1.07706800	C	-7.08063000	1.52626600	1.95014400
C	2.34788900	-2.00719700	-2.42792200	H	-6.71069900	1.46756500	2.97874200
H	3.56775800	-2.00973100	-4.18079700	H	-7.05365700	2.57414700	1.63469700
H	1.59040900	-2.62265500	-2.89588800	H	-8.11364500	1.16717200	1.91806700
C	5.62868000	-0.48838200	-3.33195300	C	-3.81593600	0.62977300	0.44385400
H	5.71651900	-0.83598200	-4.35869800	H	-3.61974000	-0.35820000	0.88328000
C	5.36483200	0.39278100	-0.68936300	H	-4.12697900	0.45390500	-0.59603900
H	5.27790900	0.74901300	0.32975500	C	-2.59432700	1.45643400	0.46971700
C	6.61128000	0.29197400	-2.76922100	C	-2.16977900	2.60983800	0.84919300
C	6.47056600	0.73820000	-1.43393200	Rh	-0.55052700	1.30044900	0.14756700
H	7.49042700	0.56927500	-3.34460300	C	-0.65285100	3.33211000	-0.46469500
H	7.24286300	1.36148000	-0.99101100	C	0.10615400	4.42094100	0.00991500
P	0.52240500	-1.95216700	-0.26186300	C	-1.24059600	3.48025800	-1.73251600
C	0.96498300	-2.81716400	1.31421700	C	0.32756300	5.55301300	-0.76758400
C	0.24233300	-2.49322100	2.47120400	H	0.54224600	4.38734800	1.00167400
C	1.96887400	-3.79561500	1.39697500	C	-1.01727400	4.60644200	-2.53545800
C	0.50085900	-3.14452400	3.67875700	H	-1.90024000	2.70408700	-2.10831300
H	-0.51442800	-1.71548500	2.41066800	C	-0.22132000	5.65089900	-2.05403800
C	2.22684900	-4.44811700	2.60318700	H	0.93095600	6.37737900	-0.39759900
H	2.56038200	-4.04208700	0.51952300	H	-1.48454700	4.66195600	-3.51318600
C	1.49056400	-4.12643100	3.74557800	C	3.38798300	-3.89829000	3.38659700

C	3.04930800	-2.68867700	2.72214200
C	2.78883400	-2.69523800	1.31388900
C	2.87909700	-3.94641800	0.63596400
C	3.20926400	-5.10359300	1.30586600
C	3.46973000	-5.08483600	2.69659100
H	3.58250200	-3.86417800	4.45607800
H	2.68366400	-3.98765500	-0.42865300
H	3.27072100	-6.04119000	0.75961200
H	3.73179500	-6.00459400	3.21257800
C	2.97090500	-1.46032700	3.41896100
H	3.18124200	-1.44291100	4.48602000
C	2.45067500	-1.46489700	0.63892200
C	2.64031500	-0.30062000	2.76432600
C	2.36586700	-0.27251900	1.36601900
H	2.59513500	0.61874800	3.33284700
P	1.75737900	1.33421500	0.60670700
C	2.10197500	2.55234900	1.97710800
C	3.23198700	3.37914100	2.03376700
C	1.13500800	2.67223400	2.99235900
C	3.39582000	4.29392000	3.07863900
H	3.98623800	3.32563000	1.25676600
C	1.30482100	3.57459300	4.04215900
H	0.23910000	2.05872600	2.93834700
C	2.43783100	4.39220400	4.08728700
H	4.27577200	4.93188800	3.09830400
H	0.54772100	3.64660400	4.81895900
H	2.56730100	5.10380900	4.89853300
C	3.05999700	1.75079400	-0.64115700
C	4.42573200	1.49363800	-0.43865700
C	2.65876200	2.38721400	-1.82512700
C	5.36940100	1.87230200	-1.39389800
H	4.75277500	0.99137300	0.46767500
C	3.60449400	2.76542300	-2.78071800
H	1.60457900	2.58560500	-1.99141300
C	4.95982500	2.51080100	-2.56696500
H	6.42246000	1.66218300	-1.22586100
H	3.27888600	3.25912800	-3.69252700
H	5.69496900	2.80339100	-3.31227000
C	1.95615600	-1.91989400	-3.63884100
C	3.25890500	-1.95108400	-3.08685300
C	3.41164200	-1.76181700	-1.67502300
C	2.25073400	-1.53785800	-0.85117500
C	0.98277900	-1.48817800	-1.43966600
C	0.86058800	-1.69362800	-2.84354500
H	1.83007000	-2.08356700	-4.70668700
H	-0.12138900	-1.68146200	-3.29879200
C	4.40340300	-2.18347600	-3.89668000
H	4.26137100	-2.32460600	-4.96562300
C	4.73237700	-1.81607300	-1.14177800
H	4.87778200	-1.67460200	-0.07764800
C	5.66186700	-2.23153300	-3.34438900
C	5.82291200	-2.04393200	-1.95083600
H	6.53072500	-2.41236600	-3.97146700
H	6.81781900	-2.07979600	-1.51489800
P	-0.52990400	-0.98313800	-0.46590000
C	-0.74415200	-2.30269900	0.81016100
C	-1.18578700	-1.91835500	2.08487600
C	-0.52228900	-3.66446000	0.55034500

C	-1.41132900	-2.87596400	3.07607500
H	-1.34012300	-0.86243500	2.29317200
C	-0.74706100	-4.62039400	1.54129100
H	-0.16752500	-3.97805100	-0.42751400
C	-1.19381200	-4.22775500	2.80541200
H	-1.74955700	-2.56382700	4.06079500
H	-0.56553600	-5.67053400	1.32899200
H	-1.36429400	-4.97349800	3.57748100
C	-1.93000700	-1.31640800	-1.64559400
C	-2.81000000	-2.40202700	-1.53265700
C	-2.16612800	-0.36872000	-2.65867700
C	-3.89717400	-2.53510300	-2.40314400
H	-2.66735500	-3.14139900	-0.75260100
C	-3.23305800	-0.51548500	-3.54382100
H	-1.51268400	0.49562900	-2.73714500
C	-4.10888400	-1.59760100	-3.41330800
H	-4.58787600	-3.36447300	-2.27960500
H	-3.39118900	0.22499000	-4.32391500
H	-4.95610000	-1.70358700	-4.08523800
O	0.05970600	6.80315900	-2.73972000
C	-0.48269300	6.95320800	-4.03807900
H	-0.13445800	7.92257500	-4.40124100
H	-0.13216500	6.16536300	-4.71943100
H	-1.58150400	6.94694800	-4.02385300
C	-2.50456700	3.81859000	1.65013700
H	-2.66277800	4.69891600	1.01772900
H	-3.42620900	3.61688100	2.20886800
H	-1.70931800	4.06702500	2.36227600

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Rh	0.66813900	1.34871700	0.09578300
C	-3.01239000	-3.69569000	-3.71704300
C	-2.71824100	-2.50306000	-3.00214500
C	-2.58577400	-2.54227800	-1.57602100
C	-2.75882400	-3.80226400	-0.93230500
C	-3.04540100	-4.94128600	-1.65126100
C	-3.17509600	-4.89266000	-3.05990300
H	-3.10708500	-3.64052800	-4.79904300
H	-2.66425100	-3.86200000	0.14546400
H	-3.17421100	-5.88709200	-1.13151500
H	-3.40236900	-5.79845500	-3.61548600
C	-2.56325300	-1.26305100	-3.66679400
H	-2.67724300	-1.22529700	-4.74783600
C	-2.28779500	-1.33299800	-0.85181700
C	-2.27832400	-0.11933000	-2.96284300
C	-2.12832000	-0.13103500	-1.54772500
H	-2.16953800	0.81463900	-3.50035300
P	-1.60528300	1.42716200	-0.65897000
C	-1.61214800	2.70769300	-2.00663200
C	-2.61180200	3.67737600	-2.17114700
C	-0.50566000	2.73457900	-2.87568200
C	-2.51423200	4.63765600	-3.18275900
H	-3.47188800	3.68847600	-1.51061000
C	-0.41491600	3.68465400	-3.89268800
H	0.29031800	2.00518700	-2.74286000
C	-1.42053400	4.64202900	-4.04911400
H	-3.30178700	5.37888200	-3.29537600
H	0.44427100	3.68045200	-4.55870200



H	-1.35052300	5.38548200	-4.83899400	H	-0.19521700	6.42401900	-0.92023300
C	-3.11631600	1.84916300	0.32534000	H	-0.49686600	4.39325600	2.85661600
C	-4.41992300	1.69552000	-0.17543200	H	1.42733000	2.94964400	2.22011500
C	-2.94388500	2.35801300	1.61933500	C	5.80396400	-1.30290900	0.80480200
C	-5.52302700	2.05841700	0.59729000	C	6.23025900	-2.25973400	-0.03250100
H	-4.57217600	1.28748800	-1.17125300	C	6.98167400	-1.94079200	-1.26793600
C	-4.04854500	2.71830000	2.39446800	C	7.19754000	-0.50135000	-1.54898400
H	-1.93841600	2.46954000	2.01231800	C	6.77325100	0.45234200	-0.70783500
C	-5.33866100	2.57190200	1.88397900	C	6.08788000	0.16903600	0.61073300
H	-6.52664200	1.93382600	0.19873000	H	5.23754100	-1.55186500	1.69986300
H	-3.89936300	3.11121900	3.39670400	H	6.03471700	-3.31358600	0.14722500
H	-6.19924100	2.84968000	2.48702100	H	7.71474700	-0.26978900	-2.47655500
C	-2.24790800	-1.63819000	3.47314800	H	6.93467400	1.50653400	-0.92879000
C	-3.47894700	-1.73133500	2.78092200	O	7.39286500	-2.81603200	-2.02491000
C	-3.47615400	-1.60226000	1.35414800	O	4.89456000	0.95723100	0.74677000
C	-2.23153300	-1.40002000	0.65144200	C	6.99183600	0.66018100	1.76254300
C	-1.03613600	-1.30790000	1.37415300	H	7.16178300	1.73673700	1.65940300
C	-1.07518600	-1.42644600	2.79451900	H	6.49074500	0.48100800	2.71895700
H	-2.24143600	-1.73631400	4.55637200	H	7.95435100	0.14021400	1.75513400
H	-0.15340600	-1.35276600	3.35766500	C	3.82346900	0.63976500	-0.16618100
C	-4.70162200	-1.95032700	3.47038500	H	4.19929900	0.70388800	-1.20242100
H	-4.67467500	-2.04847900	4.55316100	H	3.51307800	-0.39721500	-0.00524200
C	-4.73246600	-1.68285700	0.68552200	C	2.68137100	1.60142200	0.04046400
H	-4.76630000	-1.57564000	-0.39159300	C	2.83957400	2.94053000	-0.10920900
C	-5.89273400	-2.03392200	2.78797700	O	-1.51647800	6.25942700	1.47920100
C	-5.90283300	-1.89302900	1.38032300	C	-2.01248400	7.28613700	0.63773900
H	-6.82303200	-2.20262700	3.32363100	H	-2.40106800	6.88185100	-0.30644100
H	-6.84457200	-1.94956400	0.84081700	H	-2.82692700	7.75953700	1.18984900
P	0.60202300	-0.82323900	0.60677900	H	-1.24210300	8.03750800	0.41663000
C	0.90491500	-2.07483100	-0.72574000	C	4.07730800	3.65938000	-0.60567600
C	1.53974700	-1.64473600	-1.90024500	H	4.50413200	4.29619500	0.18216400
C	0.56580500	-3.43199800	-0.60274900	H	4.85305200	2.96042100	-0.92305800
C	1.85406200	-2.55113600	-2.91422300	H	3.84560100	4.32020200	-1.45190200
H	1.77177400	-0.58909200	-2.01200900				
C	0.87773100	-4.33831100	-1.61681900	<b>38-L2</b>			
H	0.03768900	-3.78258300	0.27911100	C	3.53309000	4.21683400	-2.08887600
C	1.52890500	-3.90092400	-2.77200700	C	2.88689100	5.25573100	-2.63734400
H	2.34972200	-2.20133500	-3.81594800	C	2.52223800	6.45168600	-1.84394600
H	0.60001900	-5.38327800	-1.50912400	C	2.93057700	6.44491200	-0.42119200
H	1.77213000	-4.60753200	-3.56100500	C	3.57777200	5.40391300	0.12235900
C	1.81488900	-1.33777300	1.93437700	C	4.00479100	4.17852000	-0.65312600
C	2.27056300	-2.65323700	2.11693800	H	3.77536100	3.33192900	-2.67448700
C	2.25953700	-0.34994500	2.82696400	H	2.58225300	5.26565700	-3.68090700
C	3.12669400	-2.97246100	3.17352200	H	2.65337800	7.32141100	0.15831700
H	1.97021100	-3.43697700	1.43142600	H	3.85182900	5.40438800	1.17625300
C	3.11036700	-0.66774300	3.88723900	O	1.89501400	7.38760200	-2.33655300
H	1.93994200	0.67499200	2.66853400	O	3.58580400	2.97026300	-0.00589100
C	3.54372100	-1.98286500	4.06702100	C	5.54732700	4.09359600	-0.64349300
H	3.46702300	-3.99754000	3.29677300	H	5.90277600	4.03265700	0.38992500
H	3.43931800	0.11500600	4.56568200	H	5.86483000	3.18793200	-1.17013700
H	4.20651700	-2.23439600	4.89107000	H	5.99332800	4.96749100	-1.12784000
C	1.18849300	4.82447500	-0.59680400	C	2.16524100	2.82497200	0.24264300
C	0.13818000	5.65820500	-0.22947600	H	1.82660500	3.64576700	0.89690900
C	-0.48550100	5.48951200	1.01850800	H	1.62961300	2.93345000	-0.70250000
C	-0.03430800	4.48648200	1.87873000	C	1.90163800	1.46985500	0.87037200
C	1.01770000	3.64771700	1.49891100	C	2.60415100	1.13937800	1.99256200
C	1.65894400	3.79196700	0.24234000	Rh	0.58835800	0.21876900	-0.14823400
H	1.64832200	4.96979100	-1.56998200	C	2.64011600	-0.22615400	2.58453200

C	3.78306600	-0.66558000	3.28076300	C	-2.08275700	-1.21101800	-2.52202000
C	1.59363600	-1.16482800	2.46294900	C	-2.98902000	-2.16667300	-3.00861000
C	3.90678500	-1.95761800	3.79729900	C	-1.97311600	0.01091800	-3.19916200
H	4.62600400	0.00689500	3.40216300	C	-3.76662700	-1.90127100	-4.13478700
C	1.69180800	-2.44894200	2.98372900	H	-3.08745600	-3.12757500	-2.51475700
H	0.66585900	-0.87727900	1.96737000	C	-2.74750300	0.27744900	-4.33071700
C	2.85350200	-2.86556900	3.64895700	H	-1.27810700	0.75697100	-2.82843000
H	4.82877600	-2.24569100	4.28938600	C	-3.64617600	-0.67932700	-4.80148900
H	0.86741000	-3.14752900	2.89841400	H	-4.46703900	-2.65096100	-4.49308900
C	6.35099700	-1.80267700	-0.32630200	H	-2.64758900	1.23230800	-4.84034100
C	6.76932200	-2.27372400	0.85696200	H	-4.24956100	-0.47692000	-5.68245200
C	6.31282900	-3.58207600	1.37724600	C	-4.98982400	1.88437800	-1.40741800
C	5.37781300	-4.34405300	0.51885200	C	-5.57799200	0.59860800	-1.36064900
C	4.96592900	-3.87203600	-0.66628400	C	-4.89860500	-0.43783500	-0.64440100
C	5.43665300	-2.56345100	-1.26000300	C	-3.64249800	-0.15909900	0.00341100
H	6.66583700	-0.82394600	-0.68486400	C	-3.07135000	1.11390600	-0.09721700
H	7.43806600	-1.71071500	1.50228900	C	-3.78042400	2.12772100	-0.80482900
H	5.02894700	-5.29363100	0.91561000	H	-5.50762500	2.68457100	-1.93138700
H	4.25151600	-4.42638000	-1.27315100	H	-3.36304300	3.12405200	-0.86608100
O	6.67556700	-4.00164300	2.47528900	C	-6.81771400	0.32118300	-1.99729600
O	4.31828100	-1.74657500	-1.64781100	H	-7.31688800	1.12499900	-2.53331600
C	6.17919000	-2.84054600	-2.58319800	C	-5.50457400	-1.72706100	-0.61239100
H	5.51011300	-3.35782600	-3.27835100	H	-5.00683100	-2.53140500	-0.08361400
H	6.48157100	-1.89243400	-3.03908700	C	-7.37483900	-0.93500500	-1.94003700
H	7.06655600	-3.45716500	-2.41245200	C	-6.70569200	-1.96828800	-1.24150600
C	3.42317300	-1.40216600	-0.57154800	H	-8.32391900	-1.13775100	-2.42887200
H	2.96666100	-2.31111300	-0.15912000	H	-7.14474300	-2.96158700	-1.20086900
H	3.96912300	-0.91678000	0.24699900	P	-1.37704200	1.51950800	0.61934100
C	2.38652700	-0.49018200	-1.07324800	C	-1.76768000	1.68215200	2.42604200
C	1.86539200	0.29658300	-1.90339200	C	-0.75520800	1.46413900	3.37175600
C	-3.71689200	-2.95130000	4.14032900	C	-3.03770200	2.08075600	2.87620000
C	-3.10459200	-2.62709500	2.90053200	C	-1.00936700	1.63231600	4.73512800
C	-3.64447700	-1.57531800	2.09190600	H	0.23818800	1.18339400	3.04334300
C	-4.79167700	-0.88875000	2.58323300	C	-3.28877500	2.25006900	4.23780500
C	-5.36702400	-1.22732600	3.78802500	H	-3.83271800	2.26478400	2.16018500
C	-4.82811500	-2.26912200	4.57855000	C	-2.27530500	2.02289900	5.17172600
H	-3.28620100	-3.75165500	4.73724600	H	-0.21312100	1.45383300	5.45271300
H	-5.22060100	-0.08790700	1.99377500	H	-4.27786300	2.55624800	4.56857700
H	-6.24318800	-0.68660700	4.13573100	H	-2.47303600	2.15031300	6.23288100
H	-5.29068400	-2.52482400	5.52789200	C	-1.18285600	3.30113200	0.11768400
C	-1.95928200	-3.32096500	2.43881100	C	-1.33024600	4.37107800	1.01210300
H	-1.53405900	-4.10819900	3.05682300	C	-0.85116100	3.59027300	-1.21807700
C	-3.02970400	-1.25760800	0.82554200	C	-1.15056400	5.68983100	0.58265700
C	-1.38688300	-3.00598700	1.23308100	H	-1.58393100	4.18204400	2.04913000
C	-1.92614500	-1.99034200	0.38793200	C	-0.69119800	4.90579300	-1.64981800
H	-0.50113900	-3.54323000	0.91582900	H	-0.71259000	2.77447000	-1.92178900
P	-0.91834100	-1.53194600	-1.10529900	C	-0.83324500	5.96361900	-0.74713600
C	-0.24190200	-3.16804100	-1.69052600	H	-1.26011700	6.50295300	1.29574600
C	-0.90947300	-4.39531300	-1.52353100	H	-0.43405600	5.11080000	-2.68519300
C	0.95079400	-3.15878800	-2.43128800	H	-0.67267700	6.98430100	-1.08078600
C	-0.39549600	-5.57209700	-2.06892000	O	2.85264800	-4.15049600	4.11218300
H	-1.83231300	-4.44151200	-0.95397200	C	4.02642500	-4.62640400	4.76021500
C	1.46086200	-4.33701600	-2.98323500	H	3.81210300	-5.66051400	5.03913900
H	1.49030300	-2.22995000	-2.57308600	H	4.89661000	-4.59721400	4.09339400
C	0.79257500	-5.54774900	-2.80264300	H	4.24425100	-4.04846100	5.66893000
H	-0.92753100	-6.50848600	-1.92155200	C	3.47533000	2.15762500	2.72717800
H	2.38397200	-4.29998000	-3.55617900	H	4.52891500	2.11538800	2.42409600
H	1.19028000	-6.46469400	-3.22961200	H	3.13866300	3.18107800	2.54555300

H	3.43459700	1.98216800	3.80911500	C	2.70941500	0.29981100	-0.03950000
C	1.73606400	1.00990000	-3.18749100	C	2.88801500	1.54261000	0.16463300
H	2.64653900	0.86961800	-3.78616200	C	-1.69978000	-5.88096500	1.49466300
H	0.88818900	0.63461800	-3.77418500	C	-1.36145700	-4.70836700	0.76966300
H	1.58891700	2.08616200	-3.04326400	C	-2.31058300	-3.64207300	0.65065300
<b>39-ts-L2</b>				C	-3.56218900	-3.80191300	1.31103300
C	0.96089000	5.04741400	-2.53469900	C	-3.86283100	-4.95033300	2.01101400
C	-0.13859400	5.06682900	-3.30173300	C	-2.92888300	-6.00764100	2.10063100
C	-1.39572700	5.69938600	-2.84050400	H	-0.96285200	-6.67774800	1.56372200
C	-1.35793400	6.34654300	-1.50859200	H	-4.29159900	-3.00282300	1.26430300
C	-0.25742700	6.31873800	-0.74301100	H	-4.82804600	-5.04165500	2.50206900
C	1.05158300	5.69155800	-1.16940100	H	-3.17988900	-6.90979800	2.65190200
H	1.86977400	4.55208000	-2.87348000	C	-0.08647100	-4.55865800	0.16730300
H	-0.17044100	4.59810200	-4.28147600	H	0.64580500	-5.35585900	0.27228300
H	-2.28147600	6.81757700	-1.18200900	C	-1.97553700	-2.46103500	-0.11354900
H	-0.25280900	6.77045000	0.24773600	C	0.22611600	-3.42265000	-0.53144600
O	-2.42430400	5.66428900	-3.51288900	C	-0.71923500	-2.36765200	-0.71478900
O	1.50718800	4.74435300	-0.18884400	H	1.21696100	-3.32897700	-0.96255800
C	2.14649400	6.77786300	-1.19112300	P	-0.05982000	-0.80284100	-1.44948900
H	2.25364600	7.20918500	-0.19086700	C	1.08755700	-1.35457800	-2.81208700
H	3.10410800	6.33102600	-1.47693000	C	0.97390600	-2.57373200	-3.50070400
H	1.89680600	7.57225600	-1.90095900	C	2.03847300	-0.42235200	-3.25797600
C	0.63917400	3.59742100	0.01155900	C	1.79690500	-2.85685800	-4.59226900
H	-0.35191900	3.95258200	0.32422700	H	0.24333600	-3.31245000	-3.18680300
H	0.52045400	3.09223300	-0.95166800	C	2.85436200	-0.70112100	-4.35604800
C	1.18933300	2.63091500	1.04216600	H	2.14442700	0.52280200	-2.73371400
C	1.53973200	3.07933800	2.28403900	C	2.73864700	-1.92104300	-5.02575800
Rh	0.68787100	0.68989900	0.18171100	H	1.69476200	-3.80790700	-5.10867000
C	2.25213100	2.26965400	3.30365600	H	3.58191500	0.03640200	-4.68488100
C	3.06184800	2.88988600	4.27456400	H	3.37277600	-2.13951500	-5.88104100
C	2.18501200	0.86230000	3.35682700	C	-1.36987700	-0.09403800	-2.56236100
C	3.77338900	2.16422500	5.23352700	C	-2.02840400	-0.88400600	-3.51695500
H	3.16319300	3.97025000	4.28314600	C	-1.60739500	1.28650500	-2.55156200
C	2.87589500	0.12562200	4.30712300	C	-2.91272800	-0.30792300	-4.42710200
H	1.55880000	0.35053900	2.63830900	H	-1.85360300	-1.95472900	-3.55202200
C	3.68307400	0.76921600	5.25611900	C	-2.48635900	1.86920000	-3.46943800
H	4.38833700	2.69793700	5.94989100	H	-1.09506800	1.90154300	-1.81821700
H	2.78965100	-0.95635100	4.34698800	C	-3.14093300	1.07048500	-4.40757600
C	5.99301500	-2.28020100	0.56474300	H	-3.42324200	-0.93641900	-5.15190700
C	5.93741100	-3.58182200	0.88153600	H	-2.65378100	2.94310100	-3.45824600
C	5.51853800	-4.60684200	-0.10402200	H	-3.82405800	1.52060300	-5.12304200
C	5.12134700	-4.10628800	-1.44149300	C	-5.24334600	0.36487400	-0.34624900
C	5.17929000	-2.80411900	-1.75584900	C	-5.29795400	-0.82515700	-1.10853500
C	5.69763500	-1.73883300	-0.81627800	C	-4.18564800	-1.72373700	-1.04880100
H	6.28499200	-1.53343900	1.30166300	C	-3.03471900	-1.39912400	-0.24142700
H	6.18382600	-3.94776400	1.87474900	C	-2.98637300	-0.17324100	0.43836300
H	4.76996200	-4.85588300	-2.14568300	C	-4.12744000	0.67786500	0.38794700
H	4.86111200	-2.44655800	-2.73373100	H	-6.09839400	1.03700100	-0.34965500
O	5.48233000	-5.80103500	0.17810200	H	-4.13492700	1.59379900	0.96193000
O	4.78555400	-0.62952100	-0.74432100	C	-6.42602000	-1.14441600	-1.91096200
C	6.98602400	-1.12687900	-1.40559000	H	-7.25846100	-0.44511400	-1.93576300
H	6.77134800	-0.69985900	-2.39032600	C	-4.26343600	-2.91689000	-1.82484500
H	7.34218300	-0.32427700	-0.75185400	H	-3.43352000	-3.61346000	-1.80931800
H	7.76842600	-1.88486300	-1.50407900	C	-6.46481100	-2.30702400	-2.64471500
C	3.47464800	-0.94778900	-0.24960100	C	-5.36647300	-3.19816400	-2.60039500
H	2.96230600	-1.61720700	-0.94796400	H	-7.33064300	-2.54217700	-3.25773700
H	3.55749500	-1.47823200	0.71167700	H	-5.39317500	-4.11444900	-3.18426900
				P	-1.42998100	0.41179300	1.32937800

C	-1.31700700	-0.89681000	2.64239400	Rh	0.72448300	0.28234400	0.56955200
C	-0.15978000	-1.67283200	2.77629700	C	2.54437400	0.60336900	3.28190600
C	-2.40398000	-1.15281300	3.49633300	C	1.67117100	0.09511900	4.26479300
C	-0.07722000	-2.66756100	3.75374700	C	3.88745400	0.21170600	3.37665800
H	0.66685200	-1.50334200	2.09365300	C	2.09967400	-0.78402600	5.24999700
C	-2.31844900	-2.13816700	4.47875800	H	0.62407400	0.37827800	4.24762600
H	-3.32035000	-0.57779000	3.39539100	C	4.34038600	-0.66691000	4.36486500
C	-1.15199800	-2.89611100	4.61235600	H	4.61225700	0.61158000	2.67929600
H	0.82602600	-3.26581800	3.83818900	C	3.44315600	-1.17906100	5.30744300
H	-3.16538800	-2.31960600	5.13531400	H	1.40809700	-1.17685300	5.98925300
H	-1.08783200	-3.66749000	5.37510800	H	5.39238100	-0.92909100	4.39326300
C	-1.98100400	1.90695700	2.29105000	C	5.07810800	-3.92661800	0.33441700
C	-1.83307600	1.99719500	3.68338300	C	4.70003900	-5.14284600	0.75304700
C	-2.42567200	3.05099000	1.60179400	C	3.79328500	-5.99594100	-0.05091700
C	-2.16118300	3.17220400	4.36594700	C	3.29328900	-5.40876800	-1.31607600
H	-1.45656500	1.15168500	4.24691300	C	3.67179800	-4.19100900	-1.73151500
C	-2.77155000	4.21708000	2.28391900	C	4.67749800	-3.33208100	-0.99710700
H	-2.50874100	3.03436200	0.51880200	H	5.73008300	-3.30008400	0.94139600
C	-2.64402200	4.28154400	3.67361000	H	5.02632100	-5.55773600	1.70310700
H	-2.03769100	3.21287300	5.44502600	H	2.59640700	-6.02159700	-1.88213900
H	-3.13189200	5.07718600	1.72540200	H	3.28632300	-3.76693900	-2.65671800
H	-2.90774000	5.19081800	4.20710300	O	3.46205400	-7.11901800	0.31877700
O	4.32278700	-0.04366300	6.15217500	O	4.19685500	-1.98912600	-0.83091400
C	5.12531200	0.56480000	7.14731600	C	5.93544800	-3.17765200	-1.87963900
H	5.52535400	-0.25076900	7.75342400	H	5.65766700	-2.70376800	-2.82628000
H	5.95876600	1.13038300	6.70810500	H	6.66444900	-2.53661300	-1.37331500
H	4.53754100	1.23683500	7.78765400	H	6.39317300	-4.15021200	-2.08278000
C	1.26760700	4.52102200	2.70056500	C	2.96957200	-1.86252300	-0.08128500
H	2.13977100	5.17200600	2.55230700	H	2.16696200	-2.37124800	-0.62507400
H	0.44500700	4.95738100	2.13246600	H	3.07902700	-2.38794800	0.88176300
H	0.99563500	4.56370100	3.76081600	C	2.60362900	-0.44416000	0.21121200
C	3.88884000	2.63765100	0.18196600	C	3.38191400	0.63710400	0.37927100
H	4.80855900	2.25726900	-0.27997600	C	-3.57401700	-5.07902100	1.01350800
H	3.54072300	3.52113500	-0.35787500	C	-2.84175200	-4.02580700	0.40593000
H	4.10807000	2.94841500	1.20944800	C	-3.44005900	-2.73345600	0.25595700
				C	-4.76104200	-2.55885600	0.75804700
				C	-5.44802400	-3.59894300	1.34615700
				C	-4.85560100	-4.87610500	1.47249100
				H	-3.09764800	-6.05165900	1.11146000
				H	-5.23391300	-1.58749800	0.67885700
				H	-6.45549300	-3.43354600	1.71873800
				H	-5.40903000	-5.68883100	1.93501700
				C	-1.51472300	-4.22049500	-0.05514800
				H	-1.04959400	-5.19596900	0.06597900
				C	-2.70124200	-1.66756500	-0.38248700
				C	-0.81913500	-3.19379900	-0.63578600
				C	-1.40123900	-1.90204400	-0.83087900
				H	0.20050200	-3.37189300	-0.95898700
				P	-0.20035600	-0.58623900	-1.34808200
				C	0.78766100	-1.38381100	-2.71352400
				C	0.29492600	-2.42179200	-3.52226900
				C	2.01712200	-0.79746700	-3.05121800
				C	1.01425700	-2.86175200	-4.63502900
				H	-0.65517000	-2.89218800	-3.28877200
				C	2.73101300	-1.23108900	-4.16996400
				H	2.42147800	-0.00689500	-2.42760200
				C	2.23271000	-2.26392300	-4.96636500
				H	0.61582400	-3.66621500	-5.24806400
<b>40-L2</b>							
C	3.52922000	5.02987100	-1.58017100				
C	2.67373700	5.49817100	-2.50009500				
C	1.42919100	6.20383900	-2.11610100				
C	1.21103700	6.41169100	-0.66546800				
C	2.06769000	5.93908900	0.25102800				
C	3.34287900	5.20050200	-0.08925500				
H	4.42465100	4.48462900	-1.87509900				
H	2.83460100	5.36076700	-3.56597400				
H	0.30553000	6.94805400	-0.39322700				
H	1.87819500	6.06761400	1.31549900				
O	0.60842700	6.57478300	-2.95200300				
O	3.37170900	3.92410700	0.57591800				
C	4.54747500	5.96233900	0.49640500				
H	4.43693600	6.04218900	1.58244800				
H	5.46854200	5.41020800	0.28485300				
H	4.62305900	6.96609600	0.06741100				
C	2.35433000	2.98753900	0.16360900				
H	1.36167600	3.43105500	0.29950000				
H	2.47252500	2.75791000	-0.90176500				
C	2.51548500	1.71554400	0.96657500				
C	2.06072600	1.62189100	2.28816900				

