

## Supporting Information

### **Unveiling the Mechanisms and Secrets of Chemoselectivities in Au(I)-Catalyzed Diazo-Based Couplings with Aryl Unsaturated Aliphatic Alcohols**

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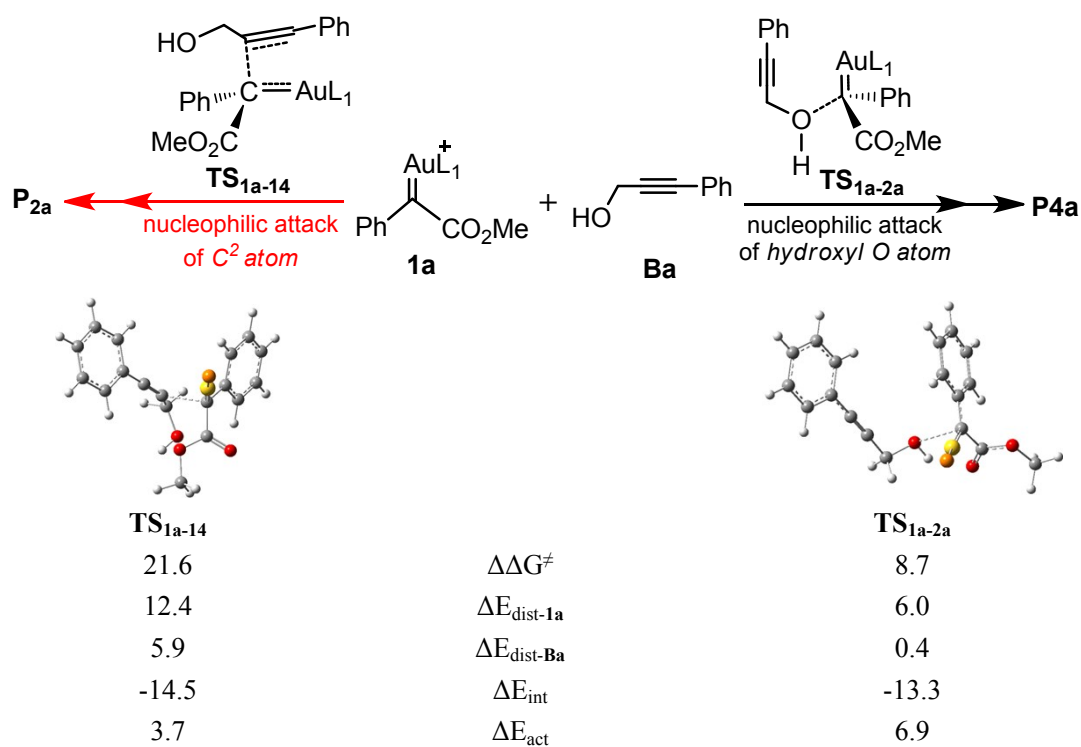
**Table S1** Calculated free energy barriers (kcal mol<sup>-1</sup>) in solvent using M06, M06-2X, M06-L, B3PW91, BP86 and B97D functionals for several steps involved in Figures 3 and 8.

	M06	M06-2X	M06-L	B3PW91	BP86	B97D
<b>2a</b> → <b>TS</b> <sub>2a-11</sub> (in DCE)	17.4	16.4	17.6	12.8	12.4	18.2
<b>21</b> → <b>TS</b> <sub>23-24</sub> (in Et <sub>2</sub> O)	12.2	12.8	13.2	9.7	8.8	16.3

**Table S2** Calculated barriers (kcal mol<sup>-1</sup>) for several selected key steps in the absence and presence of counterions.

	<b>1a→TS<sub>1a-2a</sub></b>	<b>2a→TS<sub>2a-11</sub></b>	<b>2a→TS<sub>1a-14</sub></b>	<b>20→TS<sub>20-21</sub></b>	<b>20→TS<sub>20-44</sub></b>	<b>21→TS<sub>23-24</sub></b>
AuJohnPhos <sup>+</sup>	12.8	17.4	20.2			
JohnPhosAuSbF <sub>6</sub>	14.9	5.8	18.6			
AuPCy <sub>3</sub> <sup>+</sup>				9.2	15.0	12.2
PCy <sub>3</sub> AuNTf <sub>2</sub>				11.4	22.3	18.1

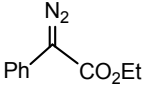
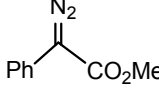
**Table S3** The distortion/interaction analysis of the propargyl C<sup>2</sup> and hydroxyl O atom nucleophilic attack transition states **TS**<sub>1a-2a</sub> and **TS**<sub>1a-14</sub> (The substituents on the phosphorous ligand are omitted for simplicity). The energies are given in kcal mol<sup>-1</sup>.

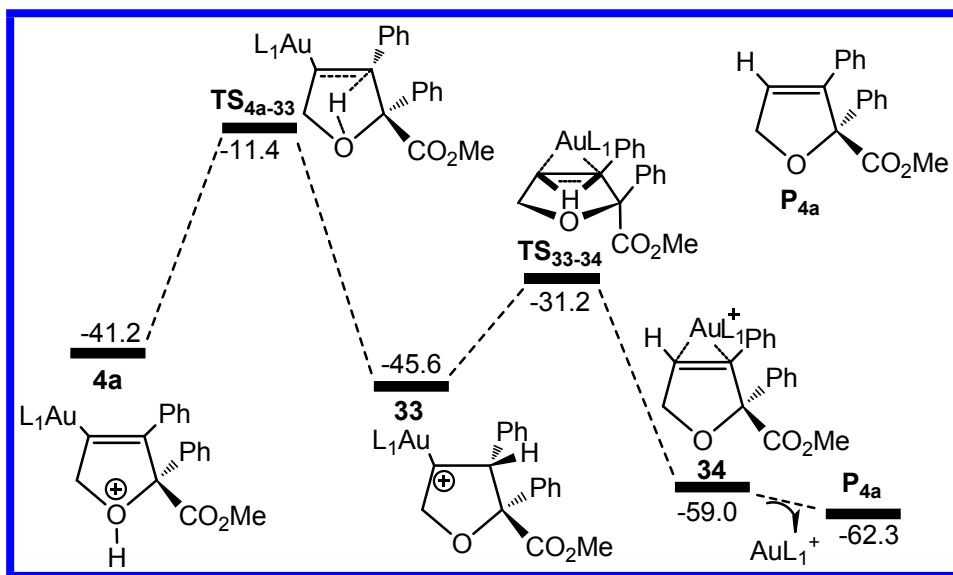


**Table S4** Comparison for the calculated energy barriers (kcal mol<sup>-1</sup>) using JohnPhos and PCy<sub>3</sub> ligands for the ring-opening and H<sub>2</sub>O-assisted [1,3]-H shift steps involved in Fig. 9.