H	3.68011500	-0.76136800	-4.41438400	H	0.94593000	3.51643400	2.28822700
H	2.78711800	-2.60050100	-5.83858700	H	0.69771300	2.53267500	3.72526600
C	-1.02986700	0.67197000	-2.43506500	H	2.22582200	3.37535200	3.50044700
C	-1.86180400	0.31469600	-3.50613600	C	4.83308600	0.90494000	0.05434400
C	-0.67149900	2.01795900	-2.27805700	H	5.35048900	-0.02110300	-0.20113800
C	-2.34416000	1.28668400	-4.38169400	H	4.91979800	1.58708200	-0.80513700
H	-2.13753600	-0.72376300	-3.66072800	H	5.35699200	1.40101800	0.88251000
C	-1.13969500	2.99195500	-3.16466500				
H	-0.01067600	2.28691600	-1.45873600	<b>41-L2</b>			
C	-1.98154200	2.62611300	-4.21555600	C	-5.18314600	4.48650100	-1.03770400
H	-3.00048300	0.99565400	-5.19751800	C	-3.89912000	4.09391900	-0.57330300
H	-0.83986200	4.02993500	-3.04281200	C	-3.78198600	3.06214500	0.41140600
H	-2.34814800	3.38012800	-4.90705600	C	-4.98394600	2.45167800	0.87371900
C	-4.93501800	2.00221400	-0.87360300	C	-6.21541400	2.84703000	0.40049100
C	-5.24629600	0.88700400	-1.68589900	C	-6.32176000	3.87902200	-0.56228300
C	-4.47113100	-0.30606900	-1.53185700	H	-5.24578300	5.27597400	-1.78299400
C	-3.39976700	-0.35080200	-0.56732900	H	-4.92456000	1.65629800	1.60726400
C	-3.08726400	0.79011600	0.18000600	H	-7.11459500	2.36057300	0.76913000
C	-3.88998700	1.95546100	0.01444200	H	-7.29976000	4.18397600	-0.92472600
H	-5.53123400	2.90723700	-0.96486200	C	-2.71678200	4.69861600	-1.05946000
H	-3.68535800	2.83361600	0.61120900	H	-2.79344800	5.50111100	-1.78957300
C	-6.29730900	0.93087500	-2.64103500	C	-2.48090100	2.65916900	0.88246900
H	-6.87398100	1.84805800	-2.73520200	C	-1.48334000	4.27964800	-0.62781500
C	-4.78672200	-1.41008200	-2.37704900	C	-1.33019900	3.24423600	0.33804300
H	-4.20895500	-2.32300300	-2.29319200	H	-0.60645000	4.76896800	-1.02820900
C	-6.57543400	-0.15671300	-3.43565400	P	0.41299900	2.64444700	0.75234500
C	-5.80435300	-1.33615500	-3.30255500	C	1.47479200	4.02424800	0.08946200
H	-7.37905300	-0.11334600	-4.16576900	C	1.64499800	4.12258500	-1.30347600
H	-6.01813300	-2.19296300	-3.93597700	C	2.16381500	4.93248600	0.90518900
P	-1.59575400	0.84825800	1.33607700	C	2.42778100	5.13101700	-1.86229100
C	-2.10520800	-0.37537200	2.62716100	H	1.16864200	3.40095800	-1.95943300
C	-1.18026000	-1.34688200	3.03391200	C	2.96770300	5.93125200	0.34542200
C	-3.38775100	-0.37612900	3.20166300	H	2.08360900	4.86978600	1.98370600
C	-1.52080500	-2.28880700	4.00838700	C	3.09277600	6.04318700	-1.03765800
H	-0.19445900	-1.36342800	2.57491800	H	2.53024000	5.19057900	-2.94249100
C	-3.72454300	-1.31143300	4.17936100	H	3.49159200	6.62327200	0.99974500
H	-4.12579700	0.35416500	2.88078200	H	3.71031300	6.82523700	-1.47162000
C	-2.79026800	-2.26858600	4.58609900	C	0.46354600	2.94614000	2.58145000
H	-0.79178900	-3.03537600	4.31124000	C	-0.01057200	4.14899200	3.13272400
H	-4.71908900	-1.29984300	4.61761300	C	1.00344200	1.97899100	3.43738500
H	-3.05673500	-3.00025400	5.34428400	C	0.07763700	4.38421400	4.50410100
C	-1.82890900	2.49398500	2.16898400	H	-0.45179800	4.90370800	2.48788800
C	-2.16286800	2.64589200	3.52215300	C	1.08605300	2.21249200	4.81233700
C	-1.56975600	3.65405800	1.41490200	H	1.34733200	1.03863300	3.02031700
C	-2.24909300	3.91666500	4.09989600	C	0.62944200	3.41642200	5.34787300
H	-2.35644300	1.77338100	4.13613300	H	-0.29434400	5.31875400	4.91530500
C	-1.67897300	4.92173900	1.98457100	H	1.50439500	1.44819900	5.46204700
H	-1.29255800	3.56475900	0.36784000	H	0.69279300	3.59906200	6.41734300
C	-2.01589400	5.05809400	3.33427200	C	-2.26616400	-0.14380200	4.17777800
H	-2.50513200	4.00875100	5.15224900	C	-2.79374000	1.15193300	4.40442000
H	-1.49228400	5.80197400	1.37495200	C	-2.85453100	2.07306500	3.30939600
H	-2.09201500	6.04482000	3.78307800	C	-2.42329800	1.65303800	1.99637900
O	3.77195600	-2.04414700	6.31385200	C	-1.96699400	0.34833000	1.80711000
C	5.11918300	-2.46980500	6.41387500	C	-1.85496000	-0.52908000	2.92808800
H	5.79916700	-1.62570000	6.59289500	H	-2.18139800	-0.83409900	5.01393400
H	5.15805000	-3.14977100	7.26731200	H	-1.41496600	-1.51022700	2.79639000
H	5.44375100	-3.00449000	5.51069000	C	-3.23909500	1.55373100	5.69164000
C	1.43331100	2.82481500	2.97345700	H	-3.18597800	0.83400900	6.50526300

C	-3.34291700	3.38378000	3.57947100	C	1.61452400	0.72988600	-5.28406200
H	-3.38159400	4.11104000	2.77793700	H	2.85497600	2.34843100	-6.01850500
C	-3.72561800	2.82234500	5.90873500	H	0.53722300	-0.80816700	-4.24939300
C	-3.77107800	3.74508600	4.83839200	O	0.96673300	0.39412400	-6.44215000
H	-4.06779100	3.11853400	6.89671800	C	1.30458900	1.10069600	-7.62172900
H	-4.14458400	4.75121400	5.01002100	H	0.69413100	0.66906600	-8.41765000
P	-1.20177400	-0.24291700	0.22783100	H	1.07722200	2.17221800	-7.53349400
C	-2.22588900	0.38960800	-1.18797500	H	2.36691100	0.98204900	-7.87548800
C	-1.59621400	1.01420200	-2.27028100	C	4.94123800	2.12420700	-1.63837700
C	-3.60149700	0.11784400	-1.26843700	H	5.42674200	1.72136400	-2.53419100
C	-2.32404800	1.36533400	-3.41051300	H	4.91800000	3.21840400	-1.74648300
H	-0.53091400	1.21185700	-2.22504700	H	5.59062500	1.88395400	-0.79629800
C	-4.32994800	0.47961500	-2.39948600				
H	-4.10528500	-0.38648900	-0.44945900	<b>42-ts-L2</b>			
C	-3.69162200	1.10170200	-3.47637800	C	-4.72003100	1.60255700	3.69265900
H	-1.81374400	1.83558500	-4.24677400	C	-3.65837700	0.88326500	3.08061300
H	-5.39554000	0.27085200	-2.44264200	C	-3.63887000	0.71591900	1.65886700
H	-4.25884900	1.37201000	-4.36334800	C	-4.69764800	1.30571800	0.90933700
C	-1.71823100	-2.02279800	0.04302200	C	-5.71038800	2.00378000	1.52883900
C	-1.10777900	-2.73928100	-0.99984500	C	-5.72869500	2.15239600	2.93638300
C	-2.74683000	-2.64569100	0.76284900	H	-4.71535600	1.71309000	4.77456200
C	-1.49063700	-4.04667900	-1.29588500	H	-4.69925200	1.20603900	-0.16975200
H	-0.33669100	-2.26356000	-1.60100200	H	-6.50336700	2.44532300	0.93106300
C	-3.12808000	-3.95728200	0.46981500	H	-6.53579500	2.70209900	3.41314300
H	-3.25878500	-2.11566500	1.55833700	C	-2.60696700	0.32087000	3.84196400
C	-2.49912100	-4.66475500	-0.55421800	H	-2.62455300	0.42217800	4.92477500
H	-1.00132600	-4.58046200	-2.10634400	C	-2.56317200	-0.01009500	1.03366400
H	-3.92258200	-4.42347100	1.04685200	C	-1.57026400	-0.33868300	3.22978800
H	-2.79612800	-5.68587500	-0.77757500	C	-1.51393600	-0.50825200	1.81721000
Rh	1.14160600	0.43261100	0.20421800	H	-0.78150000	-0.74923400	3.84666000
C	3.50684100	-0.93434400	2.82724100	P	0.01770300	-1.29459700	1.05526000
C	2.32632800	-1.45604200	3.18621500	C	0.89553200	-1.99848000	2.53740400
C	1.38277500	-2.00120600	2.18347100	C	0.94816400	-3.36479100	2.84794300
C	1.69322000	-1.73570000	0.75834900	C	1.61288000	-1.10416600	3.35297000
C	2.89593300	-1.14222200	0.38537900	C	1.66537300	-3.81901100	3.95964100
C	4.00507500	-0.87995000	1.40016800	H	0.43297300	-4.08653000	2.22480300
H	4.21081000	-0.56009900	3.56893800	C	2.30812300	-1.55295400	4.47449800
H	2.02308400	-1.54962300	4.22623200	H	1.63244400	-0.04752200	3.10247400
H	1.13310400	-2.33675000	0.05234600	C	2.33590500	-2.91589900	4.78325200
H	3.24718300	-1.26836800	-0.63401500	H	1.69186900	-4.88312300	4.18004700
O	0.42087100	-2.68800200	2.53194100	H	2.84388000	-0.84009200	5.09565900
O	4.72123600	0.33796800	1.18581200	H	2.88626400	-3.26927500	5.65120700
C	5.07911200	-1.97923400	1.22293200	C	-0.73151900	-2.78957200	0.25274000
H	5.48426300	-1.92954700	0.20715300	C	-1.65379500	-3.60294500	0.93369700
H	5.89884100	-1.80684800	1.92805500	C	-0.38472400	-3.12015800	-1.06336400
H	4.65896400	-2.97389400	1.39858500	C	-2.19061400	-4.73470600	0.32081900
C	3.88052100	1.48688200	0.98189700	H	-1.95832700	-3.34780900	1.94495000
H	3.27688700	1.66465500	1.87996300	C	-0.92773900	-4.25060300	-1.67910500
H	4.57878200	2.32334900	0.89272900	H	0.29916200	-2.47659800	-1.60731000
C	3.01395700	1.28487000	-0.24412200	C	-1.82568900	-5.06318900	-0.98748100
C	3.54025000	1.52948900	-1.47562700	H	-2.90235400	-5.35368200	0.86064200
C	2.85050400	1.25835600	-2.76627100	H	-0.65094900	-4.48935500	-2.70261800
C	3.17218600	1.98818800	-3.92700800	H	-2.24920200	-5.94200700	-1.46648700
C	1.88107000	0.24518600	-2.92562700	C	-2.82141700	-0.83341700	-3.21456900
C	2.56823700	1.74544500	-5.16370600	C	-3.74366700	-1.45022500	-2.33156400
H	3.91032800	2.78177300	-3.87330600	C	-3.64238400	-1.18080400	-0.92826900
C	1.27781500	-0.02015400	-4.14895700	C	-2.64676000	-0.25076200	-0.44857600
H	1.59380700	-0.34730200	-2.06003800	C	-1.80064600	0.38005100	-1.36129900

C	-1.87252000	0.03836600	-2.74698400
H	-2.86892600	-1.06790100	-4.27561600
H	-1.14944500	0.45746100	-3.43852500
C	-4.74220200	-2.33922300	-2.80968100
H	-4.80197600	-2.52265200	-3.88002100
C	-4.54623200	-1.85912500	-0.06130700
H	-4.47897100	-1.69554000	1.00723800
C	-5.61390300	-2.95778200	-1.94285900
C	-5.50614300	-2.71640100	-0.55400500
H	-6.37707700	-3.63356900	-2.31948700
H	-6.18513200	-3.21412600	0.13339600
P	-0.35143500	1.41618900	-0.85868400
C	-0.89945500	2.54145600	0.52326500
C	-0.14033200	2.63766900	1.69573700
C	-1.98956600	3.41192600	0.35836800
C	-0.46078000	3.57406200	2.68247100
H	0.70483600	1.97405200	1.83800600
C	-2.31644300	4.34031300	1.34485800
H	-2.58264900	3.37383600	-0.55006800
C	-1.55020800	4.42698600	2.51019100
H	0.14277700	3.63149700	3.58478300
H	-3.16910400	4.99863900	1.20190600
H	-1.80173600	5.15624000	3.27588700
C	-0.21561800	2.75992600	-2.13845900
C	0.94831000	3.54415600	-2.10167700
C	-1.23790400	3.12558100	-3.02441700
C	1.09681300	4.64618500	-2.94197000
H	1.74345300	3.29653100	-1.40357600
C	-1.08684000	4.22611000	-3.87125700
H	-2.15829100	2.55299400	-3.06563700
C	0.08094800	4.98733800	-3.83707700
H	2.00896000	5.23595800	-2.90010500
H	-1.88814400	4.48623900	-4.55822300
H	0.19770600	5.84158300	-4.49863300
Rh	1.43393200	-0.05356600	-0.41994600
C	2.83003900	-2.27026300	-3.16097100
C	1.85292200	-1.50895100	-3.66809500
C	1.76252500	-0.05682200	-3.37029400
C	2.57391600	0.44356600	-2.24335600
C	3.55360300	-0.38935100	-1.62161100
C	3.91118700	-1.75160600	-2.23822100
H	2.92459600	-3.32353300	-3.42134400
H	1.12635800	-1.89522600	-4.37918900
H	2.74405500	1.51570500	-2.24885700
H	4.40659700	0.14470600	-1.21639500
O	1.07571700	0.67666400	-4.08759700
O	4.17421200	-2.73645300	-1.23227100
C	5.22806400	-1.61541000	-3.02578000
H	6.02991500	-1.30413200	-2.34827800
H	5.50135500	-2.58281200	-3.46006900
H	5.12960600	-0.88199300	-3.83177400
C	3.20333800	-2.64523500	-0.17722000
H	2.22955500	-2.99448300	-0.53776400
H	3.54739200	-3.34251100	0.58860500
C	3.16534500	-1.19988800	0.26793800
C	4.10297400	-0.76318800	1.17059600
C	4.42855000	0.66330600	1.38757200
C	5.73118000	1.06201700	1.77712100

C	3.49932000	1.69907900	1.18918700
C	6.07271000	2.39578900	1.94482200
H	6.50305900	0.31423800	1.92793700
C	3.82207400	3.04694600	1.36118700
H	2.48337100	1.42886500	0.89617500
C	5.11882600	3.40571900	1.74347400
H	7.07941800	2.68394500	2.23231500
H	3.05062700	3.79514000	1.21343500
C	4.97557500	-1.75034000	1.94033600
H	5.84250900	-2.07781700	1.34882100
H	5.35045100	-1.30325400	2.86517000
H	4.42162000	-2.64621400	2.22786200
O	5.54869000	4.68479200	1.95185500
C	4.62500000	5.74075700	1.74725400
H	3.76679200	5.66602300	2.42853200
H	5.17126700	6.66273100	1.95586000
H	4.25827300	5.76261900	0.71229100

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C	-4.74831500	1.58036400	3.68676400
C	-3.67848300	0.87094200	3.07751900
C	-3.65043000	0.70885400	1.65534400
C	-4.70944000	1.29428700	0.90259200
C	-5.73007000	1.98318700	1.51942600
C	-5.75676800	2.12626500	2.92740400
H	-4.74979900	1.68698500	4.76906600
H	-4.70496500	1.19895100	-0.17687500
H	-6.52277500	2.42177900	0.91912100
H	-6.56996900	2.66879100	3.40201300
C	-2.62674100	0.31401500	3.84238000
H	-2.65033300	0.41195200	4.92537300
C	-2.56600900	-0.00692100	1.03305500
C	-1.58183700	-0.33511500	3.23325100
C	-1.51730100	-0.49972500	1.82041600
H	-0.79305000	-0.74133200	3.85283300
P	0.01991400	-1.28015000	1.06354900
C	0.89764500	-1.97513400	2.54979800
C	0.96148300	-3.34036700	2.86261100
C	1.60369100	-1.07300300	3.36663600
C	1.67832100	-3.78627500	3.97800700
H	0.45504400	-4.06769100	2.23872700
C	2.29849000	-1.51364700	4.49161900
H	1.61296200	-0.01650800	3.11483900
C	2.33727300	-2.87581000	4.80283100
H	1.71333900	-4.84974100	4.20042200
H	2.82468100	-0.79480800	5.11409700
H	2.88703800	-3.22283300	5.67373700
C	-0.72421300	-2.78007800	0.26456600
C	-1.63765100	-3.59935600	0.95040700
C	-0.38544500	-3.10646000	-1.05470200
C	-2.17280800	-4.73294500	0.33940600
H	-1.93666300	-3.34743500	1.96411800
C	-0.92711700	-4.23851100	-1.66867500
H	0.29086300	-2.45829700	-1.60267800
C	-1.81560700	-5.05717800	-0.97208200
H	-2.87734900	-5.35666500	0.88323800
H	-0.65672100	-4.47368300	-2.69471900
H	-2.23795900	-5.93731900	-1.44969300

C	-2.80388000	-0.80770000	-3.22091000	H	3.52938900	-3.34971600	0.58191200
C	-3.72650400	-1.43375500	-2.34483200	C	3.16641500	-1.20160500	0.27028200
C	-3.63057400	-1.17303900	-0.93952200	C	4.10479000	-0.77835200	1.17868800
C	-2.64013700	-0.24202700	-0.45049600	C	4.45860900	0.64215700	1.39277200
C	-1.79144200	0.39566400	-1.35611700	C	5.75435000	1.01105400	1.80928600
C	-1.85871300	0.06319600	-2.74438300	C	3.55804300	1.70436800	1.15658500
H	-2.84795200	-1.03448800	-4.28378500	C	6.13730200	2.34269800	1.97495000
H	-1.13538400	0.48977000	-3.43106400	H	6.50294400	0.24599500	1.98754700
C	-4.72025800	-2.32323900	-2.83192600	C	3.91826100	3.03442600	1.32347500
H	-4.77620400	-2.49952200	-3.90368600	H	2.54377000	1.45749600	0.83792700
C	-4.53406500	-1.86111600	-0.07990200	C	5.21549600	3.36931300	1.73650500
H	-4.47042700	-1.70466100	0.98991400	H	7.15238000	2.56417900	2.28561400
C	-5.59198300	-2.95119800	-1.97191900	H	3.20137900	3.83320000	1.15506600
C	-5.48895200	-2.71906100	-0.58115000	C	4.95305800	-1.77930900	1.95771900
H	-6.35136800	-3.62742300	-2.35538600	H	5.83143800	-2.10692300	1.38317000
H	-6.16757400	-3.22449800	0.10097000	H	5.30953100	-1.34331700	2.89508500
P	-0.34303900	1.42935200	-0.84576300	H	4.38726200	-2.67372900	2.22479600
C	-0.88490200	2.54467600	0.54458500	O	5.47585400	4.70214900	1.88154100
C	-0.10038100	2.65841100	1.69860000	C	6.77099000	5.08885400	2.30762700
C	-1.99291200	3.39576000	0.40033400	H	7.54384700	4.77105200	1.59475600
C	-0.41470600	3.59308100	2.68884100	H	6.75722500	6.17927900	2.36030500
H	0.76236800	2.01348900	1.82165800	H	7.00944900	4.68139900	3.29944500
C	-2.31393600	4.32141200	1.39111900				
H	-2.60527900	3.34309100	-0.49451100	<b>43-L2</b>			
C	-1.52304500	4.42536700	2.53853500	C	-6.67962100	-1.22542200	0.87025500
H	0.21019000	3.66755600	3.57510600	C	-5.29239600	-1.53032300	0.83834500
H	-3.18067700	4.96466800	1.26528800	C	-4.55260300	-1.36606600	-0.37555000
H	-1.76913100	5.15379100	3.30675500	C	-5.25722400	-0.87753400	-1.51433700
C	-0.20763900	2.78066500	-2.11675200	C	-6.60040500	-0.57818600	-1.45219500
C	0.95706400	3.56329500	-2.07645500	C	-7.32561400	-0.75767100	-0.25025000
C	-1.23291600	3.15487500	-2.99563500	H	-7.21957600	-1.36410000	1.80407900
C	1.10357500	4.67323200	-2.90659300	H	-4.72183900	-0.73115800	-2.44481900
H	1.75356100	3.30971900	-1.38224900	H	-7.10838700	-0.20142500	-2.33594900
C	-1.08359100	4.26289800	-3.83285400	H	-8.38620200	-0.52345300	-0.21621300
H	-2.15411100	2.58364700	-3.03846200	C	-4.60981700	-2.00076500	1.98413900
C	0.08489700	5.02302000	-3.79512400	H	-5.16704200	-2.16360700	2.90395300
H	2.01540500	5.26292300	-2.86009200	C	-3.14133400	-1.66673000	-0.40972000
H	-1.88702600	4.53021300	-4.51459500	C	-3.25965300	-2.24199700	1.94707500
H	0.19965600	5.88388000	-4.44843300	C	-2.48707300	-2.05847600	0.76363400
Rh	1.43881700	-0.04482400	-0.41469200	H	-2.77918900	-2.59662000	2.84840300
C	2.82032400	-2.25594700	-3.16256900	P	-0.61548700	-2.29680900	0.82708100
C	1.84942500	-1.48521300	-3.66728600	C	-0.36934400	-2.91674500	2.56601500
C	1.77060000	-0.03326600	-3.36431800	C	0.12562300	-4.19443100	2.86665200
C	2.58264300	0.45584800	-2.23322700	C	-0.59921000	-2.02835100	3.63362000
C	3.55593100	-0.38740800	-1.61323600	C	0.36647200	-4.57680100	4.19028100
C	3.90476900	-1.74877200	-2.23727700	H	0.32464900	-4.90096300	2.06854400
H	2.90719700	-3.30890500	-3.42690400	C	-0.38291900	-2.41716600	4.95485800
H	1.12028300	-1.86310900	-4.38023000	H	-0.96776900	-1.02700200	3.42751800
H	2.76021200	1.52687400	-2.23351100	C	0.10578700	-3.69558600	5.23882300
H	4.41392600	0.13913300	-1.20840300	H	0.75247100	-5.57166200	4.39725700
O	1.09181900	0.70834100	-4.08083100	H	-0.58615900	-1.71855900	5.76253100
O	4.16100900	-2.74013900	-1.23584700	H	0.28446900	-3.99765000	6.26718600
C	5.22264400	-1.61733700	-3.02377900	C	-0.46195900	-3.84877700	-0.17874900
H	6.02643900	-1.31521000	-2.34437800	C	-1.30597300	-4.95134000	0.04178100
H	5.48955400	-2.58409900	-3.46347500	C	0.50156700	-3.92867100	-1.19220900
H	5.12924200	-0.87877600	-3.82567200	C	-1.16936100	-6.11270800	-0.71719600
C	3.19110900	-2.64593300	-0.18033100	H	-2.07345100	-4.90101200	0.80931300
H	2.21456100	-2.98504600	-0.54233300	C	0.63440000	-5.09184500	-1.95615700



H	1.13376500	-3.07002500	-1.39768000	H	6.46350200	-0.85013100	-1.16383900
C	-0.19512800	-6.18669400	-1.71706100	H	6.24561800	-1.91064800	-2.57183400
H	-1.82775100	-6.95781200	-0.53330500	H	5.65516300	-0.23605500	-2.63213400
H	1.38546900	-5.13475100	-2.74035700	C	3.70213100	-2.72502400	0.46756900
H	-0.09266900	-7.09078300	-2.31148500	H	2.86506700	-3.35495100	0.13420800
C	-1.38652600	-1.50777600	-4.36681800	H	4.14679700	-3.19241500	1.35213400
C	-2.29029600	-2.55108900	-4.04532300	C	3.29940300	-1.27444900	0.69825800
C	-2.82406000	-2.61418700	-2.71768200	C	2.91392700	-0.74842900	1.90063000
C	-2.46918500	-1.59953600	-1.75257400	C	2.98669100	0.71009700	2.24545700
C	-1.57239000	-0.59109900	-2.11184000	C	1.92619300	1.36265400	2.88708900
C	-1.02219000	-0.57469900	-3.43081200	C	4.17739700	1.44097900	2.07339500
H	-0.96633500	-1.46307900	-5.36923900	C	2.00584500	2.69824900	3.28475600
H	-0.27679000	0.16912500	-3.68944000	H	1.00778100	0.81594500	3.07269400
C	-2.65966900	-3.53244000	-5.00296100	C	4.28016100	2.76895100	2.46956300
H	-2.24564500	-3.45780600	-6.00588200	H	5.04920700	0.95713000	1.64482500
C	-3.69352300	-3.70005600	-2.40922500	C	3.18898700	3.41537100	3.06664800
H	-4.09361800	-3.78987600	-1.40660700	H	1.14844800	3.16280600	3.75836800
C	-3.51505600	-4.55804100	-4.67195100	H	5.20294500	3.32481600	2.33485100
C	-4.02854100	-4.64218700	-3.35699400	O	3.38322400	4.72147900	3.41035400
H	-3.79104200	-5.30453100	-5.41190500	C	2.30635400	5.42577400	4.00608000
H	-4.69255300	-5.45997900	-3.08964100	H	2.01454900	4.98157900	4.96736200
P	-0.76676000	0.54873600	-0.89085700	H	2.66936200	6.44128500	4.17535900
C	-2.06693900	1.18844600	0.27794100	H	1.43027700	5.45907500	3.34485100
C	-1.76404800	1.29040900	1.64033400	C	2.74732700	-1.64591000	3.10913300
C	-3.27759000	1.72543000	-0.18469600	H	3.69258700	-1.65527700	3.67286800
C	-2.65433700	1.89980100	2.52796700	H	1.98032600	-1.27182200	3.78913700
H	-0.81555800	0.89601600	1.98937000	H	2.49089300	-2.67329100	2.84953400
C	-4.17204400	2.32572600	0.70029300				
H	-3.52526400	1.67977900	-1.24050200	<b>60-L2</b>			
C	-3.86293000	2.41555500	2.06009400	C	3.98695700	-1.03058800	-2.33195400
H	-2.40201300	1.97233000	3.58333500	C	2.92924300	-1.64887700	-2.87260300
H	-5.11090900	2.72531900	0.32651700	C	1.85757800	-2.23218800	-2.03449200
H	-4.55873000	2.88966400	2.74748300	C	1.87794800	-1.89874600	-0.58938500
C	-0.51030700	2.16367200	-1.76880400	C	2.93679500	-1.17723300	-0.04338500
C	0.36040000	3.08238700	-1.16441700	C	4.20122300	-0.88136600	-0.84202500
C	-1.24563700	2.56822300	-2.89066900	H	4.78974000	-0.63360900	-2.95109600
C	0.50719400	4.36844300	-1.68146700	H	2.83048900	-1.80444900	-3.94423900
H	0.92506600	2.78839200	-0.28443800	H	1.25135800	-2.50568200	0.05425000
C	-1.09266900	3.85456300	-3.41182500	H	3.09337200	-1.20855500	1.03022800
H	-1.93449900	1.88128300	-3.37164100	O	1.02559400	-2.99691600	-2.53121800
C	-0.21443800	4.75710500	-2.81195200	O	4.76967900	0.39707200	-0.56059000
H	1.19221700	5.06460900	-1.20439600	C	5.29073900	-1.88536200	-0.40009600
H	-1.66207400	4.14829300	-4.29006900	H	5.49008500	-1.75731100	0.66874500
H	-0.09441700	5.75695800	-3.22089600	H	6.21715400	-1.68459300	-0.94823900
Rh	0.96396100	-0.61442900	0.04731900	H	4.97849900	-2.91646800	-0.58980200
C	3.54933000	-2.03770800	-2.54326300	C	3.81982800	1.47058000	-0.69639000
C	2.55472300	-1.29505700	-3.04214200	H	3.42163400	1.46338200	-1.71306100
C	2.24814900	0.06364700	-2.50630300	H	4.41197600	2.38234800	-0.58364000
C	2.57367500	0.31615700	-1.09727500	C	2.72522900	1.31580700	0.34115400
C	3.76115700	-0.47206800	-0.52216200	C	2.98040900	1.71484700	1.61816900
C	4.43468500	-1.56104400	-1.41746100	C	2.12268100	1.42613200	2.80257800
H	3.82112400	-3.00003100	-2.97694100	C	2.10419100	2.29359300	3.91181600
H	1.98769500	-1.60541700	-3.91671000	C	1.34956000	0.25211000	2.92296700
H	2.63355400	1.38409600	-0.89039700	C	1.35767400	2.03117800	5.06361800
H	4.55386100	0.22526600	-0.23463900	H	2.67865900	3.21440300	3.88049900
O	1.73847900	0.89715000	-3.26930900	C	0.62397500	-0.04011300	4.07144700
O	4.72012700	-2.65941100	-0.52563100	H	1.31735800	-0.44602500	2.09234800
C	5.78486600	-1.10903800	-1.98422200	C	0.61154500	0.85164900	5.15175200

H	1.37568300	2.74582900	5.87941600	C	-2.13075000	-1.00820800	-2.11972500
H	0.05772100	-0.96361400	4.15603400	C	-1.43497400	-0.94769100	-3.33294200
C	-4.97404700	2.28554900	-4.51113600	C	-3.47165500	-1.42568000	-2.12801800
C	-3.77601600	2.31245800	-3.74745600	C	-2.06791800	-1.27926300	-4.53295600
C	-3.81423800	1.97615600	-2.35676600	H	-0.38990500	-0.65874500	-3.33419100
C	-5.07133100	1.61239700	-1.79391300	C	-4.10546500	-1.74994000	-3.32559700
C	-6.21571600	1.59206200	-2.55919900	H	-4.02043300	-1.50839300	-1.19470300
C	-6.17138100	1.93428400	-3.93235500	C	-3.40404000	-1.67773300	-4.53220700
H	-4.92364400	2.54623200	-5.56571700	H	-1.51124200	-1.23370400	-5.46518700
H	-5.12096600	1.34447900	-0.74479700	H	-5.14594100	-2.06344500	-3.31682400
H	-7.16213500	1.30933800	-2.10602000	H	-3.89646200	-1.94022100	-5.46495200
H	-7.08248500	1.91602000	-4.52432200	C	-1.71127600	-2.32221500	0.29421700
C	-2.53340900	2.67029300	-4.32144200	C	-1.10790400	-3.50197800	-0.18134100
H	-2.49728400	2.94859900	-5.37229100	C	-2.73552200	-2.44501900	1.24901800
C	-2.60347300	1.99949300	-1.58335600	C	-1.47898200	-4.74882900	0.32492900
C	-1.38169900	2.66689100	-3.57224800	H	-0.37688600	-3.45913600	-0.98398000
C	-1.38524400	2.31623300	-2.19272600	C	-3.10374800	-3.69555100	1.75204900
H	-0.45334200	2.94807300	-4.05132400	H	-3.26932900	-1.57189400	1.60365800
P	0.23121500	2.29766200	-1.21754200	C	-2.46851900	-4.85254500	1.30321700
C	1.45295300	2.87950400	-2.49268100	H	-0.99512800	-5.64244700	-0.06083500
C	1.76113900	2.02447800	-3.56737200	H	-3.89707300	-3.75821000	2.49274600
C	2.15982700	4.08519000	-2.38246900	H	-2.75356400	-5.82418500	1.69817600
C	2.71436700	2.38081400	-4.51959900	Rh	1.06508000	0.20476000	-0.37552800
H	1.25993500	1.06498500	-3.64958300	O	-0.15253200	0.48404800	6.22715300
C	3.13049500	4.43383700	-3.32707500	C	-0.15512500	1.33163300	7.36183200
H	1.96618800	4.75648600	-1.55398000	H	-0.55740200	2.32657200	7.12573400
C	3.40583100	3.58996200	-4.40163700	H	-0.80134700	0.84896300	8.09795200
H	2.92671400	1.70757500	-5.34599100	H	0.85226500	1.44627800	7.78460400
H	3.67027200	5.37079400	-3.21681900	C	4.26067700	2.48419300	1.96801000
H	4.15737200	3.86494200	-5.13680100	H	4.12873600	3.57379900	1.89344000
C	-0.03605700	3.81396800	-0.18448600	H	4.57048500	2.26860500	2.99570400
C	-0.46447200	5.02292900	-0.76194200	H	5.09528200	2.20377000	1.32488200
C	0.15814200	3.75674100	1.19873000				
C	-0.66294100	6.15380500	0.02837200	<b>61-ts-L2</b>			
H	-0.64273200	5.08155100	-1.83211900	C	5.79894200	-1.14463200	2.18786700
C	-0.04725700	4.88940700	1.99143500	C	4.49079700	-0.62391100	1.99635000
H	0.45991300	2.82525900	1.65864900	C	4.02183100	-0.34026800	0.67370200
C	-0.45062700	6.08990200	1.40892800	C	4.90885500	-0.60699600	-0.40967800
H	-0.98958600	7.08289600	-0.43186200	C	6.17102400	-1.11501500	-0.19487100
H	0.10741300	4.82178100	3.06477000	C	6.62717000	-1.38623600	1.11693800
H	-0.60967800	6.97127400	2.02494700	H	6.13112600	-1.34965600	3.20293000
C	-2.61202300	1.40053600	2.69715400	H	4.58166900	-0.41036700	-1.42340600
C	-3.26936500	2.53768700	2.16536600	H	6.82342800	-1.30855800	-1.04224900
C	-3.26655600	2.73271700	0.74606300	H	7.62638600	-1.78385300	1.27297200
C	-2.67298500	1.73355400	-0.10974800	C	3.63124200	-0.36624900	3.09021600
C	-2.11709100	0.58384500	0.44738500	H	3.98711800	-0.55943800	4.09971600
C	-2.04377400	0.46947700	1.86729100	C	2.69102300	0.18447300	0.48063300
H	-2.54346500	1.27936000	3.77542400	C	2.36471400	0.12161700	2.88849800
H	-1.51898900	-0.36837500	2.30622000	C	1.86214300	0.39436000	1.58325900
C	-3.89106500	3.49604400	3.00846700	H	1.73881200	0.30978200	3.75078700
H	-3.88712800	3.32126800	4.08184200	P	0.11131800	1.02864000	1.36607500
C	-3.85632600	3.92759500	0.24332300	C	-0.49840500	1.07071800	3.12405100
H	-3.83801100	4.12085900	-0.82211800	C	-0.86386800	2.25233200	3.78354700
C	-4.47958300	4.62337800	2.48316000	C	-0.69547400	-0.15297000	3.79205500
C	-4.45033700	4.84149400	1.08622700	C	-1.40124900	2.21418000	5.07457400
H	-4.95567200	5.35004400	3.13605600	H	-0.73572600	3.21095000	3.29342300
H	-4.89742800	5.74145500	0.67250300	C	-1.21142000	-0.18952700	5.08617600
P	-1.21169400	-0.71490600	-0.53200900	H	-0.44559400	-1.08289100	3.28934800