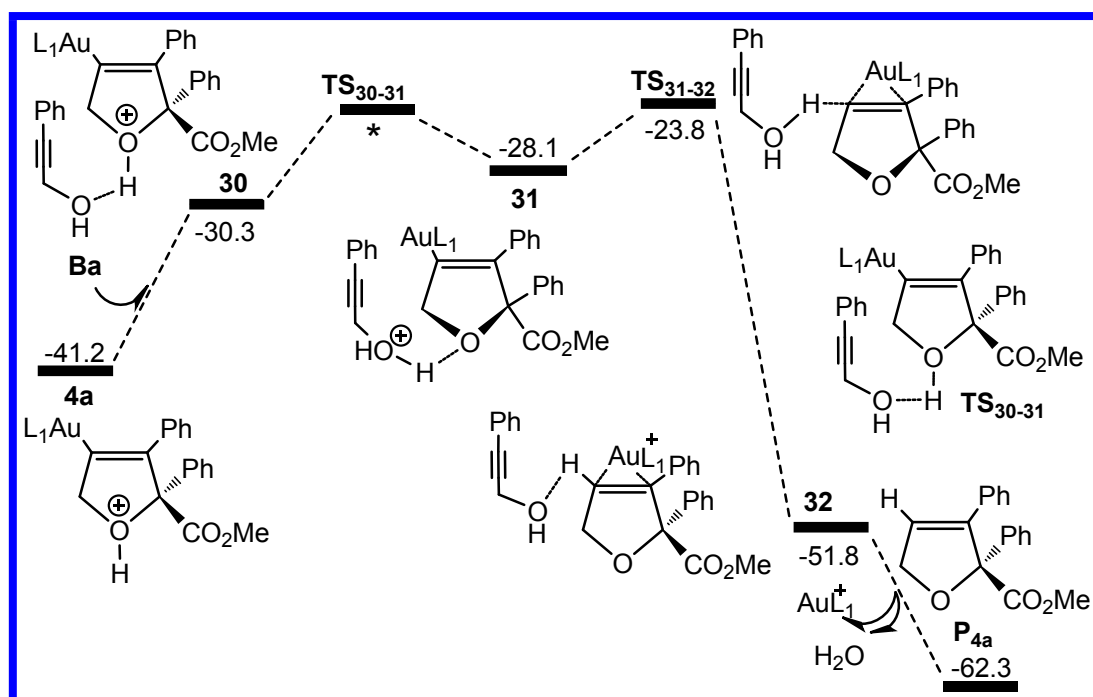
	<b>25→TS<sub>25-26</sub></b>	<b>25→TS<sub>28-29</sub></b>
AuJohnPhos <sup>+</sup>	-1.6	23.2
AuPCy <sub>3</sub> <sup>+</sup>	-1.5	22.8

**Table S5** Comparison for the calculated energy barriers (kcal mol<sup>-1</sup>) using **Aa** and **Ab** for several selected key steps in the **Db**-involved system.

	 ethyl phenyldiazoacetate ( <b>Ab</b> )	 methyl phenyldiazoacetate ( <b>Aa</b> )
<b>21</b> → <b>TS</b> <sub>21-22</sub>	11.1	12.5
<b>21</b> → <b>TS</b> <sub>23-24</sub>	12.2	12.1
<b>21</b> → <b>TS</b> <sub>25-26</sub>	-1.2	-4.2
<b>21</b> → <b>TS</b> <sub>28-29</sub>	23.1	24.2
<b>21</b> → <b>TS</b> <sub>21-43</sub>	19.6	20.9
<b>21</b> → <b>TS</b> <sub>21-47</sub>	44.0	42.4

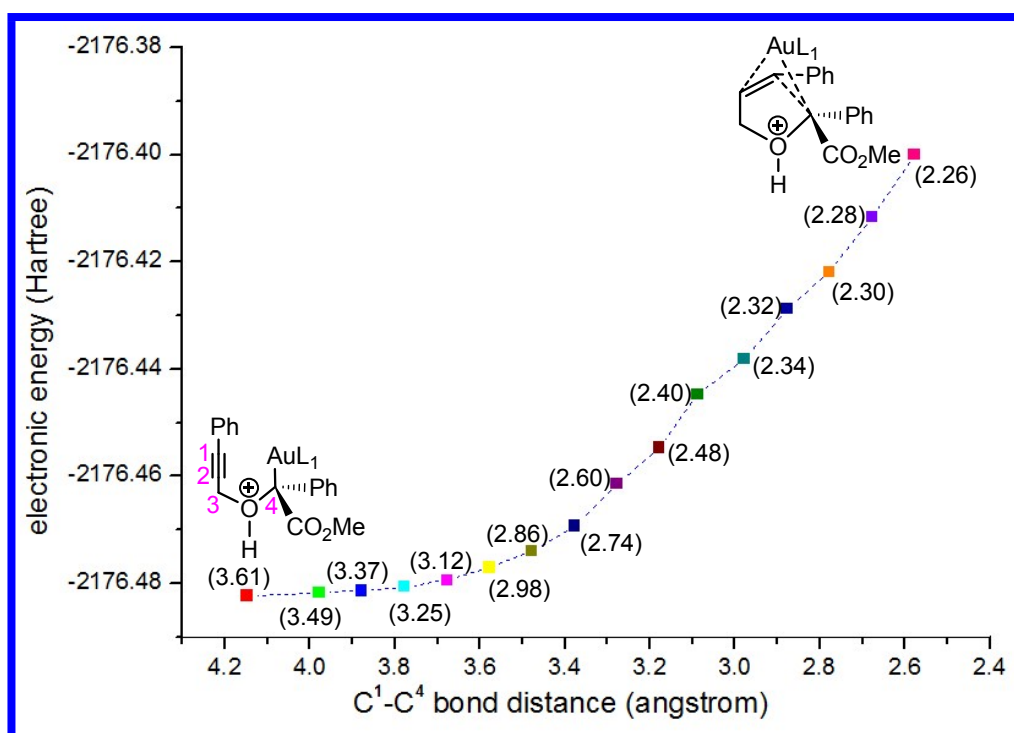


**Fig. S1** Calculated free energy profile in DCE solvent for the **4a** → **P<sub>4a</sub>** transformation via the direct [1,3]-H shift. The relative free energies are given in kcal mol<sup>-1</sup>. L<sub>1</sub> = JohnPhos

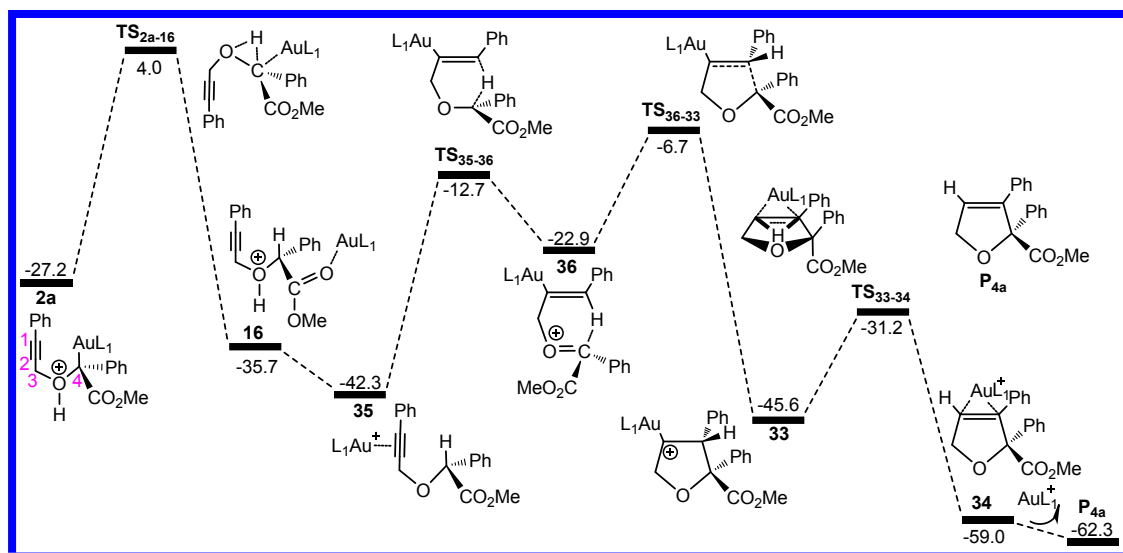


**Fig. S2** Calculated free energy profile in DCE solvent for the **4a** → **P<sub>4a</sub>** transformation via the **Ba**-assisted [1,3]-H shift. The relative free energies are given in kcal mol<sup>-1</sup>. L<sub>1</sub> = JohnPhos