C	-1.57166200	0.99703400	5.73211700	C	-3.84918000	-0.74370500	-0.02387100
H	-1.68309000	3.14293700	5.56412200	C	-4.76473700	-0.95086900	1.19732000
H	-1.34507900	-1.14574300	5.58529200	H	-4.74031600	-2.04542800	3.10365800
H	-1.98477000	0.96952300	6.73686300	H	-3.01289800	-3.71997800	2.48139900
C	0.46687000	2.82276400	1.03314500	H	-2.82518500	-1.97524700	-1.47440400
C	1.40367200	3.53916000	1.79965200	H	-4.33422600	-0.23040000	-0.84859000
C	-0.19860500	3.48537900	-0.00493500	O	-2.06262500	-3.94146000	0.08353900
C	1.65396500	4.88607100	1.54128800	O	-4.91134800	0.25797700	1.95008400
H	1.94044800	3.04215500	2.60306000	C	-6.17815300	-1.31256800	0.70954000
C	0.05617900	4.83464100	-0.26758500	H	-6.57681300	-0.49576000	0.09888000
H	-0.91260100	2.94711900	-0.61532300	H	-6.84123600	-1.45444800	1.56954700
C	0.97873500	5.53814500	0.50541100	H	-6.16507700	-2.23345200	0.11864400
H	2.37948300	5.42544800	2.14510000	C	-3.61779800	0.86744700	2.09519200
H	-0.46753100	5.32969700	-1.08098700	H	-2.98132500	0.22490600	2.70851900
H	1.17729500	6.58703500	0.30085400	H	-3.78984600	1.79595100	2.64118900
C	1.95458500	1.08932500	-3.68024000	C	-3.07136200	1.04437400	0.69446200
C	2.76234500	1.96318900	-2.91533600	C	-3.51174700	2.11594700	-0.04162300
C	2.94462600	1.68136600	-1.52276600	C	-3.42890900	2.20106600	-1.51805000
C	2.30268100	0.53414000	-0.93031200	C	-4.42466300	2.88384200	-2.24682600
C	1.44845000	-0.26123000	-1.70210200	C	-2.39680800	1.60719800	-2.27822400
C	1.31516000	0.02679200	-3.09101800	C	-4.41083600	2.96834900	-3.63922200
H	1.84239200	1.26931000	-4.74707100	H	-5.25450000	3.34539400	-1.72141800
H	0.70843700	-0.62016500	-3.71025700	C	-2.35802500	1.69919400	-3.66373000
C	3.40355100	3.08892000	-3.49921800	H	-1.60104000	1.07795300	-1.75180500
H	3.25268400	3.27905400	-4.55932300	C	-3.36660300	2.37787100	-4.36102900
C	3.76944500	2.56903600	-0.77261400	H	-5.21306000	3.49483200	-4.14414900
H	3.91077100	2.39082300	0.28630000	H	-1.53720100	1.26636100	-4.22765700
C	4.19353300	3.92196800	-2.74240900	Rh	-1.42028100	-0.31073500	0.13908900
C	4.37006700	3.65814700	-1.36310100	C	-4.24611600	3.27704800	0.62592200
H	4.67840700	4.78194000	-3.19656700	H	-4.15751900	4.19046200	0.03092700
H	4.98445400	4.32361000	-0.76268200	H	-5.31584500	3.06421100	0.76130900
P	0.29324700	-1.52385100	-0.93139500	H	-3.83741100	3.50053600	1.61422300
C	1.39911600	-2.71354600	-0.04858700	O	-3.23819800	2.41329000	-5.72035900
C	0.96663000	-3.25815200	1.16791100	C	-4.22543900	3.10204400	-6.46873400
C	2.62688400	-3.13652200	-0.58192900	H	-3.92691400	3.01201000	-7.51504800
C	1.74491600	-4.20334600	1.83861700	H	-5.21979000	2.65440200	-6.33692700
H	0.01035500	-2.95034500	1.57651300	H	-4.27215900	4.16499300	-6.19589000
C	3.40583200	-4.07929500	0.08897200				
H	2.97782900	-2.72545600	-1.52417200	<b>61-ts-L2-b</b>			
C	2.96540500	-4.61473400	1.30166900	C	5.78554600	-1.16690100	2.19465500
H	1.39397600	-4.62061300	2.77881000	C	4.48032200	-0.63888800	2.00325500
H	4.35866500	-4.38876700	-0.33181100	C	4.01702600	-0.34071300	0.68170700
H	3.57229700	-5.34935900	1.82461500	C	4.90680100	-0.60233000	-0.40076000
C	-0.26724000	-2.53644300	-2.39566700	C	6.16625800	-1.11709000	-0.18604900
C	0.14729900	-3.85813700	-2.60997000	C	6.61684400	-1.40190200	1.12470200
C	-1.19326100	-1.98140700	-3.29851300	H	6.11292200	-1.38284400	3.20899900
C	-0.32545600	-4.58953700	-3.70245200	H	4.58455100	-0.39646800	-1.41414900
H	0.83021100	-4.33487300	-1.91816200	H	6.82071200	-1.30580700	-1.03293600
C	-1.65756600	-2.70707100	-4.39548400	H	7.61386200	-1.80497600	1.28067000
H	-1.56541100	-0.97397900	-3.14168900	C	3.61770700	-0.39016100	3.09673500
C	-1.22267500	-4.01774800	-4.60286200	H	3.96827500	-0.59818000	4.10512500
H	0.00774300	-5.61482100	-3.84072000	C	2.68882300	0.19185800	0.48945200
H	-2.36670500	-2.24847700	-5.07982800	C	2.35484600	0.10720300	2.89586200
H	-1.58895100	-4.58928100	-5.45163700	C	1.85900500	0.39893300	1.59200000
C	-4.25688900	-2.03185100	2.12776000	H	1.72516900	0.28668500	3.75728000
C	-3.31656300	-2.92628000	1.80245600	P	0.11207000	1.04665100	1.38483300
C	-2.70091000	-2.95233300	0.45202100	C	-0.49342500	1.05501000	3.14491200
C	-2.94521700	-1.78011500	-0.41436800	C	-0.78377300	2.22494100	3.85971200

C	-0.74844100	-0.18450700	3.76176800	H	-1.66275400	-4.56021300	-5.41526200
C	-1.30570200	2.15897800	5.15611500	C	-4.24277000	-1.96162700	2.18652700
H	-0.60878000	3.19583600	3.40983000	C	-3.29699100	-2.85950100	1.88684500
C	-1.24844400	-0.25010400	5.06081700	C	-2.68262600	-2.92134100	0.53707100
H	-0.56246100	-1.10169200	3.21033200	C	-2.93596900	-1.77756500	-0.36372300
C	-1.53353500	0.92502400	5.76303200	C	-3.84761400	-0.73751100	-0.00373400
H	-1.53036600	3.07907200	5.68961000	C	-4.76095900	-0.91449800	1.22348500
H	-1.42912800	-1.21855500	5.51992900	H	-4.72418000	-1.94858100	3.16341500
H	-1.93447000	0.87602700	6.77190900	H	-2.98698000	-3.62996200	2.58929400
C	0.47136000	2.84777000	1.09225400	H	-2.81576600	-2.00435300	-1.41742200
C	1.46504100	3.52699400	1.81999600	H	-4.33664600	-0.25190800	-0.84265700
C	-0.26260300	3.55882900	0.13492700	O	-2.03747900	-3.91626400	0.19636900
C	1.70838100	4.88219000	1.59996000	O	-4.92098900	0.31635400	1.93678200
H	2.05138600	2.99478700	2.56389400	C	-6.17079200	-1.30558500	0.74722900
C	-0.01459100	4.91611900	-0.08992600	H	-6.57746700	-0.51210400	0.11164900
H	-1.02940100	3.05356100	-0.43847700	H	-6.83259000	-1.42723900	1.61126700
C	0.96821000	5.58101800	0.64204900	H	-6.14872800	-2.24405700	0.18502000
H	2.47885700	5.39165400	2.17331300	C	-3.63450300	0.94532100	2.06487800
H	-0.59191200	5.44839300	-0.84120500	H	-2.99676600	0.33848100	2.71174100
H	1.16149600	6.63616200	0.46684500	H	-3.82046000	1.89690400	2.56612200
C	1.97554400	1.07320400	-3.67930700	C	-3.07761700	1.07032000	0.66258000
C	2.77823300	1.95342000	-2.91617700	C	-3.52879900	2.10782600	-0.11370300
C	2.94985100	1.68285400	-1.51988300	C	-3.40858000	2.15349500	-1.58914400
C	2.30319900	0.54116900	-0.92266600	C	-4.45072000	2.71333600	-2.36897100
C	1.45087800	-0.25797800	-1.69295600	C	-2.29993600	1.65462400	-2.29436500
C	1.32817600	0.01773000	-3.08520300	C	-4.39188600	2.75736300	-3.75329700
H	1.87669100	1.24150100	-4.74961200	H	-5.33948700	3.10023100	-1.87998800
H	0.72447600	-0.63495800	-3.70187300	C	-2.21475900	1.71368400	-3.68896600
C	3.42580100	3.07323300	-3.50434100	H	-1.47133800	1.22723000	-1.73061700
H	3.28393500	3.25521700	-4.56717200	C	-3.26556200	2.26321800	-4.42959200
C	3.77219100	2.57398900	-0.77133900	H	-5.20678500	3.17478600	-4.33698900
H	3.90732200	2.40186000	0.28934600	H	-1.31604600	1.34916400	-4.17377100
C	4.21156100	3.91107800	-2.74841000	Rh	-1.41621400	-0.28619400	0.15027100
C	4.37858600	3.65756000	-1.36595200	C	-4.31138200	3.26525400	0.50563400
H	4.70100500	4.76664300	-3.20587600	H	-4.34537200	4.12458200	-0.16895900
H	4.99061000	4.32629300	-0.76683700	H	-5.34394100	2.97842100	0.74628300
P	0.29353500	-1.51363000	-0.91397600	H	-3.84968100	3.60938000	1.43572900
C	1.40909600	-2.71009500	-0.05080500	O	-3.29094300	2.37223100	-5.79057900
C	0.99587200	-3.26272100	1.16868900	C	-2.18135800	1.87742600	-6.52024200
C	2.62850200	-3.12978600	-0.60598500	H	-2.41282200	2.04894400	-7.57333100
C	1.78460800	-4.21255100	1.82048200	H	-1.25645700	2.41025900	-6.26117600
H	0.04537400	-2.96154200	1.59428900	H	-2.03329600	0.80208500	-6.35159200
C	3.41754000	-4.07748200	0.04575500				
H	2.96497300	-2.71227700	-1.55069600	<b>24-L3</b>			
C	2.99617400	-4.62085600	1.26167500	C	-2.62908500	-1.90972200	-1.20158200
H	1.44810500	-4.63608100	2.76311000	H	-2.00330300	-2.59727100	-1.76298200
H	4.36332400	-4.38459600	-0.39228700	C	-2.90764100	-2.06454700	0.16463800
H	3.61072600	-5.35939100	1.76994900	H	-2.52155600	-2.88743700	0.76161200
C	-0.28616100	-2.52017000	-2.37497600	C	-3.57001700	-0.93159700	-1.89715500
C	0.11303000	-3.84584000	-2.59363200	C	-3.30745500	0.32204700	-1.07329900
C	-1.21685100	-1.95548500	-3.26720600	C	-3.59681000	0.18979000	0.29955800
C	-0.37878100	-4.57242600	-3.68113500	C	-4.09886000	-1.24032400	0.65609800
H	0.79873800	-4.32912600	-1.90911900	H	-3.21860400	1.29489900	-1.54630300
C	-1.70041400	-2.67700600	-4.35862500	H	-3.32712700	-0.79056100	-2.95302100
H	-1.57819600	-0.94496000	-3.10378200	Rh	-1.54548200	-0.41839400	-0.09052000
C	-1.28048600	-3.99188400	-4.57140300	C	-5.34724500	-1.55895500	-0.22269800
H	-0.05755700	-5.60101000	-3.82300300	C	-5.06138800	-1.35903400	-1.74331800
H	-2.41667800	-2.21366700	-5.03271400	H	-5.66456600	-2.58903600	-0.01596600

H	-6.16822600	-0.90121800	0.08480800	C	3.91238400	-1.36606800	1.16048900
C	-4.39383600	-1.47396800	2.13580000	C	3.25793100	-1.61053800	2.37896000
H	-4.70529900	-2.51358000	2.29609800	C	4.92073800	-2.25585600	0.75140200
H	-3.50685900	-1.29002900	2.75106800	C	3.60215800	-2.71155500	3.16316500
H	-5.19590200	-0.82063000	2.49452200	H	2.45288800	-0.95108900	2.68874700
C	-5.34218700	-2.62727100	-2.55797300	C	5.26739500	-3.35560000	1.53857700
H	-6.36528000	-2.99118800	-2.41199700	H	5.43451800	-2.06948100	-0.18811600
H	-5.19062600	-2.43900300	-3.62714800	C	4.60961600	-3.58642700	2.74784800
H	-4.66441800	-3.43000400	-2.24860500	H	3.07661300	-2.89087900	4.09765500
O	-5.78322700	-0.22641300	-2.26571200	H	6.05015000	-4.03228500	1.20494500
C	-7.18376700	-0.35870200	-2.40458600	H	4.87540700	-4.44402200	3.36046500
H	-7.67616000	-0.65916900	-1.46746700	O	0.33968300	-1.25161900	0.27598400
H	-7.55860200	0.62819800	-2.69041300	C	0.67952400	-2.57073900	-0.07311400
H	-7.46327200	-1.07672700	-3.18854800	H	-0.04755200	-3.27637200	0.35757700
C	-3.91321400	1.36709900	1.15895400	H	0.70084700	-2.72957800	-1.16384100
C	-3.25843400	1.61343600	2.37691700	H	1.66886600	-2.82516500	0.32873600
C	-4.92261800	2.25560300	0.74939400				
C	-3.60331500	2.71494500	3.16012200	<b>25-L3</b>			
H	-2.45262900	0.95502300	2.68696500	C	-1.67656400	-1.81976400	0.21816300
C	-5.26993300	3.35581500	1.53568800	H	-2.16419100	-2.78619400	0.12728000
H	-5.43662800	2.06777900	-0.18974100	C	-1.08186600	-1.36640900	1.39739700
C	-4.61177800	3.58843700	2.74440900	H	-1.06757600	-1.94352500	2.31893900
H	-3.07747600	2.89572000	4.09416000	C	-1.88339500	-0.71720400	-0.81519500
H	-6.05350300	4.03141100	1.20174900	C	-0.44222700	-0.26792000	-0.99792300
H	-4.87809100	4.44639200	3.35628200	C	0.17613700	0.22195300	0.19566000
O	-0.33959900	1.25250700	0.27481900	C	-0.78218200	0.13399300	1.41650500
C	-0.67936700	2.57154600	-0.07471300	H	-0.05550100	-0.00541500	-1.97795700
H	0.04518400	3.27762900	0.35951300	H	-2.32020300	-1.08549100	-1.74607600
H	-0.69641400	2.73106300	-1.16541800	Rh	0.50671200	-1.87342500	-0.03048500
H	-1.67061300	2.82463700	0.32330000	C	-2.08345300	0.92719900	1.08799500
C	2.63012100	1.90892200	-1.20344500	C	-2.73405500	0.46116800	-0.25085500
H	2.00463500	2.59611400	-1.76562800	H	-2.78212800	0.80484100	1.92510700
C	2.90835400	2.06495900	0.16269600	H	-1.83994300	1.99394500	1.02579700
H	2.52228200	2.88855200	0.75872400	C	-0.18220400	0.58868200	2.74495000
C	3.57081600	0.92977100	-1.89782800	H	-0.91271400	0.45037100	3.55132000
C	3.30758500	-0.32298700	-1.07279200	H	0.71141800	0.00851000	2.99824500
C	3.59665300	-0.18947400	0.29998300	H	0.09843300	1.64651200	2.71947600
C	4.09912700	1.24075500	0.65524800	C	-4.19256300	0.02782100	-0.06555900
H	3.21848200	-1.29624700	-1.54486800	H	-4.79920200	0.81450000	0.39644000
H	3.32809100	0.78781400	-2.95361100	H	-4.64212000	-0.23549300	-1.02984200
Rh	1.54561800	0.41899000	-0.09116200	H	-4.24148900	-0.84822200	0.58990000
C	5.34783400	1.55813700	-0.22356500	O	-2.60444000	1.46996200	-1.27159400
C	5.06228600	1.35681900	-1.74405900	C	-3.39972100	2.63227400	-1.14051100
H	5.66540300	2.58832200	-0.01775900	H	-3.25809300	3.13583900	-0.17245900
H	6.16853500	0.90046800	0.08476900	H	-3.07998000	3.31329300	-1.93406800
C	4.39386400	1.47583400	2.13476800	H	-4.47081600	2.42422800	-1.27089800
H	4.70570300	2.51549700	2.29401200	C	1.28780500	1.21258300	0.13807500
H	3.50668100	1.29294300	2.75004300	C	2.48211500	1.05890800	0.86046500
H	5.19556900	0.82257900	2.49439100	C	1.12299000	2.36626600	-0.64849600
C	5.34370700	2.62417700	-2.55986700	C	3.47915800	2.03263000	0.80190400
H	6.36688500	2.98789000	-2.41401700	H	2.63605300	0.15628500	1.44420600
H	5.19231000	2.43495600	-3.62889800	C	2.11962000	3.34192400	-0.70292900
H	4.66614200	3.42743200	-2.25141200	H	0.19879000	2.49385300	-1.20587900
O	5.78384900	0.22343300	-2.26512400	C	3.30061900	3.17877600	0.02304900
C	7.18445500	0.35512400	-2.40381000	H	4.40103500	1.89163100	1.36002200
H	7.67673100	0.65648200	-1.46692400	H	1.97288000	4.22802700	-1.31521800
H	7.55905700	-0.63220100	-2.68844600	H	4.07937800	3.93545400	-0.02175900
H	7.46437800	1.07218500	-3.18850200	O	2.22913200	-2.27987900	-0.79593900

C	3.09918200	-1.58323800	-1.63690800
H	4.04915100	-2.13590400	-1.71167000
H	2.69997700	-1.47526400	-2.66027300
H	3.33087800	-0.57618300	-1.25324300

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C	-0.12467300	-2.09942000	-0.22665500
H	0.57636200	-2.88759600	-0.47979600
C	-0.23734100	-1.56494800	1.05965100
H	0.36481500	-1.90590200	1.89708500
C	-1.28333400	-1.71741400	-1.14011900
C	-1.17343000	-0.20077300	-1.09445000
C	-1.30766500	0.35957400	0.19583300
C	-1.50079500	-0.73135300	1.28667200
H	-1.29957100	0.39809600	-1.99074500
H	-1.17111100	-2.10848300	-2.15361700
Rh	0.77559800	-0.12770900	-0.20353700
C	-2.75002800	-1.58656700	0.90733300
C	-2.65707800	-2.15395900	-0.54156400
H	-2.84852500	-2.39691200	1.64028700
H	-3.64358600	-0.95898800	0.99830700
C	-1.60526800	-0.21097000	2.71853800
H	-1.71967700	-1.05191400	3.41307000
H	-0.70698500	0.34342900	3.00888000
H	-2.46712400	0.45235100	2.84334100
C	-2.79606500	-3.68039500	-0.57895700
H	-3.72306000	-4.01980200	-0.10404600
H	-2.78409200	-4.04170400	-1.61357600
H	-1.96506700	-4.14734800	-0.03955800
O	-3.60678300	-1.51435200	-1.41471200
C	-4.97314600	-1.83320900	-1.23493100
H	-5.31561000	-1.66289700	-0.20334600
H	-5.53226500	-1.16817100	-1.89883500
H	-5.20167500	-2.87216700	-1.51034500
C	-1.74656600	1.77024800	0.39380900
C	-1.05280100	2.67340900	1.21532600
C	-2.91332900	2.21136200	-0.25493800
C	-1.51361000	3.97885900	1.38296900
H	-0.12966900	2.35839100	1.69117600
C	-3.37565000	3.51730700	-0.08291300
H	-3.45727300	1.51509300	-0.88781200
C	-2.67728000	4.40482700	0.73730800
H	-0.95670700	4.66772000	2.01258000
H	-4.28004200	3.84019000	-0.59217900
H	-3.03321300	5.42316300	0.86904800
O	1.65737700	1.63441900	-0.84810000
C	1.15975300	2.55664800	-1.80517300
H	1.69459200	3.51010600	-1.70246900
H	1.30139400	2.18535800	-2.82525000
H	0.09842600	2.73311400	-1.60816800
C	3.12618400	-0.28900000	1.37668600
C	3.28539700	-1.49714500	2.04865700
C	3.45120400	-2.68763400	1.32105800
C	3.44306300	-2.65364400	-0.08066700
C	3.27918000	-1.42762200	-0.73501800
C	3.13138500	-0.20244400	-0.04357800
H	3.05706000	0.63174600	1.94966600
H	3.30903600	-1.54772300	3.13368400

H	3.57991200	-3.55957400	-0.66166200
H	3.31940500	-1.39539400	-1.82117600
B	3.16832300	1.24416800	-0.84295400
O	3.94737800	2.17421100	-0.06439800
H	4.02151500	3.00709300	-0.55374800
O	3.54322000	1.13999200	-2.24109400
H	4.50852000	1.17068200	-2.28784600
O	3.61478300	-3.81789900	2.06748000
C	3.83758400	-5.04560200	1.39313500
H	4.74480000	-5.00843400	0.77615700
H	3.96225100	-5.79822500	2.17395900
H	2.98367100	-5.32028300	0.75904400

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C	-0.03232500	1.82747300	-0.55686400
H	-0.88729100	2.34185200	-0.98335600
C	0.03444200	1.44742500	0.79169000
H	-0.76424000	1.64770800	1.50095500
C	1.32678800	1.81744500	-1.24610400
C	1.75533600	0.37267600	-1.03091700
C	1.84247700	-0.02037500	0.30552300
C	1.44797100	1.12535200	1.28155900
H	2.20885700	-0.20453700	-1.83038100
H	1.26747500	2.07671200	-2.30543000
Rh	-0.25466600	-0.30317500	-0.41186300
C	2.37452100	2.34791400	0.98555500
C	2.33784300	2.75983300	-0.51792200
H	2.06406500	3.18160100	1.62764400
H	3.40013000	2.08622900	1.26912100
C	1.48338100	0.75868300	2.76385800
H	1.18281700	1.62218800	3.36960600
H	0.79662100	-0.06356500	2.98957500
H	2.48722300	0.45622600	3.07958800
C	1.93412000	4.22687000	-0.70857100
H	2.58691800	4.90826600	-0.15181800
H	1.97164300	4.50082300	-1.76915700
H	0.91324100	4.38641600	-0.34588100
O	3.58768500	2.46740100	-1.17141200
C	4.70117600	3.26961600	-0.83179300
H	4.90134900	3.28147700	0.25026900
H	5.56381600	2.82633900	-1.33718000
H	4.59271300	4.30786600	-1.17569700
C	2.65561900	-1.19617000	0.72795000
C	2.13508600	-2.23355400	1.51943300
C	4.00168600	-1.26972300	0.32850700
C	2.93631700	-3.31085400	1.89784500
H	1.08908700	-2.20723900	1.80986800
C	4.80394400	-2.34637400	0.71068600
H	4.41198800	-0.46680100	-0.27820300
C	4.27370200	-3.37023800	1.49747300
H	2.51224900	-4.10988400	2.50038800
H	5.84255900	-2.38447500	0.39202500
H	4.89569000	-4.21091800	1.79340400
O	-0.54607100	-2.31394500	-0.96147500
C	0.31481500	-3.09484900	-1.79329600
H	0.00685600	-4.14502900	-1.73648300
H	0.26755600	-2.75676600	-2.83241700
H	1.33093200	-2.99547200	-1.40568200

C	-2.94762400	-0.57719100	0.95269300
C	-4.10599200	0.05961900	1.40825400
C	-4.80685200	0.90965600	0.54118100
C	-4.33824200	1.10088000	-0.76881100
C	-3.18149900	0.45746900	-1.19182800
C	-2.43421300	-0.40569300	-0.35242400
H	-2.43781200	-1.25187000	1.63734900
H	-4.45465300	-0.11626300	2.42059100
H	-4.90510300	1.75129300	-1.42962800
H	-2.85020900	0.60342600	-2.21717800
B	-1.95139300	-2.16734300	-1.32046100
O	-2.76304100	-3.10988500	-0.65813500
H	-3.68685800	-2.82659500	-0.63969200
O	-2.13477700	-1.89948500	-2.69339800
H	-2.99197700	-2.23537200	-2.98672700
O	-5.95146200	1.57898500	0.86576100
C	-6.47280100	1.42620100	2.17521800
H	-7.37165600	2.04473600	2.21459900
H	-6.74239600	0.38235100	2.38482300
H	-5.76141500	1.77175000	2.93716700

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C	-0.12259800	-2.19978100	-0.09124900
H	0.52687200	-3.05275200	-0.26222700
C	-0.19831800	-1.52984200	1.14972400
H	0.38369600	-1.83094600	2.01702400
C	-1.34722200	-1.94196800	-0.96323500
C	-1.37512100	-0.42246700	-1.05397500
C	-1.46940800	0.24293400	0.15282600
C	-1.49182800	-0.73718300	1.35790700
H	-1.53543600	0.07748400	-2.00411200
H	-1.27193900	-2.41064100	-1.94715400
Rh	0.78878200	-0.30187100	-0.26237400
C	-2.70246200	-1.70785000	1.14675000
C	-2.65220700	-2.41335500	-0.24325100
H	-2.69885800	-2.44491100	1.95933700
H	-3.63178800	-1.13413000	1.23575200
C	-1.55618500	-0.09052700	2.74080400
H	-1.60374600	-0.86903900	3.51189700
H	-0.66969800	0.51968900	2.94049800
H	-2.43989600	0.54669700	2.84999300
C	-2.67804000	-3.94167500	-0.12015600
H	-3.55246300	-4.29321200	0.43861300
H	-2.69197100	-4.40696400	-1.11251100
H	-1.78885300	-4.29257300	0.41369400
O	-3.69762900	-1.93803300	-1.11268400
C	-5.02166700	-2.32878300	-0.80964300
H	-5.31544900	-2.07158000	0.21932400
H	-5.66900300	-1.78029900	-1.49987600
H	-5.18778700	-3.40504300	-0.95855800
C	-1.88435900	1.66941100	0.23991300
C	-1.18625300	2.62161600	1.00436300
C	-3.02048200	2.09410600	-0.47298700
C	-1.60594400	3.95075200	1.04699000
H	-0.29480800	2.32070100	1.54596000
C	-3.44048700	3.42485900	-0.42936000
H	-3.57891200	1.36181700	-1.04966500
C	-2.73441700	4.35850300	0.33073400

H	-1.04400200	4.67202500	1.63445600
H	-4.32239800	3.72967500	-0.98712000
H	-3.05889300	5.39509200	0.36508900
O	1.54670300	1.73949400	-1.01678200
C	0.93072600	2.32069400	-2.17860000
H	-0.10855100	2.57409400	-1.95263300
H	1.47243600	3.21983600	-2.47795200
H	0.96647500	1.57577000	-2.97627500
C	3.13912800	-1.91820400	0.92574500
C	4.43258400	-2.43177200	0.94981500
C	5.36848400	-2.02842900	-0.01237800
C	4.98836800	-1.10001900	-0.98616800
C	3.68465900	-0.58655000	-0.97889200
C	2.71114300	-0.97354100	-0.03523800
H	2.44602400	-2.27288700	1.68585400
H	4.74227900	-3.15112200	1.70332400
H	5.68860000	-0.76725800	-1.74547400
H	3.42999900	0.14402900	-1.74419500
B	2.21841300	2.54162900	-0.09557300
O	2.75447400	1.98903800	1.02247700
H	2.70625200	1.00947100	0.99565400
O	2.31352300	3.88396800	-0.34525200
H	2.83568600	4.31258800	0.34809500
O	6.61258100	-2.59426500	0.08881500
C	7.59300300	-2.21866300	-0.85993900
H	8.49535100	-2.77606400	-0.59910800
H	7.29086400	-2.48011800	-1.88366200
H	7.80904800	-1.14204700	-0.81745400

### 29-L3

C	0.44272200	-1.82665100	-0.11701100
H	1.18367800	-2.61042100	-0.24703000
C	0.32336300	-1.07556800	1.08882300
H	0.96086000	-1.25238300	1.95245600
C	-0.84212900	-1.81720200	-0.93794900
C	-1.09319600	-0.33075700	-1.14872200
C	-1.21733300	0.41323400	0.00279100
C	-1.06133400	-0.44971100	1.28717400
H	-1.33711900	0.06716200	-2.12849100
H	-0.74329600	-2.35518900	-1.88339600
Rh	1.09820100	0.13569400	-0.42835100
C	-2.13093400	-1.59157200	1.21591900
C	-2.03133200	-2.40651300	-0.11060800
H	-1.99810600	-2.24413500	2.08791700
H	-3.12737300	-1.14316200	1.29721200
C	-1.17358000	0.30987300	2.60835200
H	-1.08709000	-0.39029400	3.44794600
H	-0.37877600	1.05473300	2.71422300
H	-2.13540800	0.82590300	2.69594400
C	-1.82002400	-3.90418800	0.14308300
H	-2.61311100	-4.32835600	0.76853500
H	-1.79523200	-4.45466100	-0.80437300
H	-0.87156300	-4.06979700	0.66450900
O	-3.16979700	-2.17201000	-0.95874200
C	-4.40596200	-2.72666800	-0.55564700
H	-4.69275800	-2.42858400	0.46420900
H	-5.15622300	-2.34059700	-1.25150600
H	-4.41329000	-3.82436300	-0.61089400

C	-1.76986900	1.79600700	0.00266900
C	-1.08913100	2.88099100	0.58106500
C	-3.01568800	2.03649400	-0.60201300
C	-1.63455900	4.16414500	0.55248400
H	-0.11604200	2.71707000	1.03666300
C	-3.56287700	3.32041200	-0.62873600
H	-3.55310900	1.20164800	-1.04368400
C	-2.87468300	4.38846100	-0.05101100
H	-1.08731700	4.99128600	0.99713700
H	-4.52799300	3.48477500	-1.10110500
H	-3.29899500	5.38869900	-0.07221400
C	3.78133600	-1.03731900	0.57047200
C	5.17585200	-0.99410400	0.68690500
C	5.88825000	0.05941400	0.10092600
C	5.19630400	1.06004400	-0.59581300
C	3.80889600	0.99576000	-0.69787300
C	3.06093200	-0.05174900	-0.11888700
H	3.25715800	-1.87026100	1.03730900
H	5.69137900	-1.77868800	1.23098600
H	5.76491600	1.86992900	-1.04425800
H	3.30016300	1.79265000	-1.24877300
O	7.25040900	0.20371300	0.15025000
C	8.00054900	-0.77786600	0.84038600
H	7.87763400	-1.77392200	0.39277200
H	9.04604600	-0.47347000	0.75587500
H	7.72472400	-0.82898200	1.90293200