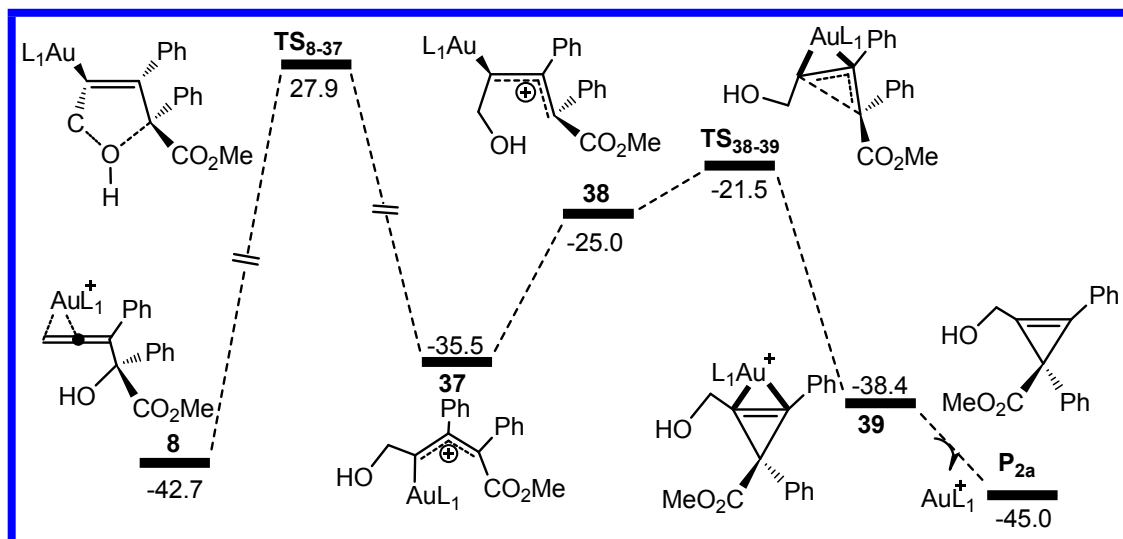




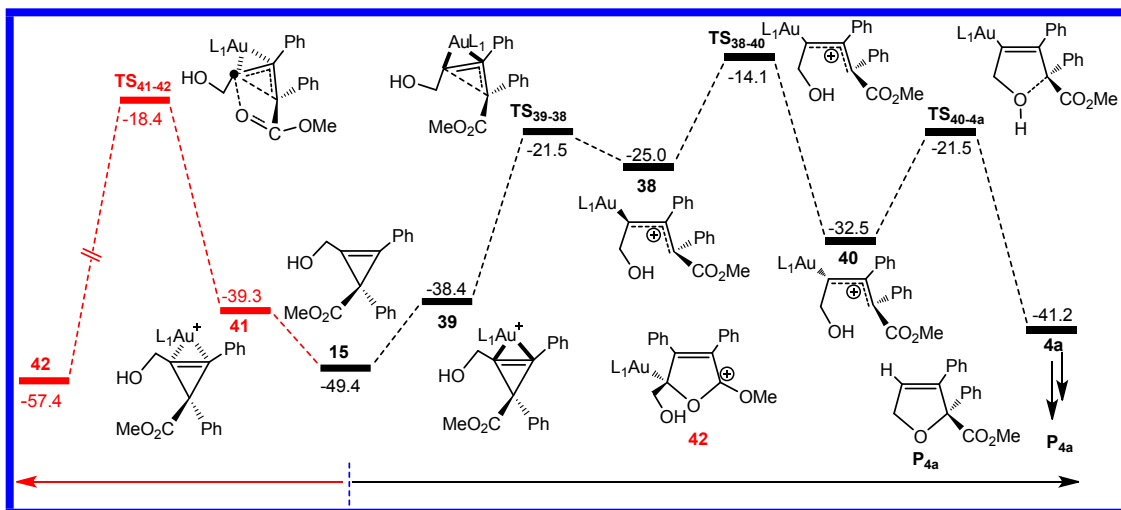
**Fig. S3** Relax energy surface scan of the C<sup>1</sup>-C<sup>4</sup> bond distances for the transition state TS<sub>2a-4a</sub> along the IRC curve. The values in parentheses are the Au-C<sup>2</sup> bond distances.