### 33-L3

C	-2.80866000	0.55934700	-0.87884600
H	-3.57005100	0.04426500	-1.45321200
C	-2.88384600	0.74915000	0.50318400
H	-3.71547500	0.38279500	1.09787400
C	-1.79156600	1.47888900	-1.53833800
C	-0.50674000	1.19459800	-0.77407100
C	-0.57057300	1.41350200	0.58576300
C	-1.98466100	1.86073100	1.04115900
H	0.43569900	1.07539800	-1.29665600
H	-1.68177300	1.29430000	-2.60902900
Rh	-1.38987600	-0.79653100	0.08299400
C	-2.31552600	3.17447100	0.25212700
C	-2.16846000	2.97869700	-1.28788400
H	-3.33491400	3.48393700	0.51288400
H	-1.64033300	3.96905500	0.58887700
C	-2.16151600	2.07168900	2.54386100
H	-3.18342600	2.41095400	2.75172000
H	-1.99970600	1.14314100	3.10075000
H	-1.46964900	2.82596200	2.93230500
C	-3.44904400	3.34366300	-2.04733100
H	-3.77336900	4.36814300	-1.83453100
H	-3.29538100	3.24655800	-3.12814900
H	-4.26492700	2.67587900	-1.75214400
O	-1.02787700	3.69296000	-1.79988700
C	-1.11858700	5.10324400	-1.86068900
H	-1.37858400	5.55289400	-0.89064300
H	-0.12781200	5.46147800	-2.15368500
H	-1.84733300	5.44553700	-2.60848400
C	0.64541200	1.62076800	1.42039000
C	0.88245800	0.92255200	2.61694200

C	1.58798700	2.57952700	1.00664800
C	2.02666900	1.17529400	3.37315100
H	0.17916400	0.16002900	2.93586500
C	2.73135400	2.83495000	1.76648000
H	1.40298100	3.13367200	0.09052400
C	2.95379900	2.13444000	2.95348400
H	2.19613600	0.61969500	4.29177900
H	3.44368400	3.58471600	1.43202000
H	3.84011500	2.33508100	3.54977800
C	-3.02816100	-3.01442600	-1.16796200
C	-4.06833600	-3.93354600	-1.29676700
C	-4.95159600	-4.15416600	-0.23178700
C	-4.77444000	-3.44410200	0.95893700
C	-3.72503800	-2.51843000	1.06728800
C	-2.83652800	-2.27307400	0.01288200
H	-2.35353200	-2.87550700	-2.01014000
H	-4.21181400	-4.49703200	-2.21484600
H	-5.43587500	-3.59685100	1.80564600
H	-3.61167600	-1.98848500	2.01099200
C	4.40833900	-2.28048300	-1.44685400
C	5.02317300	-1.44103700	-2.29192100
C	5.48802600	-0.10060800	-1.85900000
C	5.18393700	0.27744800	-0.45837400
C	4.56938700	-0.56453100	0.38421600
C	4.17799800	-1.97718800	0.01664600
H	4.05984000	-3.25804300	-1.77705100
H	5.20504100	-1.69519600	-3.33277500
H	5.47625100	1.28071900	-0.16075100
H	4.32990600	-0.26358700	1.40277700
O	6.07376200	0.65944000	-2.62347900
O	2.80996200	-2.24245100	0.38001700
C	4.98617600	-2.97221900	0.87533900
H	4.79365700	-2.78143200	1.93571900
H	4.66976500	-3.99473500	0.64645100
H	6.05758300	-2.87358600	0.67912300
C	1.84086600	-1.38918100	-0.23514100
H	2.00969700	-0.34367200	0.05112700
H	1.91720000	-1.44422600	-1.33193200
C	0.49806600	-1.82627200	0.18312200
C	-0.34751500	-2.59691100	0.68489000
H	-0.75777300	-3.50148200	1.08545100
O	-5.94075400	-5.07977900	-0.45444000
C	-6.85093600	-5.34086100	0.59586000
H	-7.41667900	-4.44181300	0.87875800
H	-7.54387400	-6.09508400	0.21623000
H	-6.34306000	-5.73453800	1.48765500

### 34-ts-L3

C	-5.34412400	-2.08672100	0.59713300
C	-6.43642600	-1.35355500	0.34067900
C	-6.81042900	-0.96860100	-1.04167500
C	-5.88005800	-1.39348700	-2.11551700
C	-4.79002900	-2.12835800	-1.85449500
C	-4.42945500	-2.63301300	-0.47565100
H	-5.07136100	-2.35402100	1.61705100
H	-7.09596900	-0.99933000	1.12836600
H	-6.13399600	-1.06891800	-3.12105400
H	-4.10830500	-2.42770900	-2.64938000



O	-7.82525600	-0.32296100	-1.28225900	H	2.96313400	-2.29585000	4.55324400
O	-3.05284100	-2.34885600	-0.16910600	H	5.61052300	-3.90881800	1.57034300
C	-4.49930300	-4.17464300	-0.46495200	H	4.71848700	-3.93175200	3.89433200
H	-3.80743700	-4.57787000	-1.21109500	O	-3.43583700	4.58544100	1.05793800
H	-4.19952800	-4.54796800	0.51934900	C	-3.67171400	5.04828300	2.37648600
H	-5.51282000	-4.51967900	-0.68834800	H	-4.29831600	5.93655300	2.27565200
C	-2.70587500	-0.96430500	-0.12195600	H	-4.20122800	4.29864700	2.97988600
H	-2.86377500	-0.48495900	-1.09794500	H	-2.73591200	5.32022500	2.88340500
H	-3.33352200	-0.42834400	0.60362400				
C	-1.27108900	-0.87962600	0.26781700	<b>35-L3</b>			
C	-0.26434400	-1.54421400	0.69484700	C	5.50832500	-1.30263200	-0.75169800
H	0.02399300	-2.52501900	1.03812000	C	6.75693700	-0.81926400	-0.69123600
Rh	0.71505400	0.10456100	0.00885900	C	7.37701700	-0.42021600	0.59498300
C	-1.06672400	1.20031500	0.31391000	C	6.52139800	-0.53693300	1.80041500
C	-1.31292200	1.60567800	1.63518500	C	5.27361400	-1.02195800	1.73509700
C	-1.69036400	1.94183700	-0.71509300	C	4.64109500	-1.54316600	0.46398700
C	-2.07956300	2.74059900	1.93306700	H	5.05601700	-1.57919800	-1.70297000
H	-0.90118000	1.02604800	2.45704800	H	7.37188500	-0.68640400	-1.57737000
C	-2.46566500	3.05858000	-0.43591900	H	6.96508900	-0.19902400	2.73320300
H	-1.55005400	1.64834400	-1.75266100	H	4.64871800	-1.09257400	2.62429800
C	-2.66000000	3.47360100	0.89349100	O	8.52841000	-0.00054700	0.65654200
H	-2.22774600	3.02487300	2.96926500	O	3.33122600	-0.99143600	0.27673900
H	-2.93235300	3.63496000	-1.22967200	C	4.38954800	-3.05954600	0.61128600
C	1.72119700	1.42248600	-1.51035700	H	3.73255100	-3.23974600	1.46798600
H	1.02532400	1.96798600	-2.13901600	H	3.89114900	-3.43565300	-0.28768600
C	2.09739200	1.84780700	-0.24528300	H	5.32964500	-3.59914800	0.75670600
H	1.72901200	2.76011900	0.21404200	C	3.26556800	0.42043400	0.11119700
C	2.61552200	0.32274500	-2.06515400	H	3.66355600	0.92227100	1.00920900
C	2.52115700	-0.75663900	-0.99826900	H	3.90508800	0.73987500	-0.72873500
C	2.91018000	-0.35692600	0.27775700	C	1.83234100	0.83208000	-0.14140600
C	3.33518500	1.14126600	0.31158600	C	0.76121000	0.00828100	-0.16396600
H	2.43679400	-1.80376300	-1.26828100	H	0.89137300	-1.05986200	0.00395500
H	2.29108900	-0.03631600	-3.04441100	Rh	-0.99097600	0.95266400	-0.31939600
C	4.50114900	1.31440000	-0.71770100	C	1.55438900	2.27121200	-0.37484000
C	4.10201600	0.80702600	-2.13744700	C	0.54128200	2.63853400	-1.29085500
H	4.78528800	2.37369800	-0.74560100	C	2.19996100	3.31958500	0.31725900
H	5.37218900	0.75447500	-0.35866700	C	0.15555000	3.97835300	-1.47777900
C	3.73544000	1.67554600	1.68527300	H	0.17119800	1.88281200	-1.99818400
H	4.02026700	2.73181800	1.60656600	C	1.83688000	4.64311700	0.12561500
H	2.90584500	1.60525200	2.39651200	H	2.98267300	3.09096200	1.03481700
H	4.58544400	1.12524900	2.10120100	C	0.80124200	4.98670600	-0.76394800
C	4.26231800	1.89083500	-3.21022900	H	-0.61840400	4.20704400	-2.20172900
H	5.27984800	2.29616400	-3.23597100	H	2.33555100	5.44370100	0.66401200
H	4.02519900	1.48765200	-4.20161800	C	-3.03069600	1.91437600	0.37380200
H	3.58458200	2.72579300	-3.00450200	H	-2.91979700	2.96149200	0.63725200
O	4.82111200	-0.39131200	-2.48917900	C	-3.21649300	1.46525900	-0.90650500
C	6.19942300	-0.26037600	-2.77565800	H	-3.28400300	2.11854400	-1.77225400
H	6.75854800	0.21989600	-1.95856200	C	-3.18675700	0.82524700	1.42750900
H	6.58336100	-1.27615500	-2.90594700	C	-2.15533200	-0.21070500	0.99358700
H	6.38516400	0.30251900	-3.70118100	C	-2.34681400	-0.70675200	-0.32670400
C	3.37343900	-1.33772700	1.30171800	C	-3.56004100	-0.02019500	-1.02210700
C	2.88260300	-1.36164400	2.61754800	H	-1.62267800	-0.79314400	1.73851100
C	4.36457600	-2.26832000	0.94364100	H	-3.00454700	1.18887400	2.44138900
C	3.36319500	-2.28801400	3.54245700	C	-4.82155300	-0.29063500	-0.13583600
H	2.10012000	-0.66529700	2.90314100	C	-4.61336500	0.18901300	1.33413400
C	4.84569400	-3.19641500	1.86930000	H	-5.68382400	0.20977900	-0.59362500
H	4.75861600	-2.24753600	-0.06885800	H	-5.02964300	-1.36634100	-0.14521500
C	4.34690000	-3.20920600	3.17242600	C	-3.80647700	-0.44163000	-2.46972500

H	-4.66185300	0.10863600	-2.88106400	C	-4.64206500	-2.60555900	-0.89824500
H	-2.93485900	-0.22873800	-3.09825700	H	-3.50903600	-1.36363000	-2.21681300
H	-4.02312200	-1.51145800	-2.54720700	C	-4.69225100	-3.26911300	0.34070900
C	-5.68270700	1.19680400	1.77414400	H	-3.59849000	-3.70539200	2.15953000
H	-6.69652800	0.80087700	1.64847100	H	-5.49707600	-2.68910300	-1.56331900
H	-5.54469900	1.46737700	2.82734900	C	-2.58799300	1.52752000	-0.88543400
H	-5.61252300	2.10742400	1.17032900	H	-3.43305900	1.17878300	-1.46971500
O	-4.53930700	-0.92532300	2.24385400	C	-2.50279900	1.38078100	0.49075800
C	-5.73792800	-1.63039300	2.50066300	H	-3.27520000	0.90875400	1.09025900
H	-6.22410800	-1.98762400	1.58053000	C	-1.56398900	2.50228700	-1.44875500
H	-5.45972300	-2.49884000	3.10424800	C	-0.24730300	1.91229400	-0.96884900
H	-6.46449500	-1.03121700	3.06724300	C	-0.12883800	1.77645400	0.41323800
C	-1.93925800	-2.09231100	-0.70470700	C	-1.42078600	2.23993800	1.14975500
C	-1.20750500	-2.37379000	-1.86959600	H	0.61682800	1.87465400	-1.62376000
C	-2.32272400	-3.16636100	0.11732400	H	-1.60654700	2.58164700	-2.53736200
C	-0.87304600	-3.68546900	-2.20412300	C	-1.66665200	3.73248200	0.74700500
H	-0.87541800	-1.54992300	-2.49390600	C	-1.73132200	3.91550500	-0.80037300
C	-1.98865200	-4.48020400	-0.21771500	H	-2.59605400	4.07143400	1.22124300
H	-2.89289100	-2.95880300	1.01883600	H	-0.85325500	4.34271300	1.15563800
C	-1.26377300	-4.74468500	-1.38039600	C	-1.41029700	2.08593800	2.66931200
H	-0.29780400	-3.88064500	-3.10569600	H	-2.35095500	2.46523800	3.08667600
H	-2.29432100	-5.29617100	0.43253500	H	-1.31639400	1.03584600	2.96448700
H	-1.00005400	-5.76640300	-1.64113000	H	-0.58734600	2.64362400	3.12760700
O	0.52782300	6.32107100	-0.86533800	C	-3.04395800	4.56424600	-1.25529400
C	-0.50663500	6.72388800	-1.74612300	H	-3.21959300	5.52674600	-0.76211400
H	-0.56689500	7.81060800	-1.66295600	H	-3.03603900	4.72775300	-2.33915200
H	-0.28099700	6.45269200	-2.78644500	H	-3.88918200	3.91345700	-1.00872600
H	-1.47261300	6.28417000	-1.46231300	O	-0.58802800	4.64009900	-1.29325900

### 36-ts-L3

C	4.67885500	-1.40568000	-1.66204100
C	5.55309200	-0.77167700	-0.86808500
C	5.80740000	-1.21434000	0.52342600
C	5.04322000	-2.39705100	0.98620700
C	4.16740900	-3.02598700	0.18982500
C	3.90185000	-2.63439800	-1.24679300
H	4.48648200	-1.05726200	-2.67585800
H	6.10507000	0.10463900	-1.19693500
H	5.22476400	-2.71026800	2.01094500
H	3.59344800	-3.87926300	0.54834500
O	6.59577600	-0.62531300	1.25742700
O	2.49081600	-2.44373100	-1.46104800
C	4.26663700	-3.81116900	-2.17322200
H	3.66924100	-4.68788000	-1.90368000
H	4.03899900	-3.54621100	-3.21055200
H	5.32880100	-4.05949200	-2.08968900
C	1.91032600	-1.34975900	-0.73582300
H	2.22147100	-1.38210500	0.31788700
H	2.27077600	-0.39031800	-1.13218500
C	0.43977600	-1.40084800	-0.81654100
C	-0.56874200	-2.05858400	-1.25400300
H	-0.89782200	-2.89097100	-1.85097100
Rh	-1.09402100	-0.09061200	-0.43780600
C	-2.41641800	-1.74439600	-0.38378300
C	-2.46858900	-2.44872400	0.82689400
C	-3.52404700	-1.86344800	-1.25131000
C	-3.59812000	-3.18866100	1.20573200
H	-1.61261600	-2.43165000	1.49614700

C	-4.64206500	-2.60555900	-0.89824500
H	-3.50903600	-1.36363000	-2.21681300
C	-4.69225100	-3.26911300	0.34070900
H	-3.59849000	-3.70539200	2.15953000
H	-5.49707600	-2.68910300	-1.56331900
C	-2.58799300	1.52752000	-0.88543400
H	-3.43305900	1.17878300	-1.46971500
C	-2.50279900	1.38078100	0.49075800
H	-3.27520000	0.90875400	1.09025900
C	-1.56398900	2.50228700	-1.44875500
C	-0.24730300	1.91229400	-0.96884900
C	-0.12883800	1.77645400	0.41323800
C	-1.42078600	2.23993800	1.14975500
H	0.61682800	1.87465400	-1.62376000
H	-1.60654700	2.58164700	-2.53736200
C	-1.66665200	3.73248200	0.74700500
C	-1.73132200	3.91550500	-0.80037300
H	-2.59605400	4.07143400	1.22124300
H	-0.85325500	4.34271300	1.15563800
C	-1.41029700	2.08593800	2.66931200
H	-2.35095500	2.46523800	3.08667600
H	-1.31639400	1.03584600	2.96448700
H	-0.58734600	2.64362400	3.12760700
C	-3.04395800	4.56424600	-1.25529400
H	-3.21959300	5.52674600	-0.76211400
H	-3.03603900	4.72775300	-2.33915200
H	-3.88918200	3.91345700	-1.00872600
O	-0.58802800	4.64009900	-1.29325900
C	-0.51358600	6.01887800	-0.98988100
H	-0.58339900	6.21949700	0.08973900
H	0.46503000	6.35799400	-1.34118600
H	-1.28915500	6.60515200	-1.50259500
C	1.20300900	1.69593000	1.07879700
C	1.49812000	0.76481400	2.08996400
C	2.21920100	2.58250400	0.67841700
C	2.76854900	0.70801000	2.66284400
H	0.73368200	0.05890000	2.39958000
C	3.49278300	2.52082100	1.24752100
H	1.99527800	3.32534300	-0.08221400
C	3.77576500	1.57940700	2.23823100
H	2.97859900	-0.02983700	3.43289600
H	4.26537800	3.20899800	0.91423300
H	4.77220900	1.51371600	2.66520800
O	-5.83970600	-3.96963800	0.59109200
C	-5.94481700	-4.65832400	1.82448700
H	-5.87855300	-3.97137200	2.67925300
H	-6.92734600	-5.13457700	1.82099900
H	-5.16935200	-5.42988600	1.92558200

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C	-4.15408200	0.54974800	-1.81131100
C	-4.82369200	-0.55781600	-1.46296200
C	-5.43087300	-0.71267600	-0.12019900
C	-5.24807600	0.41986800	0.81723300
C	-4.57679600	1.52512600	0.46483100
C	-3.99453400	1.75542100	-0.91204500
H	-3.69357600	0.64213200	-2.79404000
H	-4.93969100	-1.40190100	-2.13752900

H	-5.67292700	0.29037600	1.80903200	H	-0.80992500	-3.07039600	-0.72816300
H	-4.42555100	2.34082500	1.17040400	C	-3.01840900	-2.67103500	1.83412200
O	-6.03653600	-1.73104000	0.20340400	H	-2.69928000	-1.38197400	3.53473900
O	-2.62040200	2.15437700	-0.82412200	H	-3.04587700	-3.84627800	0.02883700
C	-4.69899000	2.96586000	-1.56113400	H	-4.00183400	-2.99949100	2.15693300
H	-4.55439600	3.85182300	-0.93454700	O	5.25320500	4.80578300	0.59615700
H	-4.25597900	3.16351800	-2.54248400	C	6.07690000	4.23830700	1.59913100
H	-5.77038400	2.77950100	-1.67987800	H	7.04474500	4.73566300	1.51187700
C	-1.71742400	1.17738200	-0.27781700	H	5.66965400	4.41338100	2.60432400
H	-2.11365600	0.79267600	0.67306200	H	6.20990800	3.15779600	1.45001500
H	-1.65766400	0.31200900	-0.95341000				
C	-0.35717700	1.76020400	-0.05558300	<b>38-L3</b>			
C	-0.09136500	3.07638300	-0.22040800	C	3.75765600	-2.95984100	-2.61609800
H	-0.82949800	3.79098700	-0.58604400	C	4.43933400	-2.21721600	-3.49957000
Rh	1.38291200	0.75570800	0.21144000	C	5.44203700	-1.21486400	-3.06519100
C	1.27737400	3.55660600	0.03684900	C	5.59947100	-1.03669900	-1.60240200
C	2.05851800	2.98170700	1.06484600	C	4.91230700	-1.77798300	-0.72163000
C	1.88541900	4.56793900	-0.74273100	C	3.97622400	-2.89750300	-1.12066400
C	3.39880000	3.35819500	1.27965500	H	3.01484200	-3.68604200	-2.94340700
H	1.56173900	2.35735900	1.81873300	H	4.28828400	-2.30547600	-4.57227500
C	3.19619700	4.95419100	-0.52690300	H	6.29156300	-0.25959400	-1.28925200
H	1.31091800	5.03965700	-1.53594000	H	5.01538000	-1.61810900	0.35051400
C	3.97254400	4.34245000	0.47925100	O	6.08977900	-0.55553000	-3.87298200
H	3.95203800	2.89859300	2.09094000	O	2.72872400	-2.80258000	-0.42396500
H	3.65920300	5.73205800	-1.12707600	C	4.57047700	-4.24167100	-0.64456600
C	3.30002100	-0.38172200	-0.47197000	H	4.69826800	-4.21865500	0.44230800
H	4.05727700	0.30203500	-0.84260500	H	3.88009600	-5.05416300	-0.89285900
C	3.12164500	-0.67452400	0.85570300	H	5.53762000	-4.43241700	-1.11837900
H	3.73341500	-0.25950500	1.65194100	C	1.97335900	-1.60576900	-0.65258900
C	2.47206100	-1.25644600	-1.40424000	H	2.61380800	-0.73140500	-0.47169500
C	1.05259600	-0.99230200	-0.91482700	H	1.66120700	-1.55955000	-1.70787900
C	0.83715500	-1.31521500	0.45584400	C	0.76790700	-1.53354100	0.24297800
C	2.14681900	-1.81766100	1.13326300	C	0.48302900	-2.52669900	1.11290500
H	0.23141700	-0.97581300	-1.62389300	H	1.14241100	-3.39446000	1.12475400
H	2.60113300	-0.99239900	-2.45629400	Rh	-0.40660200	0.08152500	0.07698200
C	2.62714400	-3.07495300	0.33428700	C	-0.63620000	-2.58056300	2.05797600
C	2.81041100	-2.76686400	-1.18325700	C	-1.34137300	-1.43675900	2.49315800
H	3.56443600	-3.43345600	0.77742400	C	-1.06286900	-3.81267400	2.58414700
H	1.88429000	-3.87031100	0.46077800	C	-2.42807100	-1.51967300	3.35546100
C	2.04592000	-2.13101400	2.62528600	H	-0.99782700	-0.44272700	2.18679200
H	3.01945900	-2.46983900	3.00074600	C	-2.14635900	-3.91747900	3.45829900
H	1.75542200	-1.24533900	3.20039700	H	-0.53955000	-4.71865300	2.28739900
H	1.31315500	-2.91841400	2.82563900	C	-2.84435100	-2.76599500	3.84492900
C	4.23037100	-3.07882800	-1.67135700	H	-2.95660900	-0.62987000	3.68493800
H	4.51716100	-4.11597700	-1.46520100	H	-2.43557900	-4.89497000	3.82818900
H	4.31300600	-2.90484900	-2.75036500	C	-1.27440400	2.38358400	-0.57161400
H	4.95285200	-2.43433200	-1.15978300	H	-2.13849400	2.26127800	-1.21557800
O	1.82031700	-3.44261100	-1.98134400	C	-1.32591800	2.33757200	0.78038100
C	1.93780700	-4.84610400	-2.11001500	H	-2.24446200	2.19687500	1.34453400
H	1.97028000	-5.35966400	-1.13750500	C	0.10782700	2.69206800	-1.11777600
H	1.04554700	-5.18012100	-2.64673500	C	1.01572000	1.63581700	-0.50230400
H	2.82349400	-5.14193800	-2.68951000	C	1.00077400	1.59318400	0.90775700
C	-0.49544400	-1.76459300	0.95344200	C	-0.00596300	2.64089200	1.48754400
C	-1.04303500	-1.30838400	2.16461400	H	1.87337700	1.28842800	-1.06754900
C	-1.23284100	-2.69519200	0.19969300	H	0.14565800	2.68539800	-2.20951200
C	-2.28901200	-1.75776000	2.60080200	C	0.47363700	4.04440200	0.97832700
H	-0.49946000	-0.56943300	2.74560900	C	0.57352600	4.09006100	-0.57655300
C	-2.48378700	-3.13917800	0.63298500	H	-0.21727400	4.81067600	1.35004700

H	1.45575800	4.25127400	1.41673700	C	4.66731100	0.79224000	1.94155900
C	-0.15175600	2.64005400	3.00933900	C	3.70707800	1.15150000	3.05394600
H	-0.87310300	3.40611700	3.31867100	H	2.79442700	0.20609900	4.82754500
H	-0.51064400	1.67389500	3.38112700	H	4.17828800	-1.85663300	4.81017700
H	0.80115500	2.85304400	3.50262800	H	6.12110600	-0.53796100	1.13986100
C	-0.27632900	5.21294700	-1.18368000	H	4.73452500	1.51735500	1.13200900
H	-0.01262300	6.19259000	-0.77068800	O	6.01828300	-2.33885700	3.02739100
H	-0.14424400	5.24905300	-2.27114000	O	2.43303100	1.55078600	2.52716400
H	-1.33604700	5.04419300	-0.96715400	C	4.22543500	2.41210200	3.77974000
O	1.94115400	4.17302400	-1.01741200	H	4.31315800	3.23627700	3.06457000
C	2.61752200	5.39901600	-0.81066200	H	3.51381300	2.70590800	4.55800100
H	2.59674400	5.72123200	0.24104900	H	5.20188700	2.22617900	4.23588300
H	3.65771100	5.22586500	-1.09940400	C	1.73425900	0.56079300	1.75726200
H	2.21429300	6.21009900	-1.43228400	H	2.44406300	0.04619100	1.09559800
C	2.22488000	1.21609700	1.68048400	H	1.31346500	-0.20002100	2.43037100
C	2.19221400	0.35516700	2.79092000	C	0.64023600	1.17906600	0.91529400
C	3.46666900	1.75918100	1.30074800	C	0.68075900	2.51397800	0.65303000
C	3.35705100	0.04507800	3.49193000	H	1.51005700	3.05299100	1.11244000
H	1.25303500	-0.09734700	3.09034900	Rh	-0.48144800	-0.21027100	-0.18211600
C	4.63407700	1.44667800	2.00086000	C	-0.22875500	3.38093400	-0.09519900
H	3.50331900	2.44024500	0.45517300	C	-1.13004700	2.95101500	-1.09498000
C	4.58389600	0.58769700	3.09985100	C	-0.20598700	4.76171400	0.18084600
H	3.30693400	-0.63145200	4.34114600	C	-1.98272300	3.83875200	-1.73827100
H	5.58093600	1.88061300	1.68884400	H	-1.13867900	1.90217400	-1.37888800
H	5.49037900	0.34451900	3.64820000	C	-1.05241200	5.66662800	-0.45670300
C	-6.10164700	-1.16446000	-0.63190400	H	0.48604500	5.13466200	0.93249200
C	-6.52453300	0.05807700	-0.28027600	C	-1.95748600	5.20480300	-1.42168400
C	-6.07768500	1.27413300	-1.00196600	H	-2.66490800	3.50112800	-2.51315200
C	-5.11968100	1.06172700	-2.11185300	H	-0.99842400	6.71815200	-0.19791700
C	-4.69059800	-0.16197200	-2.45463100	C	-1.28245600	-2.19032100	-0.98695600
C	-5.18160300	-1.43314800	-1.80136800	H	-2.17046300	-2.52405600	-0.46107200
H	-6.42335300	-2.04993300	-0.08596100	C	-1.29937900	-1.26895300	-2.01496800
H	-7.20477800	0.21970800	0.55166900	H	-2.20995700	-0.81383600	-2.39514000
H	-4.77977800	1.95815100	-2.62424400	C	0.04755300	-2.91175600	-0.84967600
H	-3.97639100	-0.30109500	-3.26279200	C	1.03611300	-1.76990000	-0.68216700
O	-6.46761900	2.39419900	-0.68664600	C	1.06028500	-0.84356300	-1.72819000
O	-4.09016800	-2.28108600	-1.39573000	C	0.00230000	-1.18898000	-2.81704100
C	-5.93109900	-2.28040100	-2.85143000	H	1.86228100	-1.86414200	0.01311200
H	-5.25800700	-2.51398600	-3.68222500	H	0.06810500	-3.60548300	-0.00647900
H	-6.25676000	-3.22157100	-2.39748600	C	0.32892800	-2.62912500	-3.33840500
H	-6.80373100	-1.74316400	-3.23366700	C	0.39510700	-3.66731200	-2.17667000
C	-3.19969700	-1.75704000	-0.40213400	H	-0.43331300	-2.91383300	-4.07408600
H	-3.73713300	-1.09635100	0.28921800	H	1.29094200	-2.60090900	-3.86192500
H	-2.85846200	-2.61976100	0.17801700	C	-0.09794400	-0.20232700	-3.97940600
C	-2.02203000	-1.06742200	-0.96918000	H	-0.85876000	-0.54263600	-4.69253200
C	-1.18842000	-0.66119800	-1.80437900	H	-0.38456200	0.79735400	-3.63662700
H	-0.71883200	-0.53913800	-2.76197300	H	0.85207600	-0.11409600	-4.51539700
O	-3.91813800	-2.74775500	4.69202700	C	-0.56087600	-4.84648000	-2.39284500
C	-4.35371900	-3.97772600	5.24418800	H	-0.38099700	-5.34955200	-3.34936900
H	-5.20172700	-3.73526500	5.88774600	H	-0.45174700	-5.58283100	-1.58857100
H	-4.68073400	-4.67957400	4.46475700	H	-1.59838000	-4.49654400	-2.40016800
H	-3.56723100	-4.45315300	5.84591600	O	1.74378800	-4.11588300	-1.94882900
				C	2.31452800	-4.97426500	-2.91750700
				H	2.28687700	-4.54620600	-3.93087400
				H	3.36003500	-5.10985500	-2.62758100
				H	1.82935300	-5.95978100	-2.94261100
				C	2.28711400	-0.05011800	-2.03173400
				C	2.26365300	1.32273700	-2.33054700
<b>39-ts-L3</b>							
C	3.54787000	0.03383300	4.06007500				
C	4.29024600	-1.08194200	4.05623200				
C	5.31258900	-1.33514600	3.01204800				
C	5.41645000	-0.31952100	1.93753500				

C	3.53022900	-0.70993200	-2.03949600	C	-2.92653800	2.53927800	0.81361300
C	3.44127400	2.01089800	-2.62038700	H	-2.59766900	3.26505100	1.55367400
H	1.32266500	1.86104200	-2.30570600	Rh	0.58985500	-0.41248200	-0.15351800
C	4.70980700	-0.02017900	-2.32718400	C	-4.35757500	2.61006300	0.48760800
H	3.55791400	-1.77609700	-1.83263100	C	-4.89509000	2.33791000	-0.78203400
C	4.66973900	1.34417700	-2.61850200	C	-5.26162000	3.03610000	1.48571800
H	3.39916300	3.07464600	-2.84002900	C	-6.26385200	2.44036300	-1.04165900
H	5.65759100	-0.55288300	-2.32970000	H	-4.23227900	2.07326100	-1.59904400
H	5.58568300	1.88364600	-2.84567500	C	-6.62329500	3.13925600	1.24560300
C	-5.94097300	-1.26390300	1.34911300	H	-4.87856000	3.27741300	2.47462000
C	-5.93007000	-2.50137000	0.83372100	C	-7.13988800	2.83410800	-0.02321300
C	-4.84809200	-3.46500700	1.14910800	H	-6.62791100	2.22960100	-2.04103400
C	-3.77878700	-2.97820100	2.05145000	H	-7.31106000	3.45708700	2.02327400
C	-3.78697000	-1.73559600	2.55666600	C	0.86003100	-2.41622100	0.42116500
C	-4.89825000	-0.74192800	2.31221700	H	-0.04578500	-2.95069800	0.69240900
H	-6.72902200	-0.55566000	1.09811300	C	1.28792200	-2.25334600	-0.92486500
H	-6.70115600	-2.85476200	0.15422200	H	0.75114000	-2.68679500	-1.76450500
H	-2.98003500	-3.68311700	2.26671800	C	2.00028600	-2.26162100	1.41827000
H	-2.98209300	-1.38785000	3.19961200	C	2.56383100	-0.88689200	1.08724500
O	-4.82842500	-4.59518900	0.67027400	C	3.00292100	-0.72555800	-0.20396800
O	-4.39105400	0.52276000	1.84509200	C	2.79077200	-2.00076400	-1.06442300
C	-5.57382100	-0.39557500	3.65497200	H	2.77752100	-0.16325200	1.86696800
H	-4.83092800	0.02012900	4.34287300	H	1.66681600	-2.33120500	2.45589100
H	-6.35002900	0.35843200	3.49059000	C	3.55184700	-3.16796000	-0.34702000
H	-6.02493200	-1.28454100	4.10530500	C	3.11782000	-3.32197700	1.14208300
C	-3.61443000	0.49997100	0.63807500	H	3.36691600	-4.09324500	-0.90654500
H	-3.92333600	-0.33499400	-0.00341800	H	4.62824600	-2.96968600	-0.39859200
H	-3.87191400	1.42655300	0.11046800	C	3.22662200	-1.89681200	-2.52521600
C	-2.14911000	0.48059800	0.85829200	H	3.07517900	-2.86101800	-3.02539800
C	-1.18721400	0.69193900	1.67403800	H	2.64384800	-1.14605800	-3.06775800
H	-0.89597600	0.85275000	2.69972300	H	4.28521700	-1.63284100	-2.61417400
O	-2.82783600	5.99542400	-2.11591800	C	2.60790900	-4.73327700	1.45794700
C	-2.82192000	7.38877800	-1.85516300	H	3.35219300	-5.50023300	1.21746700
H	-3.57828400	7.82084800	-2.51327700	H	2.35149100	-4.82130100	2.51973100
H	-3.08395700	7.60662800	-0.81103900	H	1.71219500	-4.95480800	0.86855400
H	-1.84574500	7.83867800	-2.08122000	O	4.17065900	-2.92718700	2.04023800
				C	5.28963200	-3.78587300	2.14501300
				H	5.75392400	-3.99753700	1.17007800
				H	6.01963700	-3.26243500	2.76872800
				H	5.04213300	-4.74197100	2.62674800
				C	3.90324200	0.38425800	-0.61798900
				C	3.64131400	1.20740100	-1.72663500
				C	5.08562700	0.60096300	0.11123600
				C	4.53189000	2.21493800	-2.09539100
				H	2.72081800	1.07155200	-2.28735000
				C	5.98068100	1.60636600	-0.26056500
				H	5.30279500	-0.04257400	0.95945300
				C	5.70755400	2.41438200	-1.36588900
				H	4.29575100	2.86452500	-2.93230500
				H	6.89262900	1.75404500	0.31239700
				H	6.40007600	3.20004400	-1.65523500
				C	-3.64932800	-4.06452600	-1.59904100
				C	-3.31137600	-5.08796000	-0.80209600
				C	-3.20375700	-4.92597500	0.66786200
				C	-3.45652000	-3.56564400	1.19709400
				C	-3.78689400	-2.54098700	0.39640900
				C	-3.98454900	-2.67777500	-1.09632500
				H	-3.71020900	-4.18746500	-2.67928400
<b>40-L3</b>							
C	1.87176500	3.71799300	1.30656800				
C	2.63549300	4.07814100	0.26584600				
C	2.06757900	4.79233400	-0.90207600				
C	0.60704500	5.04622600	-0.87057500				
C	-0.15339700	4.68543600	0.17301200				
C	0.40284500	4.04734200	1.42442500				
H	2.29338100	3.17933800	2.15352300				
H	3.69456000	3.84597300	0.21905700				
H	0.18934900	5.53398200	-1.74725600				
H	-1.22645300	4.86186100	0.17238500				
O	2.76060900	5.13884200	-1.85443900				
O	-0.33862000	2.86271300	1.79593700				
C	0.19137200	5.00031400	2.61900800				
H	-0.87267800	5.23417300	2.72542600				
H	0.53201900	4.51524500	3.53919000				
H	0.74963500	5.92962200	2.47481700				
C	-0.53442700	1.86074900	0.81007500				
H	0.08207300	2.07283500	-0.08200100				
H	-0.18058600	0.90738500	1.28085300				
C	-1.97827100	1.66965000	0.37633400				

H	-3.09162200	-6.07921600	-1.19011800
H	-3.34941100	-3.44564900	2.27202300
H	-3.95055800	-1.54489200	0.79970400
O	-2.90337900	-5.86379400	1.40109300
O	-3.22730200	-1.70029500	-1.83154900
C	-5.45289700	-2.35278600	-1.44232100
H	-5.69279600	-1.33742600	-1.11099300
H	-5.59145300	-2.40395900	-2.52715500
H	-6.13389500	-3.05959600	-0.95921400
C	-1.81004700	-1.65821500	-1.58686000
H	-1.48929300	-2.60601700	-1.13726800
H	-1.34155700	-1.60886400	-2.57963400
C	-1.33434800	-0.48638200	-0.75414700
C	-2.22164200	0.50073800	-0.45399800
H	-3.23742000	0.38121900	-0.81931100
O	-8.49165900	2.96526200	-0.16350500
C	-9.06533000	2.67691500	-1.42733400
H	-10.13934900	2.83568700	-1.31304700
H	-8.68163500	3.34683800	-2.20856600
H	-8.88261700	1.63599400	-1.72630100

#### 41-L3

C	4.02727900	-1.24477000	0.30854200
C	3.60427200	-2.11418400	-0.62067100
C	2.90216400	-1.66408700	-1.84555700
C	2.50070000	-0.23344300	-1.89228200
C	2.89114700	0.65608100	-0.89426000
C	3.88580800	0.25765100	0.18629100
H	4.56154700	-1.58243700	1.19532300
H	3.78431800	-3.18341300	-0.54135800
H	2.15240100	0.12107200	-2.85935200
H	2.83008300	1.72527100	-1.07760800
O	2.66725000	-2.43738900	-2.77372100
O	3.60198600	0.84524800	1.45265500
C	5.26762900	0.84276100	-0.19174500
H	5.19598900	1.93373500	-0.24491800
H	5.99810500	0.58459700	0.58158700
H	5.61122600	0.45328000	-1.15445000
C	2.27648800	0.60477100	1.96000900
H	2.14365300	-0.47075300	2.13580300
H	2.27218900	1.11178800	2.93248900
C	1.22566500	1.17086400	1.03653300
C	0.74561500	2.40026200	1.32623000
H	1.04637400	2.82308700	2.29152300
C	-0.11153900	3.31067500	0.55138200
C	-0.76467300	4.36718400	1.20793200
C	-0.28775200	3.22824900	-0.84674100
C	-1.57455000	5.28211400	0.53197900
H	-0.64001500	4.47487400	2.28333700
C	-1.08616100	4.12994600	-1.53636500
H	0.21931700	2.43697000	-1.39316700
C	-1.74237100	5.16514300	-0.85247900
H	-2.06049100	6.07497700	1.08975700
H	-1.20876500	4.06422200	-2.61376100
C	-0.76380400	-0.61961000	-2.25019500
H	-0.42545200	-0.27128300	-3.22098500
C	-0.34014600	-1.79509500	-1.67891000
H	0.38176300	-2.45679000	-2.14615300

C	-1.94136300	0.01301400	-1.52793200
C	-1.42619000	0.16386500	-0.10541100
C	-1.02698400	-1.02910800	0.50917200
C	-1.14561200	-2.23990300	-0.45998900
H	-1.65857600	1.04895900	0.47226500
H	-2.24245100	0.97127500	-1.95452300
Rh	0.71628400	-0.03376200	-0.56696000
C	-3.15426500	-0.97715400	-1.50367600
C	-2.65259200	-2.31734800	-0.88745500
H	-2.76339500	-3.14315100	-1.60032500
H	-3.25281800	-2.56707600	-0.00550800
C	-0.67020100	-3.59388100	0.06659600
H	-0.85207400	-4.36503200	-0.69139200
H	0.40394500	-3.58958400	0.27836800
H	-1.19890100	-3.88453000	0.97929000
C	-3.72680100	-1.16175000	-2.91417500
H	-4.53516700	-1.90076300	-2.93416200
H	-4.11628400	-0.21158500	-3.29714800
H	-2.94620000	-1.51679100	-3.59522600
O	-4.09263500	-0.31739500	-0.63534300
C	-5.37691200	-0.89617200	-0.50848400
H	-5.33715700	-1.95099800	-0.19790600
H	-5.89371600	-0.32625200	0.26846500
H	-5.96121100	-0.82861400	-1.43662900
C	-1.05829400	-1.19484600	1.98892300
C	-0.08683300	-1.91975200	2.70052900
C	-2.13090200	-0.63937000	2.70995100
C	-0.17477200	-2.06863800	4.08389800
H	0.75291600	-2.35176900	2.16718900
C	-2.21984400	-0.78966100	4.09432800
H	-2.90722100	-0.10674600	2.16889500
C	-1.24069100	-1.50249400	4.78749200
H	0.59407800	-2.62441800	4.61429400
H	-3.05850900	-0.35194100	4.62959800
H	-1.30786500	-1.61959500	5.86581500
O	-2.50293000	6.00061200	-1.62259200
C	-3.17356100	7.07203000	-0.98330000
H	-3.70890300	7.60547200	-1.77142000
H	-3.89445000	6.71181800	-0.23665600
H	-2.46800300	7.75913200	-0.49653300

#### 42-ts-L3

C	0.14188100	4.19157700	1.36536400
C	-0.82261800	3.50342900	1.98720300
C	-0.65199700	2.07339600	2.35308700
C	0.49238600	1.36770000	1.74463200
C	1.49683600	2.06959100	0.96790000
C	1.48407700	3.61666600	0.96485200
H	0.02294600	5.24870800	1.13230400
H	-1.75269100	3.96914300	2.30415900
H	0.78754700	0.46093700	2.27040900
H	2.49679500	1.65086500	1.06294200
O	-1.43793700	1.52966500	3.13088100
O	1.82643300	4.12334000	-0.33207400
C	2.57339500	4.13804100	1.91629400
H	3.55482500	3.78631100	1.58135000
H	2.57961700	5.23292100	1.90966000
H	2.39388900	3.79436500	2.93960000

C	1.20353200	3.32393800	-1.34154100	H	5.90412000	-5.10450900	0.50597800
H	0.12772400	3.54826600	-1.39517800	H	5.04419000	-3.89286700	1.49674900
H	1.67077000	3.61416400	-2.28884100				
C	1.47659900	1.88117400	-0.98409900	<b>42-ts-L3-b</b>			
C	2.54857100	1.28443000	-1.58159400	C	-0.05281500	4.24681000	1.12189500
H	3.01678800	1.84480400	-2.39648000	C	-1.02186000	3.57353800	1.75277400
C	3.24154800	0.04050100	-1.27020900	C	-0.82562800	2.17753100	2.22327500
C	4.46979500	-0.23452400	-1.91640900	C	0.35843800	1.46614200	1.70415900
C	2.79323700	-0.90544600	-0.32981900	C	1.37475700	2.14500400	0.92236600
C	5.20799500	-1.37128400	-1.63203300	C	1.32131700	3.68759200	0.81832100
H	4.84876200	0.47295700	-2.65045400	H	-0.19165700	5.28126100	0.81092800
C	3.52968800	-2.04979900	-0.02417700	H	-1.97704000	4.03047100	2.00022400
H	1.83251700	-0.74906400	0.15529200	H	0.65577500	0.60202300	2.29622100
C	4.74641700	-2.29138000	-0.67626500	H	2.38085900	1.76343900	1.08415300
H	6.14995600	-1.57280400	-2.13263300	O	-1.62531800	1.66525400	3.00823700
H	3.14171800	-2.74922300	0.70813200	O	1.70850600	4.11856200	-0.49319700
C	-1.46141800	0.81861900	-2.05054900	C	2.35230200	4.30099800	1.77965100
H	-1.22216800	1.64407600	-2.71374700	H	3.35689400	3.95804200	1.51068300
C	-0.76663800	-0.37814500	-2.04430200	H	2.32919700	5.39292400	1.70225700
H	0.07400000	-0.58398200	-2.70060000	H	2.13658800	4.01792300	2.81443600
C	-2.77202200	0.75781600	-1.27942500	C	1.14727000	3.23979700	-1.47254700
C	-2.32530100	0.30439300	0.10413000	H	0.07014600	3.43371400	-1.58516900
C	-1.65026600	-0.91871500	0.13139100	H	1.64734700	3.48010000	-2.41710700
C	-1.46869600	-1.51272100	-1.29611200	C	1.43686900	1.83046500	-1.00945900
H	-2.74376800	0.73952700	1.00540100	C	2.54672100	1.22360300	-1.52154000
H	-3.29292900	1.71724200	-1.25002500	H	3.03874100	1.74132000	-2.35060200
Rh	-0.19353900	0.77607900	-0.19461800	C	3.25291500	0.02179700	-1.09603700
C	-2.90401500	-1.67994700	-1.90260700	C	4.52454100	-0.24688800	-1.63790500
C	-3.70797400	-0.34472800	-1.87859000	C	2.76461600	-0.88964200	-0.13200700
H	-2.80533500	-2.05977300	-2.92682300	C	5.28612900	-1.34451000	-1.24172600
H	-3.43826100	-2.44199000	-1.32448000	H	4.93344300	0.43149100	-2.38335100
C	-0.69231400	-2.82583600	-1.38834700	C	3.51351700	-1.98092400	0.27991800
H	-0.67429100	-3.17147400	-2.42927700	H	1.76643200	-0.73891600	0.27342500
H	0.34602000	-2.70290800	-1.06479000	C	4.78376600	-2.22035600	-0.27001100
H	-1.15062400	-3.61105000	-0.77917700	H	6.26074800	-1.50459100	-1.68869000
C	-4.20104000	0.06318100	-3.27221200	H	3.13264100	-2.67839000	1.02011200
H	-4.80961500	-0.72101400	-3.73598300	C	-1.43754200	0.63765600	-2.11910900
H	-4.80185100	0.97799100	-3.21343900	H	-1.18771500	1.42416300	-2.82443200
H	-3.34952600	0.24862700	-3.93520700	C	-0.72465200	-0.54333300	-2.01300200
O	-4.79200400	-0.39727500	-0.93391500	H	0.14312700	-0.77448200	-2.62432200
C	-5.89437500	-1.22315600	-1.25339200	C	-2.77483200	0.60060800	-1.39373000
H	-5.59772500	-2.26028100	-1.47019000	C	-2.37246400	0.24193700	0.03059700
H	-6.54008000	-1.22593600	-0.37096100	C	-1.68017100	-0.96494900	0.15898100
H	-6.47262100	-0.84144400	-2.10663600	C	-1.43545600	-1.64201200	-1.22118000
C	-1.61444800	-1.76074100	1.36101400	H	-2.83417500	0.72222600	0.88674700
C	-0.45953100	-2.42898100	1.80124000	H	-3.31234000	1.55004400	-1.44412900
C	-2.79476900	-1.91818000	2.10831600	Rh	-0.24007900	0.73619800	-0.21771800
C	-0.48033100	-3.21634000	2.95124200	C	-2.84358000	-1.87255200	-1.86977700
H	0.46655500	-2.31319800	1.24753300	C	-3.66950100	-0.55393300	-1.95654700
C	-2.81727200	-2.70717300	3.25872100	H	-2.69942200	-2.31009800	-2.86520200
H	-3.69929200	-1.42169200	1.76997000	H	-3.38642600	-2.60944900	-1.26763800
C	-1.66011400	-3.35864400	3.68587900	C	-0.63489000	-2.94346700	-1.19976900
H	0.42844400	-3.71471200	3.27946800	H	-0.56086900	-3.34891300	-2.21625000
H	-3.74098500	-2.80944100	3.82225700	H	0.38415600	-2.78269000	-0.83406200
H	-1.67476100	-3.97034800	4.58402200	H	-1.10968100	-3.70001500	-0.56747500
O	5.53950000	-3.37943200	-0.46629400	C	-4.11751200	-0.24043800	-3.38942600
C	5.12792900	-4.33721000	0.49620200	H	-4.69788400	-1.06120200	-3.82514300
H	4.16819600	-4.79611600	0.22402400	H	-4.73281600	0.66642300	-3.40920200

H	-3.24520500	-0.08204300	-4.03225300
O	-4.78653100	-0.56879700	-1.04977700
C	-5.86200500	-1.43436300	-1.35540200
H	-5.54086100	-2.47824700	-1.48897900
H	-6.54270600	-1.38929500	-0.50087300
H	-6.41129600	-1.12189500	-2.25476300
C	-1.68156100	-1.73118200	1.43794700
C	-0.53445000	-2.34374300	1.97017800
C	-2.89234900	-1.87267600	2.13860600
C	-0.59275700	-3.06193900	3.16337900
H	0.41516000	-2.24063300	1.45515000
C	-2.95225700	-2.59285700	3.33197200
H	-3.79033900	-1.41888700	1.72994400
C	-1.80264000	-3.18935500	3.85015400
H	0.31022900	-3.51779600	3.56146800
H	-3.89926700	-2.68413800	3.85753700
H	-1.84652900	-3.74724400	4.78176600
O	5.43387200	-3.32431700	0.19446900
C	6.71510200	-3.62450700	-0.33566300
H	7.43423100	-2.81976100	-0.13332000
H	7.04215800	-4.53524600	0.16926100
H	6.67164000	-3.80529200	-1.41787900

**42-ts-L3-c**

C	0.49032800	4.36535300	-0.43923900
C	1.09702400	3.93369600	-1.55208700
C	0.49585200	2.87936500	-2.40847900
C	-0.63989300	2.13580300	-1.83428300
C	-1.24336800	2.50776500	-0.57366900
C	-0.84430100	3.85558600	0.06557700
H	0.92110800	5.16083200	0.16719300
H	2.02839900	4.36735800	-1.90844800
H	-1.25722100	1.62216700	-2.57035000
H	-2.30974500	2.30287700	-0.51208800
O	0.93880500	2.65323600	-3.53754700
O	-0.78564900	3.73905500	1.49041900
C	-1.93545100	4.90042000	-0.22314200
H	-2.88451500	4.56971500	0.21146400
H	-1.66321000	5.85752800	0.23368800
H	-2.06049800	5.04799500	-1.30015900
C	-0.15815400	2.50028700	1.84270100
H	0.92235300	2.56195600	1.66033400
H	-0.32089200	2.37032900	2.91756800
C	-0.82459200	1.41742800	1.02545500
C	-1.85354200	0.74325700	1.61529800
H	-1.99082700	0.92255600	2.68587400
C	-2.86585700	-0.14308300	1.05347900
C	-3.93794100	-0.54428700	1.87427600
C	-2.87483400	-0.61078700	-0.28146700
C	-4.97243100	-1.35271100	1.40825500
H	-3.96470300	-0.20488800	2.90733100
C	-3.90077300	-1.40916600	-0.76234300
H	-2.04258200	-0.35925000	-0.93492200
C	-4.96119900	-1.78927200	0.07682600
H	-5.77436700	-1.63214800	2.08217100
H	-3.90048100	-1.76782600	-1.78737400
C	0.83366800	-0.83514300	-2.20052900
H	0.27334900	-0.70733200	-3.12155500

C	1.97169000	-0.09683000	-1.90051900
H	2.36419200	0.67098200	-2.56146200
C	0.66405900	-2.05680900	-1.30759900
C	0.68287400	-1.45457600	0.09086600
C	1.83716400	-0.75046800	0.41855000
C	2.82964300	-0.68561000	-0.77770700
H	-0.01888600	-1.78680400	0.84767700
H	-0.25957700	-2.60521400	-1.50474300
Rh	0.29410900	0.62429600	-0.64443300
C	1.89690500	-3.00957500	-1.44849900
C	3.17490200	-2.16767000	-1.15480000
H	3.84395000	-2.15570600	-2.02380800
H	3.72927300	-2.61855100	-0.32430100
C	4.10918200	0.12150400	-0.56271000
H	4.74493600	0.04479900	-1.45287100
H	3.89156300	1.18290400	-0.40588600
H	4.68347700	-0.24197200	0.29518800
C	1.92703000	-3.64756400	-2.84252100
H	2.81634400	-4.27054300	-2.98808600
H	1.03880400	-4.27053400	-2.99854300
H	1.94576800	-2.87020200	-3.61329500
O	1.66704100	-3.99470100	-0.42421600
C	2.55310300	-5.09503000	-0.37051300
H	3.60662500	-4.78751800	-0.29103700
H	2.28912100	-5.65718700	0.52964400
H	2.45043500	-5.76110900	-1.23876900
C	2.25002500	-0.54475800	1.83403400
C	2.82778200	0.64837800	2.30365500
C	2.08152600	-1.59905400	2.75143100
C	3.20442900	0.78829800	3.63886600
H	2.96603400	1.48020100	1.62159900
C	2.45698700	-1.45938800	4.08803500
H	1.67312100	-2.54139800	2.39841600
C	3.01832800	-0.26393200	4.53871000
H	3.64016400	1.72461000	3.97794900
H	2.31677600	-2.29005100	4.77506800
H	3.31277000	-0.15337000	5.57894300
O	-5.91300700	-2.58304400	-0.49034100
C	-6.99709000	-3.01488700	0.31623900
H	-7.58709700	-2.16648100	0.68768300
H	-7.62303900	-3.63368800	-0.32929500
H	-6.65178400	-3.61396900	1.16927700

**42-ts-L3-d**

C	0.21290000	4.30509700	-0.76556400
C	0.70084200	3.80341900	-1.90763900
C	0.04518800	2.66630500	-2.60327000
C	-0.98173500	1.93518900	-1.83847400
C	-1.44657700	2.39069700	-0.54724400
C	-1.03376000	3.79839800	-0.06850700
H	0.68092400	5.15913000	-0.27797800
H	1.56627200	4.23474700	-2.40516800
H	-1.65796700	1.33868100	-2.44948600
H	-2.48747900	2.15311400	-0.33967100
O	0.35885600	2.36487200	-3.75777900
O	-0.81170900	3.80496800	1.34491300
C	-2.19239500	4.78077200	-0.31121400
H	-3.07213000	4.45720000	0.25473400



H	-1.91005600	5.78046100	0.03473700	C	-6.11263500	-3.34902700	-0.68524900
H	-2.44354800	4.83456500	-1.37486500	H	-5.25865900	-3.98465600	-0.95467900
C	-0.10071300	2.62143100	1.72816100	H	-7.01318900	-3.96279100	-0.62397300
H	0.95369500	2.70401700	1.43498300	H	-6.24832900	-2.58161100	-1.45880500
H	-0.15241500	2.57617700	2.82092400				
C	-0.79831100	1.45194600	1.07286700	<b>43-L3</b>			
C	-1.72761800	0.78723300	1.81859900	C	3.97458700	-2.16311700	1.08140300
H	-1.76041300	1.04462900	2.88151500	C	3.17457000	-2.94195000	0.34345700
C	-2.75839900	-0.17012200	1.43387900	C	2.44466700	-2.44614600	-0.85497700
C	-3.73719800	-0.52676600	2.39188300	C	2.35404900	-0.99473700	-1.04347400
C	-2.88261900	-0.74659700	0.15528300	C	3.24248700	-0.05774200	-0.21374300
C	-4.77927300	-1.38704400	2.09000600	C	4.21256100	-0.68969400	0.83919600
H	-3.67304000	-0.10436600	3.39207400	H	4.52553900	-2.57508600	1.92672600
C	-3.93067700	-1.60887200	-0.16663500	H	3.07006800	-4.00536600	0.54823600
H	-2.12518600	-0.53315400	-0.59561300	H	2.29078100	-0.74051300	-2.10504500
C	-4.88975200	-1.93490500	0.80134200	H	3.82311800	0.62682900	-0.84244200
H	-5.52577500	-1.65261500	2.83211200	O	1.93303400	-3.26552600	-1.63054700
H	-3.98198100	-2.02895600	-1.16504400	O	3.92636100	0.01656100	2.07127600
C	0.56474300	-1.01156900	-2.11660800	C	5.68679500	-0.43443400	0.52493200
H	-0.11883200	-1.00151200	-2.96009900	H	5.86839400	0.64275000	0.44381500
C	1.69480000	-0.20562300	-2.05021700	H	6.32603100	-0.83266200	1.32030100
H	1.95637800	0.50326700	-2.83070000	H	5.96649000	-0.91644100	-0.41785400
C	0.57679700	-2.13958300	-1.09446900	C	2.52645300	0.27488600	2.08991600
C	0.75475500	-1.39680600	0.22261400	H	1.97300500	-0.62587000	2.39568100
C	1.90827800	-0.62463700	0.31519900	H	2.33474200	1.07079800	2.81517100
C	2.72497200	-0.64690200	-1.00816200	C	2.23090300	0.68842500	0.65632200
H	0.17926300	-1.67305800	1.09883000	C	1.33947100	1.68868500	0.31497900
H	-0.33729100	-2.73713300	-1.10691800	H	0.76179800	2.08270600	1.15058000
Rh	0.16470900	0.57769000	-0.65018900	C	1.20169600	2.51954800	-0.90000300
C	1.82452200	-3.05931800	-1.30785100	C	0.29399700	3.60155500	-0.83519200
C	3.08724600	-2.14678800	-1.28818000	C	1.90128100	2.35186700	-2.10822500
H	3.62113300	-2.19959300	-2.24468900	C	0.09664200	4.46229100	-1.90340500
H	3.77976700	-2.48979000	-0.51144200	H	-0.26235000	3.76671400	0.08458200
C	3.98267500	0.22013500	-1.05155800	C	1.71639800	3.21308100	-3.19069500
H	4.49371900	0.07667800	-2.01112300	H	2.60046600	1.53473000	-2.22846700
H	3.74144200	1.28444900	-0.96502300	C	0.80923600	4.27583800	-3.09747400
H	4.68457200	-0.03837800	-0.25263900	H	-0.60122500	5.29117100	-1.83746600
C	1.69488800	-3.84465600	-2.61857400	H	2.28185100	3.04122900	-4.09951900
H	2.58419800	-4.45106200	-2.82258400	C	-0.83334900	-1.60569800	-1.59959600
H	0.82404400	-4.50944200	-2.58318300	H	-0.29443400	-2.00181000	-2.45305900
H	1.57185100	-3.15517100	-3.46027900	C	-0.76257900	-2.19003000	-0.33774700
O	1.78458800	-3.93268200	-0.16412400	H	-0.16898200	-3.07964200	-0.15051700
C	2.72086000	-4.99136400	-0.12218400	C	-1.97489300	-0.60257800	-1.71531700
H	3.75940400	-4.64325000	-0.22644800	C	-1.69890500	0.36327900	-0.57045100
H	2.61067700	-5.45883500	0.86025000	C	-1.66144400	-0.20898800	0.69461600
H	2.53065700	-5.75184500	-0.89256100	C	-1.85581200	-1.75059300	0.63597600
C	2.50206900	-0.26561400	1.63191600	H	-1.78554600	1.43456100	-0.71651700
C	3.07240000	0.99059500	1.90384300	H	-2.00233400	-0.09667000	-2.68269400
C	2.52401800	-1.23464500	2.65236400	Rh	0.42332200	-0.33970700	-0.33410100
H	3.06288000	1.75839500	1.13769800	C	-3.34644600	-1.30444300	-1.43604200
C	3.07868900	-0.95320700	3.90140300	C	-3.24103800	-2.00971600	-0.04967500
H	2.12153900	-2.22181300	2.44492600	H	-3.37854800	-3.09311800	-0.15047900
C	3.63173200	0.30230000	4.15708100	H	-4.03309600	-1.64320800	0.61264100
H	4.05450100	2.25392000	3.33985200	C	-1.76714200	-2.49021700	1.97004400
H	3.08422300	-1.71969200	4.67218100	H	-1.96194000	-3.55824800	1.81533100
H	4.06530300	0.52326400	5.12877100	H	-0.77027100	-2.39809900	2.41329100
O	-5.94731300	-2.77080300	0.59954800	H	-2.49833700	-2.11457300	2.69290200
				C	-3.68340700	-2.28691400	-2.56403000

H	-4.60360000	-2.84536100	-2.35993800
H	-3.80534300	-1.75334200	-3.51366500
H	-2.87759400	-3.01914100	-2.67954700
O	-4.27585900	-0.20524100	-1.39758100
C	-5.65070400	-0.52279700	-1.30661100
H	-5.88031800	-1.16750800	-0.44486800
H	-6.17703900	0.42709200	-1.17751300
H	-6.03044700	-1.01026900	-2.21539400
C	-1.88837300	0.60167700	1.92238400
C	-1.11103700	0.46829100	3.08655500
C	-2.93343200	1.54420000	1.92991900
C	-1.36160400	1.25443100	4.21071000
H	-0.29243300	-0.24350100	3.10014000
C	-3.18320300	2.33281700	3.05437600
H	-3.56108300	1.63499000	1.04788700
C	-2.39770500	2.19212700	4.19921300
H	-0.74249600	1.13810700	5.09659900
H	-3.99719000	3.05308800	3.03612300
H	-2.59107000	2.80447300	5.07588000
O	0.55155900	5.17126100	-4.09226800
C	1.24735400	5.03132600	-5.32067100
H	0.89160300	5.84108400	-5.96030600
H	2.33244200	5.12810000	-5.18304600
H	1.02960600	4.06788600	-5.80041500

**60-L3**

C	1.77635100	-3.61791400	-1.47746900
C	1.05327400	-4.19823200	-0.50913300
C	1.05813800	-3.68308200	0.87985200
C	1.71114100	-2.36614300	1.09631500
C	2.45288900	-1.75934800	0.08625100
C	2.71807300	-2.45646300	-1.24412700
H	1.77605500	-4.00801900	-2.49395700
H	0.44975600	-5.08485300	-0.68645700
H	1.84207100	-2.07734000	2.13703600
H	3.17319800	-0.99105300	0.34935500
O	0.54371100	-4.31434000	1.80229800
O	2.72158100	-1.57352900	-2.36563600
C	4.16315300	-3.01144100	-1.20973700
H	4.86542000	-2.18263400	-1.07543100
H	4.38925700	-3.50219900	-2.16164500
H	4.28900200	-3.73215200	-0.39652000
C	1.60925500	-0.66089000	-2.46310600
H	0.69123200	-1.22115100	-2.69086100
H	1.86000400	-0.03824300	-3.33069600
C	1.49803800	0.15437300	-1.19827400
C	2.23458700	1.28372200	-1.11301200
H	2.69290700	1.63737200	-2.04300900
C	2.60994700	2.09165000	0.05269400
C	3.35002700	3.27811200	-0.14460100
C	2.32603900	1.74233000	1.38497200
C	3.76881700	4.06961600	0.91477200
H	3.59719900	3.58012000	-1.15984800
C	2.74202800	2.52504300	2.46485600
H	1.74825800	0.84008300	1.58205000
C	3.46867100	3.69989800	2.23452100
H	4.33541400	4.98079700	0.74796800
H	2.49752200	2.20895200	3.47328200

C	-1.31573300	-0.84293900	1.87842600
H	-0.90365500	-0.94287400	2.87887000
C	-1.52578800	-1.91159300	1.04407000
H	-1.29320200	-2.93300100	1.31748400
C	-1.98425400	0.45733400	1.43606100
C	-1.39357900	0.71408800	0.02119000
C	-1.53846000	-0.41271000	-0.80263500
H	-1.44136500	-0.32845200	-1.87970200
C	-2.32786600	-1.56003700	-0.19456000
H	-2.43537600	-2.40080700	-0.88286700
Rh	0.35550200	-0.76491100	0.24348000
C	-3.50951100	0.15453100	1.22526300
C	-3.73720400	-1.01600900	0.22096700
H	-3.95661600	-0.07386100	2.20033100
H	-3.99383200	1.06313600	0.85094500
C	-1.79135700	1.57261200	2.46264500
H	-0.72954100	1.75951000	2.65385500
H	-2.24671900	2.51067600	2.13251400
H	-2.25844300	1.28467600	3.41249200
C	-4.58945400	-2.14051800	0.82130000
H	-5.55541600	-1.77174100	1.18306400
H	-4.77451400	-2.92209200	0.07563400
H	-4.07334200	-2.59193700	1.67500900
O	-4.28565000	-0.54883300	-1.02521600
C	-5.63290600	-0.11601300	-1.02003800
H	-5.82177900	0.66906300	-0.27306200
H	-5.82488300	0.29856400	-2.01334700
H	-6.33674900	-0.94118400	-0.84441400
C	-1.34719700	2.08494900	-0.56671700
C	-0.57674500	3.13522600	-0.04181500
C	-2.17051100	2.36146100	-1.67583700
C	-0.60982200	4.40529400	-0.61610600
H	0.07928800	2.95186000	0.79895200
C	-2.20450500	3.63271200	-2.24988500
H	-2.81129200	1.57533100	-2.06351200
C	-1.42080100	4.66043600	-1.72397900
H	0.01183800	5.19370400	-0.20036700
H	-2.85034200	3.81932400	-3.10428200
H	-1.44388100	5.65144000	-2.16984500
O	3.92477200	4.54210900	3.20989400
C	3.65420900	4.21015300	4.56015300
H	4.10331200	5.00335700	5.16115800
H	2.57451500	4.17278500	4.75999900
H	4.10320500	3.24711700	4.83886400

**61-ts-L3**

C	0.70036900	-4.14713400	0.22616900
C	1.59823400	-3.60293300	-0.60375800
C	1.22254800	-2.51929800	-1.54882600
C	-0.06105100	-1.84287300	-1.29179800
C	-1.04949900	-2.39103200	-0.38277100
C	-0.76375000	-3.76211700	0.27831000
H	0.96895300	-4.96220300	0.89681500
H	2.62284500	-3.95999400	-0.66508200
H	-0.42884500	-1.28316700	-2.15167600
H	-2.07355100	-2.29323300	-0.73728400
O	1.94656300	-2.22992900	-2.49950900
O	-1.18939100	-3.76805200	1.64888000