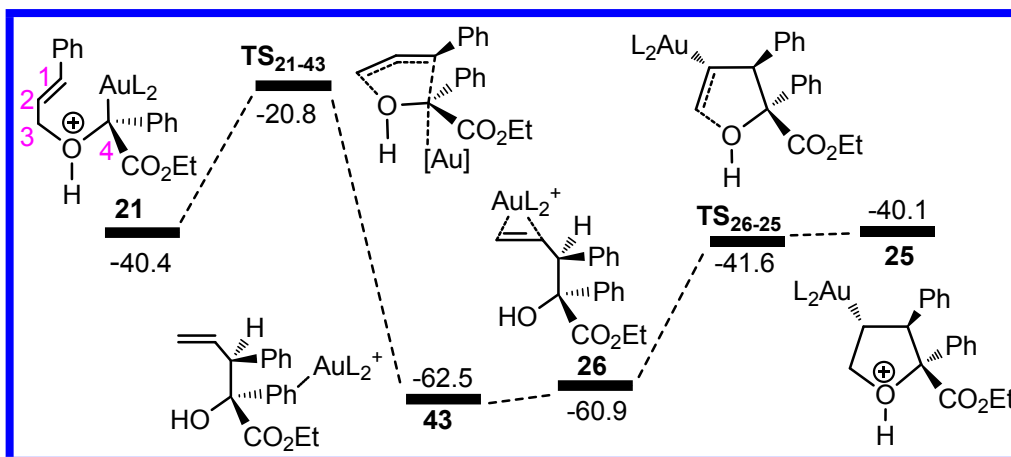
**Fig. S4** Calculated free energy profile in DCE solvent along the possible pathway for forming product **P<sub>4a</sub>** starting from **2a**. The relative free energies are given in kcal mol<sup>-1</sup>.



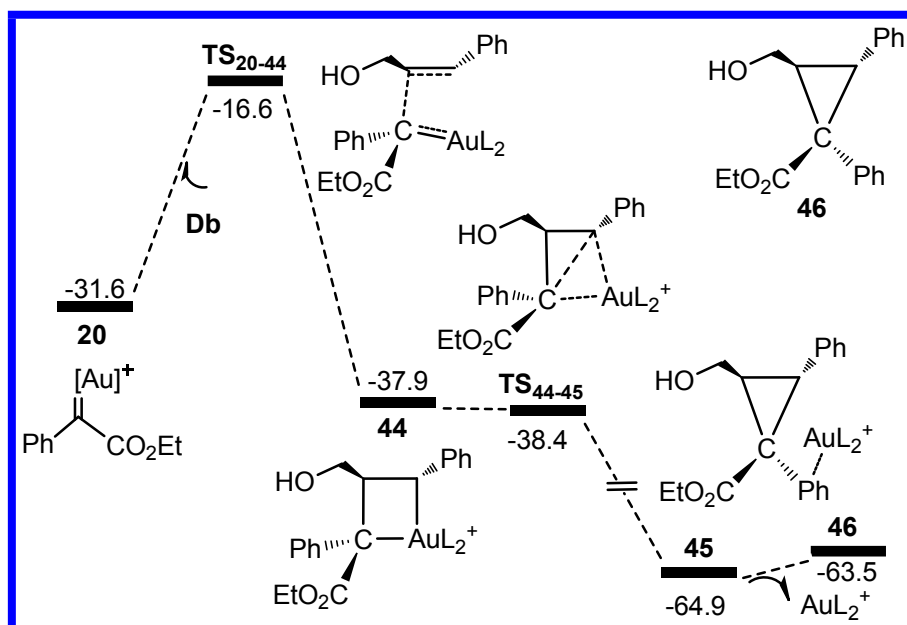
**Fig. S5** Calculated free energy profile in DCE solvent along the possible pathway for forming product **P<sub>2a</sub>** starting from **8**. The relative free energies are given in kcal mol<sup>-1</sup>.