C	-1.60168600	-4.84678400	-0.41925200	H	6.65853600	-1.24802600	-2.05198800
H	-2.66625600	-4.61053000	-0.31871900	O	-6.16605700	1.91743400	-1.91470800
H	-1.41884800	-5.81819100	0.05180100	C	-7.53641400	2.08772900	-1.58993800
H	-1.34364000	-4.91746600	-1.48036300	H	-7.96791300	2.66861300	-2.40710500
C	-0.91894800	-2.49916100	2.24826500	H	-8.05650900	1.12346500	-1.51665600
H	0.15685900	-2.39531600	2.45588200	H	-7.66287600	2.63784800	-0.64798600
H	-1.46152000	-2.48929700	3.19998500				
C	-1.42499600	-1.44812700	1.28668400	<b>61-ts-L3-b</b>			
C	-2.69559600	-0.98774600	1.47501000	C	-0.61027300	-4.16914900	-0.12276000
H	-3.18534300	-1.29471400	2.40377100	C	-1.49102000	-3.61293700	0.71757600
C	-3.55966900	-0.20496200	0.60022400	C	-1.10346000	-2.49613500	1.61789900
C	-4.91598300	-0.05297200	0.94977800	C	0.16239500	-1.81052000	1.30243300
C	-3.14114400	0.39717900	-0.61006200	C	1.13219800	-2.37362600	0.38295900
C	-5.81904600	0.64189200	0.14837400	C	0.84610000	-3.76656800	-0.22966800
H	-5.27434800	-0.50180400	1.87357000	H	-0.88686600	-5.00765300	-0.76043900
C	-4.02957000	1.08580300	-1.42142200	H	-2.50795200	-3.98225400	0.82026300
H	-2.09335900	0.34100700	-0.89480400	H	0.54580400	-1.22016000	2.13450000
C	-5.37850800	1.21519100	-1.05226600	H	2.16468400	-2.25072000	0.70383700
H	-6.85282200	0.72833800	0.46314700	O	-1.80272000	-2.18728600	2.58089800
H	-3.70126700	1.54771300	-2.34773500	O	1.23272600	-3.80843900	-1.61104900
C	0.64528200	1.01919600	1.97215800	C	1.71844000	-4.81940700	0.47485100
H	0.42014600	0.61673900	2.95586600	H	2.77633700	-4.57245900	0.33680900
C	-0.30381200	1.62168400	1.16423500	H	1.53572700	-5.80646800	0.03755500
H	-1.34724000	1.72646500	1.44047800	H	1.49150600	-4.86222700	1.54454700
C	2.08993700	1.27730500	1.54777000	C	0.93605500	-2.56078900	-2.24212200
C	2.12442600	0.74262300	0.08682900	H	-0.14479000	-2.47384300	-2.43069200
C	1.13895100	1.33389200	-0.70526300	H	1.45835200	-2.57478000	-3.20509400
H	1.17513100	1.27827700	-1.78802700	C	1.45241000	-1.47574500	-1.32494400
C	0.30020100	2.39255000	-0.00018000	C	2.71276900	-1.00693600	-1.55608300
H	-0.45720900	2.82596200	-0.65694100	H	3.18410300	-1.33442400	-2.48725800
Rh	0.13123500	-0.37604200	0.27322500	C	3.58838000	-0.19296100	-0.72223300
C	2.30239700	2.82879200	1.46338300	C	4.94074700	-0.03739800	-1.11028800
C	1.26348900	3.50964600	0.52250200	C	3.19506900	0.43341400	0.47644300
H	2.24166000	3.24145000	2.47786000	C	5.84342400	0.68266700	-0.34664700
H	3.31593800	3.02201500	1.09480700	H	5.28125100	-0.50573500	-2.03103300
C	3.08950500	0.65713400	2.52348100	C	4.09470000	1.15621900	1.26022700
H	2.90552900	-0.41300900	2.66293900	H	2.15439100	0.37533900	0.78653400
H	4.12184100	0.78182000	2.18352800	C	5.42912000	1.28523000	0.85305100
H	2.99414700	1.14068000	3.50348100	H	6.87916800	0.79454000	-0.65198000
C	0.47079600	4.61488700	1.23109000	H	3.74304600	1.62305300	2.17364100
H	1.12719200	5.37824600	1.66329800	C	-0.66259200	0.94362700	-2.02874300
H	-0.21457600	5.10459000	0.52987100	H	-0.45716500	0.51337500	-3.00491600
H	-0.11730700	4.19054600	2.05148600	C	0.29862000	1.58118800	-1.26330000
O	1.88075500	3.99631200	-0.68304700	H	1.33379100	1.68979100	-1.56795000
C	2.72753500	5.12320700	-0.57004400	C	-2.09937600	1.19531400	-1.57472300
H	3.52958500	4.97798300	0.16904100	C	-2.08923500	0.70564600	-0.09753400
H	3.18541300	5.26165100	-1.55333700	C	-1.09221200	1.33322900	0.65077200
H	2.17688400	6.03826700	-0.31052100	H	-1.10127200	1.31104100	1.73534300
C	3.35626700	0.14578900	-0.49868800	C	-0.28656800	2.38007500	-0.10820900
C	3.93019100	-1.04568500	-0.02476300	H	0.48124600	2.84363700	0.51514100
C	4.00741400	0.82621700	-1.54268900	Rh	-0.08881600	-0.39496500	-0.30125000
C	5.10801700	-1.54227300	-0.57946500	C	-2.33214700	2.74528400	-1.53089300
H	3.43189200	-1.60363000	0.76126100	C	-1.27728900	3.46824800	-0.64042200
C	5.18623700	0.32865900	-2.09883000	H	-2.30603600	3.12805000	-2.55843100
H	3.58885400	1.76272700	-1.89996300	H	-3.33772800	2.93540200	-1.13951800
C	5.74158100	-0.85743800	-1.61875600	C	-3.11403700	0.52953900	-2.50329000
H	5.52860000	-2.47214500	-0.20496900	H	-2.91742700	-0.54217200	-2.61002500
H	5.67063000	0.87105300	-2.90672100	H	-4.13910500	0.65155500	-2.14120900

H	-3.05032100	0.98021100	-3.50133600
C	-0.51810000	4.55915200	-1.40573300
H	-1.19588600	5.29938100	-1.84506100
H	0.17890300	5.08043700	-0.73962400
H	0.05375900	4.11537100	-2.22731400
O	-1.86806700	3.98663200	0.56529100
C	-2.73233000	5.09879200	0.43886700
H	-3.55264000	4.91911500	-0.27202500
H	-3.16454300	5.26463000	1.42951400
H	-2.20104700	6.01115700	0.13347600
C	-3.29840600	0.11204300	0.53640300
C	-3.86099300	-1.10532100	0.11872200
C	-3.93999000	0.82108400	1.56708400
C	-5.01925500	-1.59974000	0.71491200
H	-3.36747600	-1.68261400	-0.65627800
C	-5.09958700	0.32605000	2.16444900
H	-3.52968400	1.77673800	1.88075400
C	-5.64401900	-0.88615200	1.74020000
H	-5.43141100	-2.54965100	0.38392400
H	-5.57756700	0.89057200	2.96093000
H	-6.54578800	-1.27464700	2.20593700
O	6.38828400	1.97376900	1.53333500
C	6.03191600	2.59200300	2.75971100
H	6.94180800	3.06692900	3.13107600
H	5.25689300	3.35657900	2.61611500
H	5.68014700	1.85637700	3.49493800

**61-ts-L3-c**

C	-0.48226100	4.26011600	1.19877800
C	-1.17299600	4.27819700	0.05197800
C	-0.67960600	3.59223600	-1.16932100
C	0.44003800	2.64891300	-0.98890500
C	1.15946400	2.56263800	0.25877100
C	0.85996800	3.58245200	1.37594400
H	-0.83959600	4.78598300	2.08284600
H	-2.10262700	4.83229200	-0.05393200
H	0.97189600	2.40360800	-1.90739700
H	2.21778300	2.34267500	0.14658100
O	-1.19718900	3.81061100	-2.26698400
O	0.90521800	2.96043200	2.66667000
C	1.96835500	4.65030200	1.39834000
H	2.93376000	4.17315800	1.59655000
H	1.77165500	5.37296200	2.19695600
H	2.01587500	5.18478900	0.44460800
C	0.31409200	1.65508900	2.62548100
H	-0.78206200	1.73533000	2.60282200
H	0.61035000	1.16471400	3.55946100
C	0.87225500	0.95523700	1.40921400
C	1.98352800	0.18368300	1.57876700
H	2.27244700	-0.03291800	2.61119800
C	2.93603300	-0.31410200	0.59294300
C	4.18354300	-0.79164800	1.03838800
C	2.71799700	-0.31001800	-0.80513200
C	5.17555100	-1.22018000	0.15833900
H	4.38684700	-0.81419500	2.10657400
C	3.69742500	-0.72739700	-1.69416200
H	1.74664300	-0.00123200	-1.18894500
C	4.93909700	-1.18370000	-1.22229400

H	6.12083600	-1.57342600	0.55444800
H	3.52125400	-0.72494500	-2.76569900
C	-1.59969900	-0.01469200	-1.96711100
H	-1.14346000	0.17902100	-2.93448900
C	-2.41008000	0.90908300	-1.32234300
H	-2.62616500	1.89056500	-1.72985900
C	-1.72014600	-1.44570000	-1.44016300
C	-1.36047700	-1.30112900	0.06545800
C	-2.13895700	-0.32881700	0.68619800
H	-2.19051400	-0.25302600	1.76735900
C	-3.21422900	0.29998700	-0.18564100
H	-3.80965400	1.03759500	0.35668900
Rh	-0.46205700	0.83313200	-0.25560900
C	-3.23377600	-1.85199400	-1.49965400
C	-4.13607700	-0.84712600	-0.72155600
H	-3.53525200	-1.91461100	-2.55234700
H	-3.34281200	-2.85412000	-1.07040000
C	-0.86750900	-2.42565900	-2.24513400
H	0.18235600	-2.11548900	-2.27384300
H	-0.91077600	-3.43746900	-1.83049600
H	-1.23028600	-2.46757000	-3.27939500
C	-5.25594900	-0.27208800	-1.59651400
H	-5.87691900	-1.06076500	-2.03532900
H	-5.90169400	0.38987500	-1.00823800
H	-4.82993800	0.30544500	-2.42341500
O	-4.66026000	-1.43437100	0.48518000
C	-5.65564900	-2.42919400	0.34505200
H	-5.33816900	-3.25816800	-0.30505600
H	-5.83444800	-2.82671700	1.34798900
H	-6.60125900	-2.02558200	-0.04294200
C	-0.72671900	-2.39600100	0.85254800
C	0.56162400	-2.89478100	0.59675700
C	-1.47150100	-2.99175600	1.88895600
C	1.08961900	-3.93810000	1.35655600
H	1.16768100	-2.44697600	-0.18124700
C	-0.94274000	-4.03493100	2.64987400
H	-2.48418900	-2.64421900	2.07166600
C	0.34228600	-4.51198400	2.38753300
H	2.09405200	-4.29612600	1.14607100
H	-1.53978100	-4.47885300	3.44256400
H	0.75696700	-5.32488400	2.97798300
O	5.83022300	-1.57688400	-2.17614800
C	7.09740800	-2.05707700	-1.75664500
H	7.63944200	-2.30959100	-2.66977400
H	7.65645200	-1.29074800	-1.20340000
H	7.00246000	-2.95477900	-1.13131800

**61-ts-L3-d**

C	-0.22721600	4.29405300	1.14761300
C	-0.87709300	4.32872800	-0.02262500
C	-0.38601400	3.58705000	-1.21183400
C	0.66695800	2.58141500	-0.97241100
C	1.33835500	2.48028200	0.30019000
C	1.06496800	3.54131900	1.38473500
H	-0.58094800	4.86002600	2.00802800
H	-1.76698900	4.93565600	-0.17156900
H	1.21287600	2.28293500	-1.86674900
H	2.38376900	2.19158800	0.22935300

O	-0.85278800	3.80984500	-2.33121300	H	1.82772900	-4.40411700	1.33704700
O	1.03062700	2.94767100	2.68886800	H	-1.91469900	-4.37746700	3.46003400
C	2.23453900	4.54141900	1.42260300	H	0.35108600	-5.34973600	3.10521600
H	3.16229200	4.01203400	1.66332900	O	5.95670700	-2.04245100	-1.69850100
H	2.05597000	5.29229700	2.19915900	C	5.84972800	-2.01108400	-3.11276300
H	2.34488800	5.05051100	0.46023800	H	6.77412700	-2.44964200	-3.49296100
C	0.36053500	1.68071600	2.65553200	H	4.99555300	-2.60368000	-3.46665000
H	-0.72658900	1.82948100	2.59040700	H	5.75433200	-0.98330100	-3.48711800
H	0.59202000	1.19646700	3.61072400				
C	0.91588400	0.91758500	1.47662500	<b>24-L4</b>			
C	1.97232800	0.08577700	1.70154600	C	2.41521500	-1.91845400	-1.02844300
H	2.21023400	-0.12546900	2.74794100	C	2.76930200	-2.21616400	0.30479900
C	2.92657900	-0.49084500	0.76147100	C	3.37500100	-0.88893300	-1.64963100
C	4.12048900	-1.05654100	1.26770800	C	3.22423900	0.27941700	-0.68331400
C	2.77105600	-0.48691400	-0.63827400	C	3.60262500	-0.02497000	0.64134200
C	5.10365000	-1.56155500	0.43298200	C	4.02464400	-1.49794700	0.78297000
H	4.27475000	-1.08354500	2.34387800	H	4.26774100	-1.74795100	1.81791700
C	3.75571300	-0.98460100	-1.49308200	Rh	1.48875500	-0.48459900	0.33414800
H	1.84237100	-0.11332100	-1.06712900	C	4.82718900	-1.44411300	-1.62416900
C	4.93446700	-1.52346200	-0.96100000	C	5.22329100	-1.79276100	-0.16269600
H	6.01818400	-1.98907700	0.83234200	H	4.88626600	-2.32784400	-2.27040500
H	3.58679000	-0.96137800	-2.56398200	H	5.50515200	-0.69256600	-2.04563700
C	-1.49692500	0.03805400	-1.96743200	H	3.07499000	-0.61901400	-2.66432800
H	-1.00109300	0.18987400	-2.92279100	H	5.49863200	-2.85014900	-0.07236900
C	-2.27044800	1.01774300	-1.36024200	H	6.09109000	-1.20649100	0.16156800
H	-2.41484900	2.00380900	-1.78788200	C	1.54932100	-2.76242400	-1.88982500
C	-1.72151700	-1.37580500	-1.42777300	C	0.81095700	-2.19423600	-2.94405600
C	-1.40528400	-1.23295000	0.08726000	C	1.46361600	-4.15174200	-1.69857900
C	-2.14287800	-0.20797400	0.67025500	C	0.00932600	-2.98309400	-3.76665800
H	-2.22439700	-0.11493800	1.74823600	H	0.84993200	-1.11957500	-3.09918100
C	-3.14748700	0.47326500	-0.24517900	C	0.66097100	-4.94328800	-2.52135600
H	-3.71612600	1.25186700	0.26777200	H	2.04377800	-4.61712200	-0.90705300
Rh	-0.36666100	0.84251400	-0.23192100	C	-0.07086700	-4.36319600	-3.55837300
C	-3.25425800	-1.69041500	-1.53621200	H	-0.55648000	-2.52035900	-4.57136900
C	-4.11916700	-0.62069200	-0.80274600	H	0.61437600	-6.01647700	-2.35489200
H	-3.52236600	-1.74902100	-2.59813200	H	-0.69400300	-4.97902000	-4.20131500
H	-3.44009200	-2.67795700	-1.09950100	C	3.98439000	0.97219800	1.67248400
C	-0.90028800	-2.41556700	-2.18886800	C	3.77523300	0.71017000	3.03868200
H	0.16621100	-2.16702200	-2.17933500	C	4.59347100	2.18787300	1.31713200
H	-1.01822400	-3.41721200	-1.76427000	C	4.15305500	1.63299600	4.01126900
H	-1.22567800	-2.45022500	-3.23577100	H	3.28536900	-0.21362400	3.33372600
C	-5.16486200	0.01552000	-1.72654700	C	4.97396900	3.11249000	2.29135300
H	-5.81932800	-0.73466500	-2.18390500	H	4.78416700	2.40153600	0.26919800
H	-5.78802300	0.72512700	-1.17023100	C	4.75485200	2.83953300	3.64210800
H	-4.67007400	0.55484400	-2.54095900	H	3.97225600	1.41307700	5.06022000
O	-4.72505100	-1.15780200	0.38821400	H	5.44767700	4.04413800	1.99254600
C	-5.77689700	-2.08775000	0.21850300	H	5.05147500	3.55817100	4.40140000
H	-5.48715900	-2.94531600	-0.40702800	H	3.13377300	1.29942300	-1.04659300
H	-6.02333500	-2.45724300	1.21777300	H	2.38703400	-3.08491100	0.83371000
H	-6.67668600	-1.62926500	-0.21479700	O	0.39802800	1.21309000	0.88144800
C	-0.86826200	-2.35507800	0.90671000	C	0.83964100	2.53563000	0.69456900
C	0.40112100	-2.92441600	0.71219400	H	0.92438200	2.80901300	-0.36752900
C	-1.69255600	-2.90297600	1.90855100	H	0.13671100	3.23654800	1.16861300
C	0.83540100	-3.99116900	1.49844800	H	1.81986800	2.67378500	1.16960500
H	1.06556600	-2.51231400	-0.03741100	C	-2.41567400	1.91913400	-1.02687600
C	-1.25811300	-3.97047900	2.69510000	C	-2.76941600	2.21567600	0.30669000
H	-2.69149000	-2.49825800	2.04337000	C	-3.37538500	0.88978600	-1.64846700
C	0.00969400	-4.51825300	2.49410200	C	-3.22399700	-0.27919700	-0.68300100

C	-3.60210000	0.02411300	0.64201200
C	-4.02442900	1.49690200	0.78476200
H	-4.26727500	1.74614500	1.81995500
Rh	-1.48836200	0.48451000	0.33437600
C	-4.82773500	1.44448400	-1.62215100
C	-5.22345800	1.79203000	-0.16031800
H	-4.88732300	2.32861400	-2.26778200
H	-5.50560800	0.69299500	-2.04388100
H	-3.07566300	0.62058200	-2.66343600
H	-5.49908100	2.84927000	-0.06917100
H	-6.09097700	1.20528100	0.16384900
C	-1.55029800	2.76403200	-1.88781900
C	-0.81290200	2.19711000	-2.94339300
C	-1.46403700	4.15305200	-1.69472200
C	-0.01169600	2.98686900	-3.76553900
H	-0.85230100	1.12268600	-3.10001800
C	-0.66183300	4.94551000	-2.51702700
H	-2.04347900	4.61752600	-0.90215200
C	0.06903800	4.36665800	-3.55542300
H	0.55335500	2.52508400	-4.57132500
H	-0.61483100	6.01846100	-2.34914300
H	0.69182400	4.98320800	-4.19801000
C	-3.98366800	-0.97382100	1.67250500
C	-3.77431900	-0.71275800	3.03886900
C	-4.59283600	-2.18926200	1.31639400
C	-4.15203800	-1.63624900	4.01086300
H	-3.28440200	0.21082500	3.33448400
C	-4.97322400	-3.11454400	2.29004200
H	-4.78367700	-2.40218400	0.26832600
C	-4.75391800	-2.84251200	3.64095600
H	-3.97109700	-1.41705500	5.05993900
H	-5.44699300	-4.04597500	1.99064800
H	-5.05045500	-3.56167000	4.39978900
H	-3.13351900	-1.29895000	-1.04703700
H	-2.38715800	3.08405600	0.83620000
O	-0.39748100	-1.21293700	0.88166400
C	-0.83877700	-2.53560800	0.69422700
H	-0.91951900	-2.80973700	-0.36796500
H	-0.13771100	-3.23619500	1.17156400
H	-1.82078100	-2.67310300	1.16573300

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C	1.56746600	0.67595600	0.09345800
C	0.78877700	0.73696900	1.26439000
C	0.88004400	1.40127100	-1.07312600
C	-0.42500000	0.61417200	-1.14593400
C	-1.22672000	0.70675100	0.03620600
C	-0.50521900	1.52722900	1.11643200
H	-1.07080200	1.55454100	2.04994700
Rh	0.09630000	-0.98352200	0.10906400
C	0.60480200	2.88847500	-0.71830100
C	-0.22462600	2.96423500	0.59343700
H	1.55849200	3.41803400	-0.61102800
H	0.06823100	3.36169100	-1.54919200
H	1.44080700	1.30650700	-2.00459800
H	0.31472600	3.52325800	1.36651400
H	-1.17740500	3.48092600	0.42875400
C	2.98639300	0.25227100	0.06284400

C	3.87623200	0.73287400	-0.91406300
C	3.49545300	-0.63949000	1.02961800
C	5.21592500	0.34262000	-0.92417600
H	3.52760800	1.43151000	-1.66816900
C	4.83097700	-1.03151400	1.01693800
H	2.83075600	-1.04125100	1.78980100
C	5.70127100	-0.54222500	0.03864600
H	5.88115900	0.73438800	-1.68928700
H	5.19281000	-1.72592800	1.77070800
H	6.74320600	-0.84977800	0.02735700
C	-2.69283000	0.49110300	0.07773000
C	-3.33618100	0.14904400	1.28178600
C	-3.48473200	0.64268800	-1.07377800
C	-4.71533200	-0.03812300	1.33059800
H	-2.74423600	0.00366300	2.18094900
C	-4.86704900	0.45827000	-1.02493900
H	-3.01748700	0.92699200	-2.01183700
C	-5.48875100	0.11708700	0.17663400
H	-5.18784300	-0.31022400	2.27066500
H	-5.45792300	0.58714000	-1.92798100
H	-6.56506500	-0.02653300	0.21542200
H	-0.84486700	0.32830300	-2.10681400
H	1.19837800	0.53108600	2.24958400
O	-0.77723300	-2.63335100	-0.38372300
C	-1.96387100	-2.92300400	-1.05723000
H	-1.88686000	-2.73322900	-2.14261100
H	-2.20174600	-3.99095400	-0.92838600
H	-2.81975300	-2.34481400	-0.67093500

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C	0.72120100	1.77572200	-0.03661700
C	0.26126400	1.25644300	1.18657400
C	-0.34898400	2.64705600	-0.71455500
C	-1.51140200	1.66892000	-0.83035000
C	-1.97949500	1.18478700	0.41466600
C	-1.13509100	1.72731200	1.57770600
H	-1.45292000	1.31153600	2.53582600
Rh	-0.39506000	-0.09680500	-0.36891700
C	-0.72040500	3.83293200	0.22103900
C	-1.20469000	3.28208300	1.58934100
H	0.15556300	4.48018500	0.34278300
H	-1.50050900	4.43454200	-0.25946600
H	-0.01900700	3.00356500	-1.69190000
H	-0.58143900	3.65927400	2.40821200
H	-2.23433300	3.59369200	1.79941700
C	2.14291100	1.86173900	-0.45157100
C	3.16400200	1.99921600	0.50291900
C	2.49935500	1.84277800	-1.81179500
C	4.49940000	2.10347500	0.11310400
H	2.90849400	2.03676500	1.55776800
C	3.83325700	1.94164100	-2.20120300
H	1.72901200	1.71286200	-2.56653000
C	4.83965500	2.07285100	-1.24026100
H	5.27314200	2.21191000	0.86857400
H	4.08830800	1.91060900	-3.25710200
H	5.87959100	2.15353800	-1.54512600
C	-3.31723500	0.58719600	0.64447000
C	-3.52310500	-0.33723000	1.68450500

C	-4.41858100	0.94399600	-0.15297700
C	-4.77957200	-0.89401700	1.90974100
H	-2.68190700	-0.64218800	2.30062400
C	-5.67851000	0.38850000	0.07421800
H	-4.29096200	1.67741600	-0.94389500
C	-5.86387800	-0.53410400	1.10458100
H	-4.91238900	-1.61543000	2.71149900
H	-6.51644400	0.68291500	-0.55216300
H	-6.84423800	-0.96783300	1.28136400
H	-2.10335500	1.61102300	-1.73957400
H	0.92371300	0.79468500	1.91283100
O	-1.32694100	-1.64387400	-1.41133200
C	-2.36480800	-1.52650700	-2.36830800
H	-2.01121000	-1.01521700	-3.27400100
H	-2.71165000	-2.53118300	-2.63490300
H	-3.19566400	-0.96585700	-1.92954500
C	0.58449500	-2.32339900	0.77807400
C	1.48688600	-2.25040100	1.85112100
C	2.81585900	-1.89777900	1.59966300
C	3.22889700	-1.61451600	0.28326000
C	2.32012000	-1.68344800	-0.75887900
C	0.96147900	-2.05116300	-0.56094400
H	-0.42426900	-2.67922700	0.97349100
H	1.14989300	-2.49193400	2.85357800
H	4.26517800	-1.33566900	0.11837200
H	2.64604200	-1.46818400	-1.77206900
B	-0.04674500	-2.42042800	-1.82060300
O	-0.46693200	-3.80497600	-1.90176000
H	0.30118200	-4.34899000	-2.12526000
O	0.52307200	-1.89493600	-3.04732100
H	0.15359500	-2.40568100	-3.78190400
O	3.78718800	-1.80089600	2.55384900
C	3.44626400	-2.10965100	3.89464400
H	4.36112600	-1.97762700	4.47569000
H	2.67120000	-1.43397200	4.28160900
H	3.09885300	-3.14631500	3.99561600

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C	-0.22001500	1.92767600	-0.17333400
C	0.14856900	1.22039600	-1.33849200
C	0.97946900	2.68695700	0.42041300
C	1.99666800	1.57725900	0.64190000
C	2.36709700	0.90021500	-0.52312000
C	1.60321900	1.42543800	-1.75050800
H	1.85350400	0.86583100	-2.65385800
Rh	0.53567700	-0.06190200	0.32727700
C	1.51472500	3.70187100	-0.63283400
C	1.90413000	2.94256000	-1.92997800
H	0.74200700	4.45346500	-0.83139300
H	2.37794100	4.23061500	-0.21244000
H	0.71876500	3.19121400	1.35271100
H	1.33876500	3.31810800	-2.79059100
H	2.96750200	3.07451300	-2.16139300
C	-1.60343900	2.32468200	0.18813500
C	-2.58872700	2.50624400	-0.79658000
C	-1.95481800	2.56671100	1.52866800
C	-3.88087700	2.90612500	-0.45488100
H	-2.33546600	2.34700700	-1.84045700

C	-3.24533800	2.96521300	1.87135200
H	-1.21648400	2.41062700	2.31010100
C	-4.21575100	3.13739000	0.88028800
H	-4.62404500	3.04566400	-1.23591400
H	-3.49520500	3.13861900	2.91490900
H	-5.22092400	3.45317400	1.14689500
C	3.55926000	0.02778300	-0.65575300
C	3.58525400	-1.02106800	-1.59294000
C	4.69903900	0.22937100	0.14307500
C	4.70251000	-1.84397700	-1.71763300
H	2.70909400	-1.20867200	-2.20704100
C	5.81826600	-0.59456300	0.01842800
H	4.71504600	1.05252500	0.85181000
C	5.82479200	-1.63546700	-0.91153100
H	4.69504400	-2.65418800	-2.44190600
H	6.68952200	-0.41584700	0.64331800
H	6.69666700	-2.27632100	-1.01044300
H	2.55052000	1.50196000	1.57331400
H	-0.58257100	0.84352400	-2.04777300
O	1.10182600	-1.70738200	1.54538600
C	2.08638000	-1.66287500	2.57823800
H	1.76044000	-1.02006400	3.40198400
H	2.25769000	-2.67897700	2.95161300
H	3.01163800	-1.27996700	2.14125500
C	-1.11100500	-2.22877000	-0.91376200
C	-2.21442600	-2.64395800	-1.64697900
C	-3.49827400	-2.19646100	-1.29042300
C	-3.65223400	-1.33828700	-0.19453600
C	-2.52059000	-0.92329600	0.51525900
C	-1.21605500	-1.34500700	0.19440000
H	-0.13377600	-2.62009600	-1.18836300
H	-2.11902900	-3.32131100	-2.49126400
H	-4.63290200	-0.98403600	0.10498800
H	-2.66249400	-0.25819100	1.36248400
B	-0.26690200	-2.07201100	1.88623800
O	-0.49441000	-3.45764700	1.78904600
H	-1.43116300	-3.65374200	1.65478800
O	-0.78324700	-1.34540400	2.98119600
H	-1.40208000	-1.89978100	3.47531200
O	-4.52307300	-2.66340500	-2.06294500
C	-5.83995500	-2.23274900	-1.76437200
H	-6.48728700	-2.71247000	-2.50134800
H	-6.14911800	-2.54099600	-0.75651500
H	-5.93859300	-1.14231200	-1.84988800

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C	-0.37185600	2.03624500	-0.04069200
C	0.12591900	1.49155200	-1.25501500
C	0.75219100	2.73604700	0.74530600
C	1.82388900	1.66630800	0.89310100
C	2.31123200	1.16822800	-0.29865100
C	1.59966000	1.79543400	-1.50759500
H	1.94887400	1.36956400	-2.45049600
Rh	0.31821100	0.01490200	0.23359600
C	1.30736800	3.90583000	-0.12484600
C	1.82831000	3.33862200	-1.47330900
H	0.50951900	4.63972000	-0.28610500
H	2.10856600	4.41404000	0.42392000

H	0.40386100	3.09997800	1.71395900
H	1.30238200	3.79361200	-2.32059700
H	2.89544300	3.55053400	-1.60653500
C	-1.78706900	2.41709100	0.20809700
C	-2.65041700	2.74968000	-0.84861100
C	-2.28993500	2.49399100	1.51907500
C	-3.97077700	3.13053800	-0.60658100
H	-2.28046600	2.72292100	-1.86934600
C	-3.60707200	2.87479100	1.76310000
H	-1.64665100	2.22578500	2.35273900
C	-4.45594700	3.19423000	0.69992400
H	-4.61851400	3.38372300	-1.44209600
H	-3.97490700	2.91623000	2.78512900
H	-5.48387100	3.49129800	0.88976600
C	3.52738700	0.33494900	-0.44394600
C	3.64193800	-0.60528700	-1.48466900
C	4.60761700	0.46883300	0.44770100
C	4.78504300	-1.39158400	-1.61791500
H	2.81507200	-0.73814400	-2.17631800
C	5.75141500	-0.31883900	0.31447800
H	4.55743000	1.21552800	1.23531100
C	5.84511900	-1.25371700	-0.71813000
H	4.84623800	-2.11702500	-2.42488600
H	6.57539200	-0.19255200	1.01209700
H	6.73716400	-1.86483500	-0.82468500
H	2.28824700	1.46672900	1.85454600
H	-0.52944200	1.25979900	-2.09023000
O	1.14355400	-1.86320900	1.29355800
C	1.93895300	-1.67367500	2.47551800
H	1.39332200	-0.99098400	3.13003300
H	2.09517500	-2.63012400	2.97851000
H	2.90711000	-1.24038800	2.20835400
C	-2.14131200	-1.08721900	-1.25702000
C	-3.36190900	-1.76978400	-1.37780900
C	-3.95275500	-2.33289100	-0.24434200
C	-3.30459600	-2.21816400	0.99418100
C	-2.08597500	-1.55359700	1.08586000
C	-1.46031300	-0.95468700	-0.03405100
H	-1.72093700	-0.65393800	-2.16283200
H	-3.83376700	-1.84705900	-2.35194700
H	-3.77397300	-2.66399400	1.86718700
H	-1.60634700	-1.50025700	2.06172700
B	1.28835000	-3.03441500	0.54732000
O	0.52816200	-3.25025200	-0.55422400
H	-0.16809700	-2.56920600	-0.66189000
O	2.21762400	-3.95071800	0.96122900
H	2.19689900	-4.72476300	0.38030000
O	-5.14298200	-3.01380000	-0.23486000
C	-5.83549000	-3.15596400	-1.46000600
H	-5.24391400	-3.71273900	-2.20030800
H	-6.74364200	-3.71809300	-1.23113000
H	-6.11198600	-2.18181900	-1.88712500

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C	-0.10208100	1.77197200	0.04408400
C	-0.53865000	1.03514500	1.19313100
C	-1.30735200	2.30668500	-0.75254400
C	-2.13427500	1.06548800	-1.04865500

C	-2.56012700	0.37660800	0.06818500
C	-2.05525100	1.02613600	1.36692000
H	-2.36039700	0.46267900	2.25048800
Rh	-0.34121900	-0.30512400	-0.39359700
C	-2.12218000	3.26616600	0.16800100
C	-2.58300500	2.49267300	1.43333600
H	-1.49599000	4.12512200	0.43511500
H	-2.98154600	3.65407900	-0.39040800
H	-0.99123900	2.81351600	-1.66669800
H	-2.20097700	2.96661500	2.34492300
H	-3.67597900	2.47871300	1.51242600
C	1.20528600	2.46919300	-0.06237600
C	1.86890500	2.94940900	1.07948000
C	1.79429900	2.70484400	-1.31778700
C	3.08386700	3.62999500	0.97230000
H	1.42136900	2.80285700	2.05835100
C	3.00528000	3.38307900	-1.42616800
H	1.30772700	2.32386100	-2.21153100
C	3.65756900	3.84868400	-0.28011200
H	3.57686300	3.99416800	1.87004600
H	3.44666700	3.54318000	-2.40639700
H	4.60267400	4.37815000	-0.36531900
C	-3.54979300	-0.72679700	0.06669600
C	-3.52516600	-1.72408100	1.05962200
C	-4.54436600	-0.80682800	-0.92511500
C	-4.44973000	-2.76721000	1.05205400
H	-2.75876200	-1.69539200	1.82893500
C	-5.46865300	-1.85049100	-0.93273200
H	-4.60418000	-0.03074600	-1.68275900
C	-5.42574000	-2.83663300	0.05526900
H	-4.40470500	-3.52999300	1.82491300
H	-6.23082000	-1.88721800	-1.70681500
H	-6.14858600	-3.64784700	0.05152400
H	-2.48212200	0.84786200	-2.05418300
H	0.10723400	0.87964000	2.05385300
C	2.63625500	-0.73863500	0.49677700
C	3.75777500	-1.57490400	0.55014600
C	3.70280700	-2.85459600	-0.01693600
C	2.52192500	-3.28904600	-0.63457100
C	1.41716300	-2.44154000	-0.67308600
C	1.44324600	-1.14712200	-0.11217700
H	2.71375600	0.25434200	0.93253800
H	4.66442600	-1.21840900	1.02810200
H	2.49505400	-4.28467000	-1.06841800
H	0.50649500	-2.81299700	-1.15681800
O	4.73983400	-3.75143200	-0.02157400
C	5.95310300	-3.36984500	0.59838600
H	5.81429400	-3.15597400	1.66730200
H	6.62944400	-4.22028500	0.48752700
H	6.39881700	-2.48935400	0.11502800