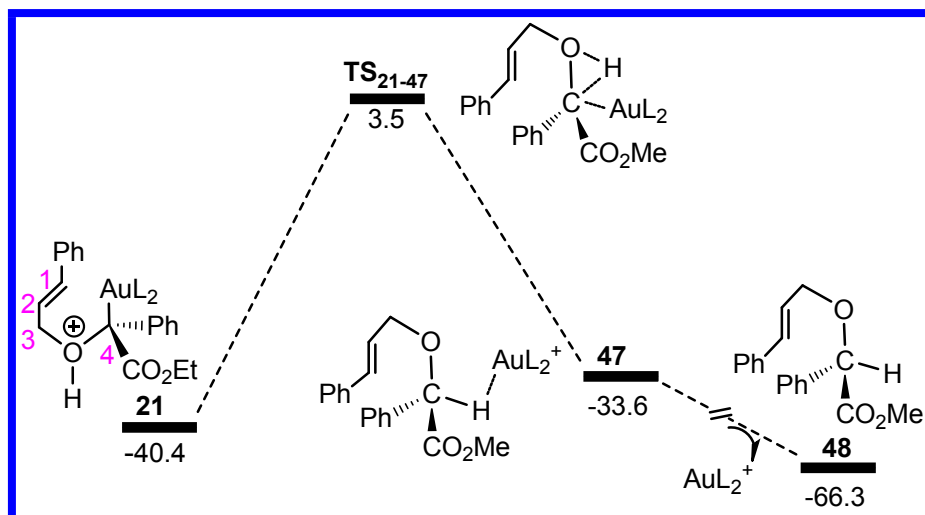
**Fig. S6** Calculated free energy profiles in DCE along two possible pathways bifurcated from **15**. The relative free energies are given in kcal mol<sup>-1</sup>.



**Fig. S7** Calculated free energy profile in Et<sub>2</sub>O solvent along the possible pathway via [2,3]-σ rearrangement for step **21**→**25**. The relative free energies are given in kcal mol<sup>-1</sup>.



**Fig. S8** Calculated free energy profile in Et<sub>2</sub>O solvent along the possible pathway starting from **20**. The relative free energies are given in kcal mol<sup>-1</sup>.



**Fig. S9** Calculated free energy profile in Et<sub>2</sub>O solvent along the possible pathway for [1,2]-H shift of intermediate **21**. The relative free energies are given in kcal mol<sup>-1</sup>.

## Cartesian coordinates for all complexes calculated in this study:

### AuL<sub>1</sub>

P	-1.20021000	-0.20307400	0.10940800
C	-1.88716400	-0.40238300	1.94150600
C	-2.35325400	-0.84366600	-1.35438500
C	-2.68902500	-2.31578900	-1.06814900
H	-3.37192400	-2.42872400	-0.22228600
H	-3.19011100	-2.73393000	-1.94804500
H	-1.79340200	-2.91573800	-0.87947000
C	-3.64722000	-0.03166100	-1.53162800
H	-3.45236700	0.98253900	-1.88459000
H	-4.24943400	-0.52860100	-2.30058500
H	-4.25580700	0.01506800	-0.62643400
C	-1.51113200	-0.73280900	-2.63669900
H	-0.61781500	-1.36426700	-2.59489000
H	-2.11809700	-1.07197300	-3.48351000
H	-1.20617500	0.29810400	-2.84007000
C	-3.35348400	0.04085700	2.05917500
H	-4.02939400	-0.59264400	1.47958000
H	-3.65376400	-0.04326800	3.10974800
H	-3.50033200	1.08317700	1.76651400
C	-1.74205300	-1.87678200	2.35232900
H	-0.70296200	-2.21481700	2.29165800
H	-2.06676000	-1.97886100	3.39383900
H	-2.35810900	-2.54735700	1.74975400
C	-0.99296100	0.47415300	2.83292100
H	0.06312200	0.19826400	2.74924100
H	-1.09646500	1.53748900	2.60381700
H	-1.29169100	0.32472300	3.87623800
C	-0.82067500	1.62956100	-0.17203000
C	0.48557800	2.18535500	-0.27177100
C	-1.92626500	2.49654200	-0.22840300
C	0.60750700	3.57326000	-0.45572900
C	-1.77778300	3.87024900	-0.41219500
H	-2.92785800	2.10188400	-0.11924100
C	-0.50163400	4.41133700	-0.53685900
H	1.60461900	3.99528100	-0.53519100
H	-2.65646600	4.50588600	-0.45385800
H	-0.36518000	5.47776200	-0.68538400
C	1.77377300	1.43367000	-0.11793500
C	2.26374400	0.55613000	-1.12038600
C	2.54030400	1.60591100	1.03983500
C	3.44970100	-0.18100400	-0.91010600
H	1.77636800	0.52672100	-2.09121800
C	3.73091200	0.89122000	1.23685100