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C	-1.81069400	1.67365500	0.78127100
C	-1.74047400	1.94879600	-0.59542100
C	-0.60833800	2.28733800	1.51436600
C	0.61942800	1.77049600	0.77873400
C	0.67051900	2.10656800	-0.55841600
C	-0.58963000	2.85856900	-0.99918900



H	-0.58661000	3.06179900	-2.07188800	H	6.16899300	-3.68286300	-0.46591600
Rh	-0.62879400	0.08903600	-0.29784500	C	2.37609100	-1.22190500	0.16570200
C	-0.67806500	3.83859900	1.33815500	H	2.33328800	-1.36784000	1.25569700
C	-0.66946000	4.18340400	-0.17512700	H	2.80628800	-0.22844400	-0.01560800
H	-1.58592100	4.21168100	1.82504300	C	1.01855800	-1.30068000	-0.39786800
H	0.17638500	4.29486100	1.85108700	C	0.09334700	-1.80247100	-1.06966700
H	-0.58830300	2.01674500	2.57069200	H	-0.44712300	-2.54000300	-1.62702100
H	-1.57878500	4.72329200	-0.46193400	O	-5.89997000	-3.24637300	-0.98078000
H	0.18139000	4.82491700	-0.43157300	C	-6.68657900	-3.15977500	-2.15197100
C	-3.03475900	1.31289500	1.53669800	H	-7.54737300	-3.81223800	-1.98855600
C	-4.31393100	1.59683900	1.02883100	H	-7.04076700	-2.13460400	-2.33140500
C	-2.94957200	0.70237800	2.80108200	H	-6.13744500	-3.50432500	-3.03983600
C	-5.46224400	1.27080500	1.74875600				
H	-4.40990800	2.08854200	0.06588900	<b>34-ts-L4</b>			
C	-4.09612100	0.38006500	3.52379300	C	4.37478800	-1.66488300	-2.15787400
H	-1.97550500	0.45125500	3.21135300	C	5.47525400	-0.91505300	-2.00649500
C	-5.36004100	0.66123600	3.00022100	C	6.32397500	-1.01140200	-0.79412400
H	-6.43962400	1.50055700	1.33249900	C	5.85569700	-1.94047900	0.26238100
H	-4.00239600	-0.09784000	4.49558500	C	4.75392300	-2.68764600	0.10698900
H	-6.25505800	0.40956000	3.56265600	C	3.92083600	-2.70116600	-1.15477500
C	1.87890600	2.06373600	-1.41580200	H	3.75208400	-1.57932500	-3.04728700
C	1.78392000	1.77954700	-2.79021700	H	5.79731500	-0.19825100	-2.75711000
C	3.14778900	2.35157400	-0.88246400	H	6.45524900	-1.97207600	1.16814300
C	2.91885300	1.76793800	-3.59782000	H	4.41255300	-3.35871500	0.89387300
H	0.81522000	1.53760000	-3.21769600	O	7.34900700	-0.34968600	-0.66718900
C	4.28479200	2.34454100	-1.69298100	O	2.52395900	-2.53990600	-0.85125400
H	3.23798400	2.60893700	0.16915700	C	4.00038900	-4.10067900	-1.80008900
C	4.17511200	2.05102900	-3.05323500	H	3.63310300	-4.85122900	-1.09309900
H	2.82399300	1.53521500	-4.65504200	H	3.36716100	-4.12954900	-2.69245800
H	5.25322100	2.58487000	-1.26183600	H	5.02980000	-4.34168900	-2.08016000
H	5.05805000	2.05197100	-3.68667500	C	2.17404800	-1.31078300	-0.21164700
H	1.47363000	1.38312500	1.32510700	H	2.70262600	-1.20639700	0.74601300
H	-2.59548400	1.82652100	-1.25212300	H	2.45853400	-0.44969700	-0.83163900
C	-2.80357200	-1.91979200	0.40132000	C	0.70155000	-1.32192500	0.00543300
C	-3.99418700	-2.62781500	0.25014400	C	-0.36299800	-2.02962100	-0.04227000
C	-4.74390000	-2.50665100	-0.92677300	H	-0.72664000	-3.03255800	-0.19892300
C	-4.28111800	-1.67119700	-1.94689500	Rh	-1.20317300	-0.17454300	-0.05946300
C	-3.08104300	-0.96383500	-1.77450900	C	0.48112300	0.47689000	1.03892000
C	-2.32402300	-1.05695500	-0.59998900	C	1.30978000	1.55680100	0.66232100
H	-2.24725200	-2.03807700	1.32791400	C	0.45100700	0.13278300	2.40127600
H	-4.36227800	-3.28339200	1.03464000	C	2.02256100	2.28259600	1.60739900
H	-4.83256200	-1.56195000	-2.87524600	H	1.38203400	1.84894500	-0.38111800
H	-2.74202000	-0.33241600	-2.59350800	C	1.14671400	0.86952800	3.36791000
C	5.29452200	-1.09595000	-0.06438800	H	-0.12303200	-0.73277500	2.71989000
C	5.98637900	-0.52569400	0.93224500	C	1.93960700	1.95116300	2.97042600
C	5.98747600	-1.08552900	2.30516000	H	2.64812900	3.12144100	1.31650300
C	5.14312000	-2.28459100	2.52520200	H	1.07806800	0.57733400	4.41026500
C	4.45423900	-2.85362500	1.52589700	C	-2.03723100	1.76692800	-0.98894100
C	4.50729200	-2.37677900	0.09202500	C	-2.53442000	1.58495300	0.30236300
H	5.28250900	-0.66119200	-1.06248400	C	-2.88669200	1.01303900	-2.02363800
H	6.57072900	0.37928400	0.78823800	C	-2.89633600	-0.42466700	-1.52879600
H	5.11234200	-2.66579300	3.54241800	C	-3.42818500	-0.59021500	-0.25177700
H	3.82623400	-3.72631900	1.69893100	C	-3.81731800	0.76413200	0.36641900
O	6.63457900	-0.57304600	3.21277600	H	-4.17679300	0.65715800	1.39112300
O	3.17936300	-2.23640300	-0.44457800	C	-4.34006400	1.58106400	-1.97742400
C	5.14386300	-3.47521900	-0.78550000	C	-4.90173900	1.42569200	-0.53854300
H	4.54998700	-4.39164000	-0.71224100	H	-4.32422800	2.63264200	-2.28580700
H	5.14938600	-3.15111900	-1.83083600	H	-4.95967400	1.04156500	-2.70296900

H	-2.47191700	1.08994300	-3.02996600	C	0.68040400	-3.20481900	0.18742100
H	-5.17365000	2.39915000	-0.11460100	C	-0.46089100	-1.64735100	-1.24952300
H	-5.80565500	0.80537700	-0.53120500	C	-0.26952000	-4.16935100	-0.11207100
C	-1.08851900	2.82480800	-1.40435700	H	1.47851000	-3.45651800	0.87982200
C	-0.94580400	4.01044600	-0.66144900	C	-1.44053400	-2.61195800	-1.54000200
C	-0.30668900	2.68095400	-2.56668200	H	-0.42615800	-0.73535900	-1.86578200
C	-0.05150000	5.00535600	-1.05580900	C	-1.34927400	-3.88017200	-0.96662700
H	-1.55368800	4.15972700	0.22547600	H	-0.20876900	-5.16567500	0.31594500
C	0.58549700	3.67536500	-2.96324000	H	-2.23858800	-2.36186100	-2.22923300
H	-0.38105900	1.76708800	-3.14923000	C	-3.34052700	0.74395000	0.43668600
C	0.71912900	4.84413800	-2.20851400	C	-3.15408600	1.28286900	-0.81515700
H	0.03708900	5.91238000	-0.46344500	C	-2.91419900	1.72100000	1.54400100
H	1.18150400	3.53601800	-3.86158800	C	-1.46122600	2.05094300	1.21121300
H	1.41332600	5.62064500	-2.51807300	C	-1.29107900	2.63970600	-0.07638100
C	-3.91302700	-1.87498400	0.31208800	C	-2.63463600	2.71288800	-0.82369700
C	-4.02098500	-2.06535300	1.70189300	H	-2.51547600	3.09405600	-1.83976200
C	-4.29612400	-2.93626300	-0.52730200	C	-3.78062700	3.01282600	1.42087900
C	-4.47820900	-3.27090900	2.22997300	C	-3.60763000	3.61350100	-0.00028600
H	-3.71796100	-1.26974800	2.37623000	H	-4.82979400	2.76693100	1.62154800
C	-4.74857000	-4.14570100	0.00024800	H	-3.46455600	3.72637400	2.19055100
H	-4.25784600	-2.80556100	-1.60472700	H	-3.01341100	1.27897600	2.53743000
C	-4.84190100	-4.32012400	1.38198100	H	-4.56970300	3.67494200	-0.52158400
H	-4.54546500	-3.39359700	3.30791700	H	-3.19983300	4.62970700	0.04599200
H	-5.04038800	-4.94859400	-0.67198900	C	-4.06506100	-0.51404200	0.72742100
H	-5.19966800	-5.25986400	1.79385500	C	-5.11579900	-0.95009700	-0.10021600
H	-2.74727500	-1.24895400	-2.21918300	C	-3.73800000	-1.29907500	1.84820600
H	-2.22333700	2.18978800	1.14770700	C	-5.80271300	-2.13310000	0.17313500
O	2.67766500	2.73046700	3.81582300	H	-5.41248100	-0.34065100	-0.94928600
C	2.64094100	2.43566300	5.20116400	C	-4.42235900	-2.48225600	2.12047500
H	3.02130000	1.42670300	5.41092300	H	-2.92199400	-0.99236600	2.49636000
H	3.28847400	3.17112900	5.68264000	C	-5.45779000	-2.90657000	1.28431700
H	1.62465500	2.52629700	5.60822100	H	-6.62088600	-2.44140000	-0.47316500
				H	-4.14345900	-3.07681800	2.98630800
				H	-5.99554300	-3.82549200	1.50121700
<b>35-L4</b>				C	-0.18296300	3.55625500	-0.44954800
C	5.55640700	-1.14803600	1.67357500	C	0.16141500	3.75556000	-1.79943500
C	6.47960500	-2.06158700	1.34295300	C	0.54172900	4.26553500	0.52363300
C	7.09343100	-2.09831200	-0.00656400	C	1.18960400	4.62247700	-2.16059800
C	6.58692700	-1.10621500	-0.98480500	H	-0.36843200	3.20417100	-2.57118500
C	5.66070600	-0.19679100	-0.65034400	C	1.57516900	5.13218100	0.16386900
C	5.09425700	-0.04832200	0.74430100	H	0.28245900	4.15168200	1.57188200
H	5.10430000	-1.13671400	2.66438700	C	1.90391900	5.31618700	-1.17940900
H	6.81904200	-2.82287800	2.04031100	H	1.43854500	4.75370400	-3.21057000
H	7.00316800	-1.16983300	-1.98668200	H	2.11698400	5.67099300	0.93710400
H	5.28145000	0.51749900	-1.37963200	H	2.70538400	5.99403100	-1.46070300
O	7.95978200	-2.91578800	-0.30110400	H	-0.74896900	2.20937200	2.01657100
O	3.66352900	0.03181400	0.70914300	H	-3.50357200	0.80619400	-1.72632900
C	5.53061700	1.31627100	1.32049500	O	-2.22322200	-4.90545900	-1.18340400
H	5.15816000	2.11937200	0.67670500	C	-3.35213600	-4.65528600	-2.00540100
H	5.09916300	1.44773900	2.31792700	H	-3.05486900	-4.39271100	-3.03003900
H	6.62034500	1.38132300	1.38708600	H	-3.91938800	-5.58793500	-2.02616700
C	2.98352200	-1.12604700	0.23380400	H	-3.97947100	-3.85545400	-1.59159300
H	3.44322200	-1.48272100	-0.70306600				
H	3.09104800	-1.94723000	0.96123300	<b>36-ts-L4</b>			
C	1.52493900	-0.79888800	0.00346000	C	4.80824100	2.32065600	-0.29820900
C	0.97348200	0.43154000	0.09564600	C	5.73195100	1.61234800	0.36644800
H	1.59399300	1.28652500	0.36251300	C	6.31784100	0.37424300	-0.19805500
Rh	-1.00267300	0.51152900	-0.14208800	C	5.85264100	-0.01614900	-1.55015200
C	0.60810600	-1.90630300	-0.36030000				

C	4.93081200	0.69666300	-2.21243900
C	4.30980300	1.96901800	-1.68195700
H	4.36083300	3.21126100	0.14068700
H	6.07664100	1.89433400	1.35761600
H	6.28932500	-0.92306100	-1.96007400
H	4.57879000	0.38416800	-3.19466200
O	7.12847300	-0.30400500	0.42751900
O	2.87310700	1.87462600	-1.68934400
C	4.61521200	3.13104900	-2.64721000
H	4.22008100	2.89690200	-3.64074000
H	4.12599300	4.04236700	-2.28921300
H	5.69279700	3.30558200	-2.72010500
C	2.32799200	0.82544300	-0.87522900
H	2.60654900	-0.15736000	-1.27968700
H	2.74721700	0.87162600	0.14026500
C	0.86084300	0.94249800	-0.81179400
C	-0.16685400	1.60977900	-1.18223100
H	-0.54548000	2.39545000	-1.81202100
Rh	-0.68014100	-0.24574100	-0.14987100
C	-1.84429400	1.51267300	0.02578200
C	-3.07334500	1.72314300	-0.63355800
C	-1.59057800	2.27015000	1.17897500
C	-4.01669900	2.60910000	-0.13110400
H	-3.29906300	1.18020900	-1.54655000
C	-2.54190100	3.15190500	1.70952200
H	-0.62961400	2.18027100	1.67787200
C	-3.76298900	3.32449600	1.05152000
H	-4.96724700	2.76168100	-0.63416900
H	-2.30787000	3.70462300	2.61298500
C	-2.29142900	-1.89345900	-0.23681800
C	-2.01736200	-1.53580800	1.08452000
C	-1.30927100	-2.96262800	-0.73795500
C	0.06398400	-2.35729500	-0.49836400
C	0.33210200	-2.04272100	0.83074900
C	-0.88525900	-2.33081800	1.72496000
H	-0.71117700	-2.02573700	2.75824900
C	-1.47148800	-4.23437100	0.15382600
C	-1.20818200	-3.85440700	1.63614800
H	-2.48177600	-4.63796700	0.02149800
H	-0.76940500	-5.00443900	-0.18604300
H	-1.46669100	-3.20336200	-1.79071900
H	-2.08337200	-4.06971400	2.25978200
H	-0.36859100	-4.42606800	2.04851000
C	-3.55893800	-1.62926600	-0.95511600
C	-4.76249800	-1.42517500	-0.25704700
C	-3.60133400	-1.59365300	-2.36196500
C	-5.95723100	-1.18485500	-0.93533100
H	-4.76338400	-1.47139400	0.82766600
C	-4.79492800	-1.35653900	-3.04094400
H	-2.68321000	-1.72583000	-2.92730200
C	-5.98065900	-1.14973900	-2.33051400
H	-6.87340700	-1.03258900	-0.37064800
H	-4.79863600	-1.32814700	-4.12759200
H	-6.91207600	-0.96696600	-2.85952000
C	1.68477300	-1.82105700	1.40124600
C	1.86941700	-1.03233800	2.55175900
C	2.82263600	-2.40081000	0.81155700
C	3.14312200	-0.80924900	3.07298500

H	1.00921800	-0.56579400	3.02373300
C	4.09852300	-2.17093600	1.32743000
H	2.70377400	-3.04632200	-0.05409500
C	4.26637900	-1.36931900	2.45814000
H	3.25938700	-0.18763800	3.95719500
H	4.96608100	-2.61620300	0.84851200
H	5.26277200	-1.18341800	2.84811900
H	0.83790100	-2.42123500	-1.25730700
H	-2.70593100	-0.96406500	1.69780800
O	-4.76026400	4.16710500	1.46079400
C	-4.55595200	4.91708500	2.64449500
H	-5.46338000	5.50736800	2.78793900
H	-4.40640000	4.26614200	3.51689000
H	-3.69536100	5.59393200	2.55315100

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C	-4.83006500	2.19950300	-0.55888900
C	-5.82093000	1.29706600	-0.55479700
C	-6.21870600	0.58397400	0.68066500
C	-5.46117900	0.92221800	1.90872200
C	-4.47242300	1.82709500	1.90012900
C	-4.06830300	2.62037800	0.67762900
H	-4.52529900	2.69641000	-1.47869200
H	-6.36231800	1.02562600	-1.45681400
H	-5.74569500	0.38106100	2.80741800
H	-3.90754100	2.05199500	2.80383600
O	-7.11232500	-0.25934700	0.68451100
O	-2.65466900	2.54114700	0.45928800
C	-4.32700600	4.11906500	0.94275100
H	-3.74824800	4.44159700	1.81422500
H	-3.99981400	4.70436800	0.07750600
H	-5.38900400	4.30788600	1.12506100
C	-2.12662200	1.23070000	0.19075100
H	-2.29076000	0.58200100	1.06406300
H	-2.67736900	0.76822900	-0.64115500
C	-0.66823900	1.29707600	-0.13930300
C	0.00541200	2.46717800	-0.21467700
H	-0.45270600	3.42855300	0.01898400
Rh	0.62429000	-0.25942500	-0.27420300
C	1.43562100	2.44048400	-0.56617900
C	2.38084600	3.30546200	0.01323800
C	1.92336300	1.48164100	-1.49093900
C	3.73964300	3.20707500	-0.27641600
H	2.04388900	4.05988800	0.72004200
C	3.28732100	1.36713800	-1.77604900
H	1.20310900	0.93299400	-2.11276600
C	4.20594800	2.22245100	-1.16472000
H	4.43158200	3.89452500	0.19788000
H	3.65113600	0.63612500	-2.49123900
C	2.13059100	-1.90732100	0.52091100
C	1.76385400	-2.24952100	-0.76428300
C	1.07622600	-2.34679200	1.54891100
C	-0.20046200	-1.66329000	1.06575900
C	-0.58508400	-2.04626100	-0.25221400
C	0.44922400	-3.00535700	-0.86926800
H	0.20179700	-3.25114600	-1.90405500
C	0.90850100	-3.89472400	1.46198800
C	0.51898600	-4.29011100	0.01185200

H	1.84411400	-4.37789900	1.76625600	Rh	0.06056900	-0.32117500	-0.43273500
H	0.13795600	-4.20875600	2.17557100	C	0.18875300	-2.10597800	2.39028300
H	1.34256600	-2.04124300	2.56238200	C	0.18889700	-3.18667500	3.28906900
H	1.25304900	-4.98071500	-0.41860600	C	1.44432900	-1.71417200	1.87825700
H	-0.45355000	-4.79475800	-0.01365700	C	1.35625200	-3.86936800	3.63499000
C	3.45990900	-1.39349200	0.92489500	H	-0.75547000	-3.51162000	3.72008100
C	4.61554900	-1.72396000	0.19451000	C	2.61688700	-2.38615600	2.20049300
C	3.60593700	-0.57106400	2.05674900	H	1.51648300	-0.82304400	1.24498100
C	5.86695400	-1.24043600	0.57216700	C	2.58189400	-3.47567000	3.08293200
H	4.53278600	-2.38306000	-0.66477800	H	1.29802400	-4.70056300	4.32910400
C	4.85749900	-0.08894000	2.43623700	H	3.57343300	-2.07009800	1.79538000
H	2.72760300	-0.28545900	2.62815300	C	2.20734200	-1.18210200	-1.99095100
C	5.99467900	-0.42111600	1.69604500	C	1.39570400	-0.49429800	-2.83413300
H	6.74535000	-1.51372600	-0.00652000	C	1.64692600	-2.57304700	-1.69111500
H	4.94363600	0.54941700	3.31173200	C	0.20713200	-2.39764900	-1.20463300
H	6.97196000	-0.05343600	1.99770900	C	-0.62673700	-1.73999800	-2.11461100
C	-1.98148300	-2.06706500	-0.76107300	C	0.17962900	-1.25185600	-3.32644700
C	-2.24575100	-1.92622700	-2.13577000	H	-0.41779800	-0.65064700	-4.01291000
C	-3.07099600	-2.26674800	0.10365800	C	1.57961800	-3.35203100	-3.04864300
C	-3.54974700	-1.96833900	-2.62408700	C	0.70309400	-2.54769300	-4.04381500
H	-1.41850900	-1.75627700	-2.81995000	H	2.59222600	-3.49693000	-3.44179800
C	-4.37921100	-2.30580600	-0.38272400	H	1.15680900	-4.34590700	-2.86489500
H	-2.89021500	-2.40390400	1.16598100	H	2.23752200	-3.10971500	-0.94810500
C	-4.62370000	-2.15517800	-1.74846200	H	1.27653500	-2.25444700	-4.92958200
H	-3.72951200	-1.84833200	-3.68947000	H	-0.15285700	-3.13785900	-4.38967600
H	-5.20954600	-2.44547900	0.30333400	C	3.53352500	-0.72837400	-1.51750400
H	-5.64260700	-2.18238600	-2.12435700	C	3.86232100	0.64092300	-1.47506800
H	-0.92160400	-1.29485400	1.79119700	C	4.52299300	-1.65443300	-1.14163900
H	2.42579800	-2.14905000	-1.61888400	C	5.13124700	1.06692000	-1.08973300
O	5.51641500	2.04412800	-1.51042600	H	3.10653200	1.37895300	-1.72817100
C	6.49208900	2.84866100	-0.87225200	C	5.79429800	-1.22902500	-0.75212400
H	6.48535300	2.70144900	0.21611500	H	4.31098600	-2.71850600	-1.17187900
H	7.45542500	2.52726600	-1.27343600	C	6.10428400	0.13055400	-0.72591400
H	6.34930000	3.91523900	-1.09371900	H	5.36002500	2.12873200	-1.06996800
				H	6.54258800	-1.96603200	-0.47264800
				H	7.09325700	0.46192500	-0.42159700
				C	-2.09362200	-1.93360700	-2.24176300
				C	-2.88236700	-1.04256700	-2.99458200
				C	-2.73770200	-3.03698400	-1.65171100
				C	-4.25287500	-1.24366300	-3.15065200
				H	-2.42235600	-0.17187800	-3.45231100
				C	-4.10899500	-3.23709800	-1.80276200
				H	-2.15588700	-3.75472800	-1.08304700
				C	-4.87476700	-2.34451800	-2.55661600
				H	-4.83548200	-0.53847900	-3.73749700
				H	-4.57715400	-4.10282800	-1.34155900
				H	-5.94099700	-2.50929000	-2.68722200
				H	-0.17499600	-3.07264000	-0.44558100
				H	1.64536600	0.47719300	-3.24886700
				C	2.51201700	4.90860800	1.64540200
				C	3.75145200	4.86096400	1.13697700
				C	3.98645500	4.69813400	-0.31610500
				C	2.78221200	4.58124600	-1.17014000
				C	1.54362100	4.62250600	-0.65716600
				C	1.25468200	4.84558700	0.80854700
				H	2.34603700	5.00488400	2.71706200
				H	4.63895500	4.92125400	1.76105400
				H	2.96387000	4.44773700	-2.23333600
<b>38-L4</b>							
C	-4.62744700	1.66358500	2.21398200				
C	-5.16302400	2.72226000	1.58993200				
C	-5.98836700	2.57067100	0.36794100				
C	-6.13900800	1.19185900	-0.15385900				
C	-5.60239400	0.13575500	0.47346100				
C	-4.85600800	0.23070700	1.78487800				
H	-4.00857300	1.78594800	3.10167800				
H	-5.01045500	3.74011700	1.93887800				
H	-6.69660400	1.09275200	-1.08146300				
H	-5.69574300	-0.86895800	0.06505500				
O	-6.50003800	3.53571400	-0.19257800				
O	-3.62084500	-0.49172400	1.73144500				
C	-5.67002900	-0.49515400	2.87894400				
H	-5.81371800	-1.54198600	2.59308000				
H	-5.11642100	-0.46943300	3.82304100				
H	-6.64592100	-0.02185100	3.02008600				
C	-2.67884900	-0.04238600	0.74464100				
H	-3.05781000	-0.27425100	-0.25899600				
H	-2.57402200	1.05040500	0.80159400				
C	-1.32955400	-0.68106300	0.94901200				
C	-1.07049300	-1.44594200	2.03311000				
H	-1.89676700	-1.61932700	2.72262900				

H	0.66857600	4.51612800	-1.29408500	C	0.16827900	-2.00474300	-2.58891400
O	5.12098600	4.63556300	-0.78482400	H	0.77108700	-2.87344200	-2.32151500
O	0.36700600	3.84101900	1.33538100	C	-1.18911200	-0.86291600	-4.40247100
C	0.46519200	6.16022100	0.97577400	C	-0.32266200	-2.10608600	-4.06897400
H	-0.46725700	6.10379100	0.40555400	H	-2.19650700	-1.15539700	-4.72043700
H	0.21442300	6.30446600	2.03137300	H	-0.74765800	-0.28114000	-5.21965600
H	1.05170700	7.01446400	0.62533400	H	-1.89549000	0.93152100	-3.33965800
C	0.79034700	2.47515500	1.22541400	H	-0.89494100	-3.03212100	-4.19350900
H	1.88528400	2.40601200	1.18729200	H	0.54828000	-2.17238100	-4.73073700
H	0.46767800	1.98675300	2.15207100	C	-3.31010900	-0.70147700	-1.61714500
C	0.18166600	1.75997300	0.08189900	C	-4.05198500	-1.85430300	-1.29610800
C	-0.57372400	1.62901400	-0.91935600	C	-3.98369500	0.53386100	-1.62195200
H	-1.25868900	1.98088800	-1.67065200	C	-5.40485300	-1.76868200	-0.96649200
O	3.78590400	-4.07029200	3.34714000	H	-3.57371900	-2.82889800	-1.32339200
C	3.80850500	-5.15358600	4.25910800	C	-5.33657800	0.61806600	-1.29598800
H	4.85219000	-5.46678600	4.32950300	H	-3.44111700	1.44139000	-1.86846800
H	3.45329600	-4.85374200	5.25455000	C	-6.05413700	-0.53285100	-0.96192200
H	3.20158000	-5.99748200	3.90302700	H	-5.95483400	-2.67513100	-0.72740300
<b>39-ts-L4</b>				H	-5.83149400	1.58580400	-1.30424500
C	4.43394100	-0.59583700	2.31982900	H	-7.10956900	-0.46780600	-0.71190700
C	5.41607900	-1.28183500	1.71936200	C	2.41921700	-0.66475600	-2.47419700
C	6.43121300	-0.60992500	0.87428100	C	3.18416900	-1.70277700	-1.90875800
C	6.30838500	0.86034700	0.74383300	C	3.11068900	0.38040700	-3.11641000
C	5.32438600	1.54168000	1.34670800	C	4.57680400	-1.68699100	-1.96424500
C	4.29281400	0.90752300	2.25132600	H	2.68468500	-2.52043300	-1.39722000
H	3.67984700	-1.10488500	2.91874500	C	4.50390200	0.39940700	-3.16872900
H	5.50553900	-2.36164800	1.80385700	H	2.54923500	1.17571000	-3.59688400
H	7.04734000	1.34615300	0.11253000	C	5.24600900	-0.63215400	-2.58942500
H	5.22861700	2.61919300	1.22080500	H	5.14747800	-2.48952700	-1.50582500
O	7.31161600	-1.24156000	0.29574300	H	5.00995200	1.21841000	-3.67376100
O	2.96276300	1.28173100	1.85245600	H	6.33154100	-0.61918600	-2.61695600
C	4.43765200	1.49324300	3.67197000	H	0.48801800	1.41570900	-2.82058800
H	4.29351000	2.57767500	3.63768400	H	-1.34686600	-2.68889800	-1.04562000
H	3.67079500	1.06603200	4.32618600	C	-3.50420100	-3.27017400	2.88544700
H	5.42593800	1.27356600	4.08629400	C	-3.56403700	-4.17722200	1.90049400
C	2.55916400	0.87550100	0.52219800	C	-2.35090900	-4.59681000	1.16064100
H	3.22527300	1.33713700	-0.21866000	C	-1.06370200	-4.04594400	1.63989300
H	2.65907000	-0.20892500	0.42377400	C	-1.00809100	-3.12950800	2.61728600
C	1.12555700	1.32405900	0.30420300	C	-2.22302200	-2.61853800	3.35548700
C	0.90209800	2.66541200	0.38093100	H	-4.40581800	-2.93164200	3.39313100
H	1.79891500	3.27082400	0.54521300	H	-4.50161800	-4.61735400	1.57139900
Rh	-0.22280200	-0.07061700	-0.51774600	H	-0.17351300	-4.39204800	1.12157200
C	-0.31387000	3.47609500	0.36413300	H	-0.05878300	-2.69598100	2.92249700
C	-0.20653600	4.83883100	0.70100700	O	-2.41541200	-5.33162100	0.17713900
C	-1.60786800	3.00086300	0.05500200	O	-2.34164800	-1.18537400	3.23537600
C	-1.31165400	5.68775600	0.75286000	C	-2.04728600	-2.85459500	4.86671200
H	0.77340300	5.24486000	0.94241400	H	-1.14378100	-2.34531400	5.21626600
C	-2.71869200	3.82895400	0.11252800	H	-2.90519700	-2.44009900	5.40539100
H	-1.72885400	1.96385300	-0.24024500	H	-1.96646600	-3.92318900	5.08815700
C	-2.58408000	5.18147200	0.46272600	C	-2.42200600	-0.66260300	1.89847700
H	-1.17047800	6.72868300	1.02154100	H	-2.90438800	-1.38053700	1.22824000
H	-3.71019500	3.45175300	-0.12054700	H	-3.08736800	0.20638200	1.96672200
C	-1.87713600	-0.80075900	-1.99420100	C	-1.11911100	-0.21145400	1.35017200
C	-1.04048700	-1.86315100	-1.67949100	C	0.05603300	0.20019000	1.63661200
C	-1.29404300	0.04431900	-3.13582000	H	0.81737500	0.32878700	2.38777200
C	0.10740700	0.41166800	-2.66535300	O	-3.73854900	5.91182900	0.48020800
C	0.93806300	-0.68791900	-2.43088400	C	-3.65602100	7.28491500	0.82092600
				H	-4.67711800	7.66860500	0.77397500

H	-3.26258200	7.42714500	1.83654000
H	-3.02748700	7.84117000	0.11233900

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C	5.30949600	-0.01363400	-2.29703800
C	5.99566800	1.09931400	-2.59180700
C	6.41474900	2.05777300	-1.54036300
C	5.98916700	1.74011000	-0.15616600
C	5.30218000	0.62655500	0.13501700
C	4.94268800	-0.42514500	-0.88865400
H	4.99355500	-0.70514200	-3.07674800
H	6.27296900	1.35809300	-3.61024900
H	6.26171600	2.46837200	0.60317900
H	4.98203300	0.40645300	1.15164600
O	7.06321200	3.06504100	-1.80439800
O	3.54576500	-0.76214200	-0.81662400
C	5.66298800	-1.74350400	-0.53807800
H	5.36499300	-2.06528800	0.46466700
H	5.37238600	-2.52033300	-1.25270600
H	6.74856500	-1.61380600	-0.57071200
C	2.63290500	0.31042800	-1.01100800
H	2.63590500	0.98188900	-0.14055300
H	2.92993400	0.92001300	-1.88109200
C	1.23056500	-0.19498400	-1.28480500
C	0.91257700	-1.52482900	-1.07088400
H	1.69908200	-2.09415500	-0.58166700
Rh	-0.52897300	-0.40572400	0.48460900
C	-0.12222100	-2.39768100	-1.67627100
C	-0.08729700	-3.76141800	-1.33486500
C	-1.07509600	-2.00832700	-2.64453800
C	-0.95805100	-4.69873000	-1.89404700
H	0.65581900	-4.10457600	-0.61817300
C	-1.93832600	-2.92967900	-3.21685000
H	-1.13708600	-0.96988900	-2.94443200
C	-1.89740600	-4.28349500	-2.84333400
H	-0.88377500	-5.73801400	-1.59413900
H	-2.66307600	-2.62279700	-3.96504000
C	-2.41852000	-0.43747200	1.57438400
C	-1.53512200	0.49732600	2.15836000
C	-2.23177500	-1.83298200	2.19434300
C	-0.74889600	-2.12289000	2.02241300
C	0.09506400	-1.21546500	2.63517800
C	-0.69689900	-0.07573100	3.29537100
H	-0.04708400	0.68120900	3.73622200
C	-2.56576600	-1.74368400	3.71534800
C	-1.63922400	-0.68831200	4.37755700
H	-3.62160400	-1.47518300	3.83544600
H	-2.42939500	-2.73058000	4.17209900
H	-2.85031200	-2.58065200	1.69409800
H	-2.22410000	0.11745000	4.83575700
H	-1.03215400	-1.13731500	5.17199700
C	-3.69782500	-0.10044300	0.89785800
C	-4.45186200	1.01744000	1.29295800
C	-4.20789700	-0.91730000	-0.12778600
C	-5.66690500	1.31884300	0.67472200
H	-4.08936800	1.64697900	2.10073300
C	-5.42113500	-0.61766200	-0.74383600
H	-3.62937600	-1.77281300	-0.46507500

C	-6.15627300	0.50357000	-0.34635900
H	-6.23354000	2.18788100	0.99903700
H	-5.79129500	-1.25719900	-1.54094700
H	-7.10304400	0.73569300	-0.82666500
C	1.53828300	-1.42197300	2.89884300
C	2.38577700	-0.34173000	3.20920500
C	2.10058800	-2.71299000	2.89718100
C	3.73198700	-0.54401600	3.51190000
H	1.99145300	0.66967700	3.20753500
C	3.44880600	-2.91528900	3.18679900
H	1.46578000	-3.57110600	2.69753600
C	4.27325500	-1.83203800	3.50148000
H	4.35764600	0.30800100	3.76681400
H	3.85141400	-3.92494800	3.18851600
H	5.31907400	-1.99111200	3.74991200
H	-0.41696500	-3.07104600	1.61232900
H	-1.69508800	1.56990600	2.08771700
C	-2.73672100	4.78856500	-1.28165500
C	-2.84808900	5.38823000	-0.08787600
C	-1.69333900	5.50871500	0.83342600
C	-0.42283500	4.90043700	0.37375800
C	-0.31653800	4.29647500	-0.81895800
C	-1.44457800	4.21700500	-1.82205800
H	-3.59502300	4.68756000	-1.94390100
H	-3.78713500	5.80407700	0.26783300
H	0.41306300	4.96549800	1.06539700
H	0.61755300	3.83622000	-1.13224000
O	-1.78982000	6.06417400	1.92401300
O	-1.65438700	2.87055300	-2.27788500
C	-1.04465300	4.98900300	-3.09647500
H	-0.12847900	4.55972800	-3.51447400
H	-1.83920100	4.89667400	-3.84377100
H	-0.87773600	6.04759200	-2.87704100
C	-1.94569500	1.88545500	-1.26558400
H	-2.24652300	2.37720400	-0.33347900
H	-2.82764400	1.33381800	-1.61771300
C	-0.82839300	0.91958000	-1.02358700
C	0.29145500	0.83913300	-1.77191200
H	0.57225700	1.50826800	-2.58947700
O	-2.79921400	-5.10065600	-3.46208900
C	-2.79930300	-6.47643900	-3.12146900
H	-3.02038500	-6.62961100	-2.05638300
H	-3.58712900	-6.93507700	-3.72207200
H	-1.83870100	-6.95247400	-3.36029200

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C	-2.63800400	2.94233200	-1.10460900
C	-3.36350700	2.41196100	-0.10948100
C	-2.72955700	1.94815100	1.14783900
C	-1.24928300	1.85071800	1.13935700
C	-0.49539100	2.43370100	0.12419800
C	-1.15004100	3.20685100	-1.01638400
H	-3.10842300	3.29258500	-2.02217100
H	-4.44387400	2.31721500	-0.16202900
H	-0.79970400	1.63965900	2.10726600
H	0.53735100	2.70062700	0.32198000
O	-3.38585100	1.68684100	2.15180300
O	-0.52097200	3.00424100	-2.28505100

C	-0.94684300	4.71754100	-0.74655000	H	-7.53499400	-0.33877400	1.22080300
H	0.12486200	4.93749600	-0.71012200	O	6.17703400	1.10235300	2.22094000
H	-1.38915800	5.29776700	-1.56266300	C	5.93148000	0.92679000	3.60417600
H	-1.41342800	5.01567800	0.19690500	H	5.47531000	-0.05039800	3.81557400
C	-0.19176600	1.64552800	-2.63122600	H	6.90647000	0.98026100	4.09299700
H	-1.11311200	1.07675900	-2.82473700	H	5.28221300	1.71716600	4.00495800
H	0.35897100	1.74467000	-3.57554800				
C	0.66022400	1.02439700	-1.54780500	<b>42-ts-L4</b>			
C	1.99389200	1.22963700	-1.60152700	C	2.32717600	-3.00550700	-1.52035100
H	2.38008500	1.63709700	-2.54262800	C	3.06421900	-2.59668200	-0.48017800
C	3.02800600	1.11738200	-0.56594300	C	2.43246800	-2.18835800	0.80045800
C	4.37890500	1.31445100	-0.92532700	C	0.98575100	-1.90375000	0.75540300
C	2.76145300	0.91054900	0.79827900	C	0.16911100	-2.33871200	-0.34935400
C	5.39977000	1.29789900	0.01324400	C	0.81917800	-3.14212600	-1.49480000
H	4.62493000	1.48740800	-1.97072500	H	2.79059300	-3.33218500	-2.45023000
C	3.77504100	0.90068700	1.75851700	H	4.15010200	-2.58848300	-0.50375600
H	1.73507400	0.73971600	1.11377000	H	0.52261100	-1.87030600	1.74149000
C	5.10597200	1.09283500	1.36926500	H	-0.81163600	-2.70802400	-0.06059800
H	6.43523600	1.44981800	-0.27637400	O	3.08559800	-2.11868800	1.83995700
H	3.51589400	0.74309600	2.80009200	O	0.28827700	-2.75289300	-2.76947600
C	-0.60580000	-1.70093900	-1.34412700	C	0.44987500	-4.62874000	-1.33898900
C	0.40912800	-1.93346600	-0.40068300	H	-0.63808200	-4.74391900	-1.38614600
C	-1.96831500	-2.24953100	-0.94961400	H	0.89296700	-5.20833700	-2.15540600
C	-2.35446700	-1.51699600	0.33399500	H	0.81710500	-5.02502500	-0.38736800
C	-1.34343500	-1.58795900	1.27044800	C	0.05616800	-1.34091100	-2.82096600
C	-0.19087100	-2.50703200	0.88875200	H	1.00772500	-0.80401000	-2.94777700
H	-2.70282400	-2.11206400	-1.74370100	H	-0.56246800	-1.17352400	-3.71013000
Rh	-0.53940700	0.13068800	-0.14312300	C	-0.66139500	-0.96206600	-1.54593200
C	-0.77688800	-3.91706800	0.54539300	C	-2.02386200	-0.97923300	-1.55907300
C	-1.81449500	-3.76653200	-0.59634300	H	-2.49791900	-1.06309800	-2.54107100
H	0.04163100	-4.58450400	0.25424500	C	-2.97193700	-1.02650100	-0.45246500
H	-1.23778500	-4.33846400	1.44581600	C	-4.32877800	-1.31185800	-0.73107200
H	-2.79016700	-4.17119900	-0.30487100	C	-2.62367100	-0.85932200	0.90090700
H	-1.49500500	-4.30579700	-1.49514900	C	-5.27261700	-1.43641200	0.27495900
H	0.53758300	-2.57595800	1.69647500	H	-4.63705000	-1.44485800	-1.76548600
H	-0.38823900	-1.54303400	-2.39531500	C	-3.55984300	-0.99174700	1.92680000
H	-1.47032700	-1.25601800	2.29636400	H	-1.60213300	-0.58341500	1.15206000
C	1.84015000	-2.15774400	-0.72799900	C	-4.89503300	-1.28303800	1.61898200
C	2.79964600	-2.34916100	0.28216100	H	-6.31156100	-1.65753000	0.05045200
C	2.27483700	-2.26105800	-2.06312500	H	-3.24207200	-0.85195100	2.95424100
C	4.12982300	-2.62985300	-0.02394600	C	0.76840200	1.95753500	-1.28643800
H	2.51504700	-2.25584500	1.32447900	C	-0.27699400	2.18475300	-0.39369900
C	3.60477200	-2.53498400	-2.37221500	C	2.14515300	2.31766900	-0.75376900
H	1.56354500	-2.13905300	-2.87261400	C	2.34330300	1.41279600	0.46649000
C	4.54113600	-2.72340800	-1.35360200	C	1.27316900	1.53205300	1.35508200
H	4.84771000	-2.76462400	0.78037400	C	0.26263500	2.60953500	0.97803800
H	3.90799000	-2.61046600	-3.41329200	H	2.91964200	2.17046900	-1.50737500
H	5.57811100	-2.94168200	-1.59374100	Rh	0.58855100	0.03048700	-0.13641500
C	-3.76226000	-1.13640900	0.58294100	C	1.01224500	3.96987100	0.80284800
C	-4.60797700	-0.74273700	-0.47043200	C	2.13021100	3.80019900	-0.25823800
C	-4.31694700	-1.23530000	1.87152900	H	0.29383500	4.74129300	0.50332600
C	-5.95305600	-0.45663600	-0.24342100	H	1.42872400	4.27284200	1.77021300
H	-4.20540300	-0.63521200	-1.47293500	H	3.11344400	4.05001300	0.15595200
C	-5.66011600	-0.94677100	2.09983500	H	1.96301200	4.45974700	-1.11733200
H	-3.69269200	-1.55688400	2.69880400	H	-0.52513300	2.69654100	1.72715100
C	-6.48570400	-0.55841900	1.04355800	H	0.61224100	1.84766500	-2.35505100
H	-6.58557100	-0.15275200	-1.07352200	H	1.31897100	1.15554700	2.37275700
H	-6.06277200	-1.02917800	3.10550400	C	-1.68911100	2.42589100	-0.77826500

C	-2.71777900	2.44529000	0.18061700	H	-6.29572000	-1.52882100	0.14805900
C	-2.04080400	2.69762000	-2.11431500	H	-3.22715400	-0.71019200	3.04900500
C	-4.03729900	2.71517300	-0.17785900	C	0.83787900	1.93488900	-1.28100300
H	-2.49365200	2.22118400	1.21797800	C	-0.18495900	2.19976000	-0.37237400
C	-3.35976900	2.96223700	-2.47621700	C	2.23253500	2.26751600	-0.77794300
H	-1.26987900	2.72568600	-2.87763000	C	2.43064900	1.37405600	0.45048900
C	-4.36706800	2.97349500	-1.50887900	C	1.38070200	1.53157500	1.35670700
H	-4.81072600	2.71229800	0.58529200	C	0.39003900	2.62877600	0.98368800
H	-3.59855800	3.17347300	-3.51545700	H	2.98964300	2.09157100	-1.54301500
H	-5.39529300	3.18574900	-1.78895900	Rh	0.63066000	0.02815700	-0.10301100
C	3.69382800	0.89753800	0.79380100	C	1.16984800	3.96765300	0.77669800
C	4.58597500	0.50711200	-0.22176200	C	2.26343600	3.75622600	-0.30192300
C	4.14751000	0.84412800	2.12301600	H	0.46525500	4.75277600	0.47991900
C	5.87717600	0.07869400	0.08007600	H	1.61119300	4.27260600	1.73233000
H	4.25887000	0.51649900	-1.25724400	H	3.26005700	3.98646200	0.09110300
C	5.43679500	0.41256500	2.42643500	H	2.09713400	4.40878200	-1.16653300
H	3.48870600	1.15760400	2.92652700	H	-0.38102700	2.74457700	1.74611400
C	6.30942100	0.02996800	1.40709500	H	0.65922400	1.81408000	-2.34487400
H	6.54650300	-0.21887900	-0.72321000	H	1.43468300	1.16578800	2.37786900
H	5.76072700	0.37878400	3.46306500	C	-1.59801200	2.46998100	-0.73389400
H	7.31661400	-0.30230600	1.64351600	C	-2.60563900	2.53803200	0.24497600
O	-5.89414800	-1.42455700	2.53750800	C	-1.97045200	2.72138700	-2.06843200
C	-5.56728600	-1.29529400	3.91117400	C	-3.92458300	2.83641600	-0.09261800
H	-5.18307200	-0.29270000	4.14288600	H	-2.36676800	2.33128000	1.28255400
H	-6.49787200	-1.45879900	4.45792100	C	-3.28901000	3.01406900	-2.40923000
H	-4.82706000	-2.04408100	4.22278600	H	-1.21540500	2.71094100	-2.84787500

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C	2.27189600	-3.07883800	-1.46384300
C	3.03322600	-2.67184100	-0.44072300
C	2.42989600	-2.22391100	0.84040800
C	0.99048100	-1.90311700	0.81010000
C	0.14750500	-2.33537200	-0.27603200
C	0.76123600	-3.17339600	-1.41719200
H	2.71403400	-3.43411200	-2.39360700
H	4.11852500	-2.69356400	-0.47830500
H	0.54182700	-1.84095200	1.80147400
H	-0.83722800	-2.67687600	0.03245500
O	3.09952200	-2.15243000	1.86924600
O	0.22562200	-2.78748900	-2.69124200
C	0.35348200	-4.64676900	-1.23543600
H	-0.73767800	-4.73289900	-1.26817700
H	0.77094500	-5.24988500	-2.04834200
H	0.72118200	-5.03929300	-0.28245300
C	0.03355700	-1.37028600	-2.75871700
H	0.99892100	-0.86251800	-2.90053300
H	-0.58830300	-1.19592800	-3.64430000
C	-0.66045000	-0.95600700	-1.48164000
C	-2.02298300	-0.93933700	-1.48183200
H	-2.50909800	-1.02645400	-2.45769900
C	-2.95980900	-0.94874500	-0.36502900
C	-4.31713700	-1.22003700	-0.62025800
C	-2.59067500	-0.75808100	0.98659500
C	-5.26277700	-1.31542900	0.39906200
H	-4.63928500	-1.37036700	-1.64813200
C	-3.51713500	-0.85932100	2.01303400
H	-1.56210600	-0.49225000	1.21987200
C	-4.86366400	-1.14037300	1.73058300

H	-6.29572000	-1.52882100	0.14805900
H	-3.22715400	-0.71019200	3.04900500
C	0.83787900	1.93488900	-1.28100300
C	-0.18495900	2.19976000	-0.37237400
C	2.23253500	2.26751600	-0.77794300
C	2.43064900	1.37405600	0.45048900
C	1.38070200	1.53157500	1.35670700
C	0.39003900	2.62877600	0.98368800
H	2.98964300	2.09157100	-1.54301500
Rh	0.63066000	0.02815700	-0.10301100
C	1.16984800	3.96765300	0.77669800
C	2.26343600	3.75622600	-0.30192300
H	0.46525500	4.75277600	0.47991900
H	1.61119300	4.27260600	1.73233000
H	3.26005700	3.98646200	0.09110300
H	2.09713400	4.40878200	-1.16653300
H	-0.38102700	2.74457700	1.74611400
H	0.65922400	1.81408000	-2.34487400
H	1.43468300	1.16578800	2.37786900
C	-1.59801200	2.46998100	-0.73389400
C	-2.60563900	2.53803200	0.24497600
C	-1.97045200	2.72138700	-2.06843200
C	-3.92458300	2.83641600	-0.09261800
H	-2.36676800	2.33128000	1.28255400
C	-3.28901000	3.01406900	-2.40923000
H	-1.21540500	2.71094100	-2.84787500
C	-4.27512500	3.07465600	-1.42201200
H	-4.68077400	2.87258200	0.68684900
H	-3.54366100	3.20897200	-3.44791700
H	-5.30266100	3.30999500	-1.68598100
C	3.77367000	0.82893500	0.76006100
C	4.63594900	0.40080300	-0.26596000
C	4.25061400	0.78275700	2.08139400
C	5.92128100	-0.05642800	0.01818000
H	4.28932700	0.40373400	-1.29513600
C	5.53393300	0.32225400	2.36720600
H	3.61511400	1.12413100	2.89223200
C	6.37702200	-0.09730500	1.33759900
H	6.56750700	-0.38278200	-0.79281000
H	5.87629600	0.29461100	3.39808800
H	7.37968200	-0.45205100	1.56030500
O	-5.69583400	-1.21056100	2.80968700
C	-7.06799900	-1.48716800	2.58339500
H	-7.20956000	-2.46386500	2.10169000
H	-7.53801600	-1.50017200	3.56858000
H	-7.54085900	-0.71102600	1.96666900

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C	-2.93564100	3.22210000	-0.21232200
C	-3.25084200	2.37514200	0.77569100
C	-2.22652900	1.63960700	1.56243800
C	-0.86380200	1.60053800	1.02410200
C	-0.43830100	2.61489800	-0.04710900
C	-1.53103900	3.53867100	-0.67290500
H	-3.71736000	3.76004400	-0.74849200
H	-4.28195400	2.21546600	1.07960500
H	-0.14336300	1.48266500	1.84071500
H	0.40579600	3.23358100	0.27861600



O	-2.54567300	1.08524200	2.62169500	H	4.81681600	-2.12177400	1.62557900
O	-1.45227200	3.29157300	-2.10075100	H	4.41900900	-3.55456100	-2.41049200
C	-1.23437900	5.02696300	-0.48076700	H	5.85864800	-3.00551200	-0.45439300
H	-0.24464100	5.26338500	-0.88612300	O	6.33847500	1.68549000	0.78122700
H	-1.97658600	5.63865100	-1.00512700	C	6.57820400	2.22465100	2.07017500
H	-1.25759200	5.28984900	0.58215700	H	6.15857000	1.58761500	2.86055300
C	-1.09777100	1.92288600	-2.28092100	H	7.66347100	2.26699900	2.18107000
H	-1.98356000	1.28100700	-2.17425100	H	6.16446100	3.23723200	2.16891500
H	-0.69291700	1.80640600	-3.29107100				
C	-0.05968100	1.68961800	-1.19353700	<b>60-L4</b>			
C	1.11983300	0.97485400	-1.34131600	C	-3.33174600	1.39638200	2.27560600
H	1.21556700	0.44054200	-2.28673400	C	-3.15241400	2.44591200	1.46079500
C	2.42930800	1.15552200	-0.66895900	C	-1.80086100	2.94278900	1.11770900
C	3.58233600	0.82377100	-1.41295100	C	-0.65063400	2.11728500	1.56812100
C	2.63786700	1.66380300	0.62410200	C	-0.84474300	0.99420700	2.36694200
C	4.86123300	1.01083600	-0.91263500	C	-2.20392100	0.65974800	2.96522700
H	3.46548800	0.41480900	-2.41326800	H	-4.33012700	1.04592300	2.53260600
C	3.92005700	1.85796500	1.14326800	H	-3.98479600	2.99885400	1.03274800
H	1.79621900	1.89705100	1.26288300	H	0.32868000	2.58049600	1.48171700
C	5.04364900	1.53632600	0.37446900	H	0.00001100	0.56609800	2.90010700
H	5.73763700	0.75523500	-1.49989200	O	-1.64904800	3.99571900	0.49301200
H	4.02439200	2.25254600	2.14776900	O	-2.46866400	-0.73895000	3.01228600
Rh	-0.39393800	-0.22057800	-0.04045400	C	-2.19107700	1.08538100	4.45324100
C	-1.33072600	-1.69028800	1.27792900	H	-1.40795400	0.53175400	4.98090100
C	-2.21109500	-1.60487700	0.18922900	H	-3.15372200	0.83874700	4.91237500
C	-0.24573400	-2.75245100	1.10149600	H	-2.00916100	2.15920100	4.55524700
C	0.51773700	-2.33919600	-0.16769400	C	-2.35024500	-1.42964200	1.75432500
C	-0.34197200	-2.18028500	-1.24582700	H	-3.09096800	-1.03378500	1.04585100
C	-1.78784800	-2.53799300	-0.95062500	H	-2.62520700	-2.46326800	1.99586900
H	0.40981800	-2.80720100	1.97176400	C	-0.94469600	-1.34306200	1.21451200
C	-1.85071700	-4.00518100	-0.41109800	C	-0.10711100	-2.37262700	1.46838600
C	-0.92123100	-4.13349100	0.82344100	H	-0.55423200	-3.25588700	1.93867100
H	-2.88813600	-4.24830600	-0.15533900	C	1.33793500	-2.52222800	1.23768400
H	-1.54498200	-4.68999400	-1.21009200	C	1.91081400	-3.81206900	1.28024300
H	-0.14368900	-4.88813600	0.65847900	C	2.21713900	-1.44941100	1.01369000
H	-1.48509100	-4.43597600	1.71293800	C	3.26885400	-4.02099300	1.08599800
H	-2.42216500	-2.42464500	-1.83072000	H	1.26636200	-4.66813400	1.46885900
H	-1.56836200	-1.27847000	2.25397100	C	3.58702600	-1.63932100	0.81931100
H	0.00644300	-2.07946000	-2.26941800	H	1.81933000	-0.43761500	0.99286200
C	-3.60103500	-1.09014700	0.22466400	C	4.12249900	-2.93292500	0.85113900
C	-4.24924200	-0.67634000	-0.95544600	H	3.69621600	-5.01872300	1.11711600
C	-4.33516200	-1.06527700	1.42350300	H	4.22154900	-0.77376100	0.66106400
C	-5.57626600	-0.25511000	-0.93863200	C	0.81079800	1.50009100	-1.53606000
H	-3.70118200	-0.66478000	-1.89345300	C	-0.52233300	1.83338000	-1.69176100
C	-5.66522000	-0.64532800	1.44071500	C	1.10990000	0.14208300	-2.18219500
H	-3.86280400	-1.38333100	2.34519900	C	0.10535800	-0.81835700	-1.55838700
C	-6.29267800	-0.24087300	0.26153700	C	-1.23811800	-0.48324400	-1.78878100
H	-6.05141200	0.06525800	-1.86213500	C	-1.33744200	0.85692900	-2.52488100
H	-6.21078300	-0.63767400	2.38037600	H	-2.36792400	1.19567800	-2.63766500
H	-7.33043800	0.08166800	0.27549500	Rh	-0.51249900	0.37734700	0.16917300
C	1.98976800	-2.48580300	-0.25679600	C	0.82045500	0.25152100	-3.71243000
C	2.81773600	-2.18696400	0.83992200	C	-0.65148000	0.69321100	-3.91988100
C	2.59535100	-2.97989800	-1.42611700	H	1.51678100	0.96628600	-4.16559900
C	4.19697100	-2.36903000	0.76814400	H	1.00902100	-0.72321200	-4.17629000
H	2.37831200	-1.78393800	1.74756700	H	2.12462400	-0.20588700	-1.99621700
C	3.97595600	-3.16171600	-1.49886400	H	-0.70644500	1.64897800	-4.45248300
H	1.97468300	-3.25296300	-2.27462600	H	-1.20877500	-0.04146300	-4.51196300
C	4.78334700	-2.85886100	-0.40113200	C	1.88040000	2.41820700	-1.07189600

C	3.23756300	2.04989800	-1.13600500	H	-1.76748800	0.61330600	-0.10136600
C	1.57606300	3.70761300	-0.58376000	C	-4.13120400	2.85802900	-1.05731800
C	4.24660300	2.92586500	-0.73288400	H	-3.74571900	4.88873600	-1.63810400
H	3.52215400	1.07276000	-1.50970400	H	-4.18018300	0.77467000	-0.44718200
C	2.58494100	4.57602300	-0.17566200	C	-0.58102400	-2.18705400	-0.60650300
H	0.54332600	4.02869700	-0.49289000	C	0.68401000	-2.53572200	-0.11633700
C	3.92742000	4.19372500	-0.24907900	C	-0.48616600	-1.68987100	-2.05591400
H	5.28524300	2.61265300	-0.80122400	C	0.53911700	-0.56616400	-1.99798300
H	2.31790600	5.56014200	0.20026400	C	1.80444400	-0.95884200	-1.56527100
H	4.71198400	4.87627200	0.06596100	C	1.80429100	-2.43500900	-1.14725500
C	-2.37918800	-1.43106100	-1.78159900	H	2.75995300	-2.75050200	-0.72720400
C	-3.70453200	-0.96684000	-1.68937200	Rh	0.50011500	-0.35506900	0.22829900
C	-2.17405300	-2.81766900	-1.89779400	C	0.06398900	-2.84588000	-2.94795700
C	-4.78052900	-1.85284600	-1.70619200	C	1.43829500	-3.30295600	-2.39251300
H	-3.89440900	0.09647000	-1.57756300	H	-0.65495500	-3.67311000	-2.95483600
C	-3.24955100	-3.70437400	-1.91320900	H	0.15426300	-2.48695600	-3.97957500
H	-1.16411800	-3.20312200	-1.99120300	H	-1.43676000	-1.31315500	-2.43297200
C	-4.55843400	-3.22711700	-1.81763300	H	1.41109600	-4.35605500	-2.09125600
H	-5.79419800	-1.46866900	-1.62827000	H	2.22572000	-3.20253300	-3.14828200
H	-3.06359600	-4.77097400	-2.00797100	C	-1.87951600	-2.59395200	-0.00733800
H	-5.39663400	-3.91836700	-1.83348100	C	-3.05739100	-2.61352900	-0.77833000
H	0.42045100	-1.81684300	-1.28009200	C	-1.96988800	-3.01075800	1.33744600
H	-0.92586700	2.80956700	-1.44979700	C	-4.27392500	-3.03083700	-0.23405200
O	5.44453600	-3.23646600	0.67637000	H	-3.03422800	-2.32103300	-1.82247300
C	6.35091100	-2.16973700	0.46184800	C	-3.18643000	-3.41948000	1.87773100
H	6.36655100	-1.47379000	1.31156800	H	-1.09495600	-2.98058100	1.98043100
H	7.33607500	-2.62794600	0.35363300	C	-4.34694300	-3.43453100	1.09810800
H	6.11030700	-1.61050800	-0.45302800	H	-5.16281200	-3.04409500	-0.85998200

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C	2.47726000	0.69423100	3.27547100
C	2.19115200	-0.61176800	3.33669900
C	0.84730900	-1.13334200	2.98579700
C	-0.06821000	-0.20628500	2.29610600
C	0.27825700	1.18388200	2.09596900
C	1.49800000	1.76524900	2.84470400
H	3.45476600	1.07390300	3.56892900
H	2.90673200	-1.34548800	3.69981900
H	-1.12199700	-0.47082800	2.35217600
H	-0.57762800	1.85469400	2.08541500
O	0.53868100	-2.29300800	3.28701000
O	2.18955500	2.71451800	2.02835400
C	1.01399100	2.54724000	4.07750300
H	0.36683200	3.37103700	3.75898800
H	1.87292700	2.97005600	4.60880200
H	0.46251800	1.89603700	4.76257000
C	2.27822200	2.21500300	0.68668900
H	3.01914800	1.40739400	0.62949000
H	2.62737900	3.05270000	0.07469800
C	0.89138300	1.76000000	0.30071500
C	0.10084200	2.66082700	-0.35278900
H	0.59989000	3.57361600	-0.69235500
C	-1.33440800	2.66479400	-0.61336100
C	-1.93251700	3.86272400	-1.07263800
C	-2.19156200	1.56705500	-0.40714000
C	-3.29628800	3.96379800	-1.29011500
H	-1.30314800	4.73251400	-1.24728400
C	-3.56773300	1.65356400	-0.61592000

H	-1.76748800	0.61330600	-0.10136600
C	-4.13120400	2.85802900	-1.05731800
H	-3.74571900	4.88873600	-1.63810400
H	-4.18018300	0.77467000	-0.44718200
C	-0.58102400	-2.18705400	-0.60650300
C	0.68401000	-2.53572200	-0.11633700
C	-0.48616600	-1.68987100	-2.05591400
C	0.53911700	-0.56616400	-1.99798300
C	1.80444400	-0.95884200	-1.56527100
C	1.80429100	-2.43500900	-1.14725500
H	2.75995300	-2.75050200	-0.72720400
Rh	0.50011500	-0.35506900	0.22829900
C	0.06398900	-2.84588000	-2.94795700
C	1.43829500	-3.30295600	-2.39251300
H	-0.65495500	-3.67311000	-2.95483600
H	0.15426300	-2.48695600	-3.97957500
H	-1.43676000	-1.31315500	-2.43297200
H	1.41109600	-4.35605500	-2.09125600
H	2.22572000	-3.20253300	-3.14828200
C	-1.87951600	-2.59395200	-0.00733800
C	-3.05739100	-2.61352900	-0.77833000
C	-1.96988800	-3.01075800	1.33744600
C	-4.27392500	-3.03083700	-0.23405200
H	-3.03422800	-2.32103300	-1.82247300
C	-3.18643000	-3.41948000	1.87773100
H	-1.09495600	-2.98058100	1.98043100
C	-4.34694300	-3.43453100	1.09810800
H	-5.16281200	-3.04409500	-0.85998200
H	-3.22540900	-3.72758500	2.91938100
H	-5.29291600	-3.75803600	1.52430000
C	3.06154000	-0.20627000	-1.78949500
C	4.22788300	-0.49994200	-1.05781800
C	3.13405000	0.81753900	-2.75282300
C	5.41121100	0.20514600	-1.27263900
H	4.20538300	-1.27230300	-0.29525800
C	4.31541800	1.52608800	-2.96483800
H	2.26072900	1.04864100	-3.35440200
C	5.46149700	1.22432100	-2.22587100
H	6.29501200	-0.04046700	-0.68975500
H	4.34314400	2.30874200	-3.71857400
H	6.38404800	1.77275100	-2.39505100
H	0.35187200	0.37101700	-2.51119400
H	0.82192500	-3.11855600	0.78910800
O	-5.45796500	3.05416900	-1.30068400
C	-6.35116100	1.97808300	-1.06118600
H	-7.34695600	2.35694900	-1.29869300
H	-6.12784500	1.11703300	-1.70500500
H	-6.32446300	1.65787500	-0.01142000

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C	-2.53415300	-0.48116500	3.31063600
C	-2.41240600	0.84606100	3.19023600
C	-1.12990200	1.48022600	2.79772400
C	-0.07749800	0.58932700	2.27604400
C	-0.24436700	-0.84849300	2.26384200
C	-1.41770800	-1.47074900	3.05462200
H	-3.46885800	-0.93660200	3.63428200
H	-3.22613100	1.52657200	3.42899600

H	0.93349700	0.98816000	2.33139000	H	-0.18834800	1.91343900	-4.26454400
H	0.68594700	-1.40036700	2.37582800	H	1.42469800	1.18145900	-2.48586800
O	-0.98133100	2.70102900	2.93271900	H	-1.76979700	3.86820100	-2.74317500
O	-1.95992000	-2.59696500	2.35840800	H	-2.37699800	2.48049600	-3.64732300
C	-0.89568300	-2.01845400	4.39361900	C	1.56343000	2.84597800	-0.26578100
H	-0.14444100	-2.79261400	4.20573300	C	2.77827000	2.89623800	-0.97549700
H	-1.71978000	-2.46854300	4.95678800	C	1.51929600	3.46051300	1.00328800
H	-0.45186700	-1.22065800	4.99695800	C	3.90260700	3.53128800	-0.44404800
C	-2.04382600	-2.29571900	0.95917800	H	2.85604900	2.45331700	-1.96231900
H	-2.86866800	-1.59705700	0.76794300	C	2.64462300	4.08762300	1.53164200
H	-2.26764300	-3.24288800	0.45812500	H	0.61465100	3.41483400	1.60244700
C	-0.70176000	-1.73462100	0.55538900	C	3.84352300	4.12956300	0.81355700
C	0.21133700	-2.61374700	0.04852900	H	4.82371300	3.55782100	-1.02069500
H	-0.16715900	-3.61586000	-0.17549900	H	2.58212700	4.54496800	2.51574400
C	1.64418500	-2.48108500	-0.19150200	H	4.71838900	4.62155200	1.23026100
C	2.38230200	-3.63875600	-0.50736500	C	-2.94991000	-0.36247500	-1.89084700
C	2.36846500	-1.26889400	-0.10415500	C	-4.18299600	-0.11606100	-1.25786100
C	3.76017600	-3.61210300	-0.71303600	C	-2.84697100	-1.51082400	-2.69821800
H	1.86087100	-4.59036500	-0.58443000	C	-5.26230600	-0.98381500	-1.41793700
C	3.73991000	-1.22622000	-0.29989700	H	-4.29328200	0.75100900	-0.61395600
H	1.83431600	-0.34246200	0.09351500	C	-3.92415300	-2.38138900	-2.85507700
C	4.45155900	-2.39776800	-0.60588900	H	-1.91893200	-1.71361100	-3.22328200
H	4.28003000	-4.53277300	-0.95274800	C	-5.13862900	-2.12343100	-2.21545400
H	4.28285000	-0.28797700	-0.23579200	H	-6.20110300	-0.77064900	-0.91350700
C	0.36053800	2.20075100	-0.85520100	H	-3.81700400	-3.25820400	-3.48848700
C	-0.96485700	2.45763600	-0.48167000	H	-5.98016400	-2.79899900	-2.34178500
C	0.41529600	1.49013100	-2.21518800	H	-0.14994400	-0.70173900	-2.39016700
C	-0.47654000	0.26976500	-2.03487200	H	-1.22585100	3.14437200	0.31771100
C	-1.80361400	0.56178000	-1.72313600	O	5.79405100	-2.24761500	-0.79011800
C	-1.99874400	2.07187100	-1.53517600	C	6.56227500	-3.39491100	-1.11449700
H	-3.00889500	2.32589100	-1.21188200	H	7.59219100	-3.04744500	-1.21479900
Rh	-0.55348300	0.38513000	0.19143400	H	6.51144600	-4.15284300	-0.32152000
C	-0.20582500	2.42715900	-3.29659300	H	6.23720400	-3.84384300	-2.06254700
C	-1.65610900	2.78714300	-2.88073300				
H	0.41221400	3.32674900	-3.39604400				