H	2.19614000	2.29584000	1.80438000
C	4.17585600	-0.01869800	0.28164100
H	3.83209400	-0.81627000	-1.70356900
H	4.30396400	1.04806600	2.14531300
H	5.09373300	-0.57634200	0.43642200
Au	0.92517500	-1.29271700	-0.15502700
<b>Aa</b>			
C	0.50043900	0.40249700	-0.00030100
C	-0.94291300	0.07906000	-0.00007500
C	-1.38617100	-1.25623400	-0.00048200
C	-1.90504400	1.10688500	0.00049000
C	-2.75129500	-1.54034000	-0.00033500
H	-0.65934900	-2.05698200	-0.00088500
C	-3.26514400	0.80998900	0.00062400
H	-1.59679200	2.14835300	0.00086000
C	-3.69900900	-0.51676900	0.00020500
H	-3.07222500	-2.57828300	-0.00066700
H	-3.98653300	1.62209000	0.00106300
H	-4.75997700	-0.74781400	0.00030000
C	1.62127900	-0.55010000	-0.00012500
O	1.51766000	-1.76223900	-0.00011500
C	2.81561300	0.09477500	0.00021300
O	3.97023500	-0.75934800	0.00059600
H	4.82814900	-0.08726800	0.00084900
H	3.97991100	-1.39461800	0.88969700
H	3.98046100	-1.39464900	-0.88847800
N	0.84832000	1.67389600	-0.00045100
N	1.11823800	2.77968200	-0.00056300
<b>Ba</b>			
C	0.84060400	-0.00022400	-0.22061400
C	2.04781200	-0.00034500	-0.32808100
C	3.50049400	-0.00050300	-0.47930100
H	3.79678700	-0.88603200	-1.06624300
H	3.79680300	0.88386000	-1.06798900
O	4.12085300	0.00075900	0.80394600
H	5.07616200	0.00062700	0.65883800
C	-0.58340300	-0.00009600	-0.09685500
C	-1.29667300	-1.21298600	-0.03486900
C	-1.29647900	1.21294000	-0.03527600
C	-2.68418800	-1.20861600	0.08446600
H	-0.75002700	-2.14945200	-0.07994600
C	-2.68398600	1.20883300	0.08406800
H	-0.74966800	2.14929300	-0.08067100
C	-3.38212400	0.00017100	0.14385400



H	-3.22264000	-2.15081200	0.13186200
H	-3.22229800	2.15112400	0.13115300
H	-4.46427400	0.00028300	0.23708000
N <sub>2</sub>			
N	0.00000000	0.00000000	0.55265300
N	0.00000000	0.00000000	-0.55265300
<b>Au-Ba</b>			
Au	1.35609500	-0.60563700	-0.11524800
P	-0.90291500	0.16252900	-0.55971300
C	-2.06413600	-1.09048800	0.28605400
C	-3.40564700	-0.93459900	0.72269100
C	-1.45785400	-2.35626700	0.42832200
C	-4.05612600	-2.05633000	1.27341200
C	-2.13094100	-3.45122100	0.96277300
H	-0.42792200	-2.50121600	0.11866200
C	-3.44561300	-3.30030400	1.39206200
H	-5.07953100	-1.92863800	1.61162000
H	-1.62085200	-4.40596600	1.04350500
H	-3.99199300	-4.13587200	1.81840400
C	-0.94722900	2.00823200	0.12755100
C	-1.19255300	-0.01030600	-2.49721800
C	-0.98193500	1.89355200	1.65959800
H	-0.91744400	2.90067400	2.08709400
H	-1.90254700	1.43802700	2.02069000
H	-0.13265800	1.31585400	2.03970500
C	-2.12273300	2.83935700	-0.40700500
H	-2.07779200	3.83215200	0.05574400
H	-2.05644500	2.98687200	-1.48851100
H	-3.09325000	2.40833500	-0.17146600
C	0.37319100	2.69263500	-0.27947400
H	0.48166900	2.80533500	-1.35899200
H	0.37718400	3.69743600	0.15801500
H	1.25013800	2.16167400	0.10320600
C	-0.31748600	1.01541700	-3.23340400
H	-0.65999900	2.04191800	-3.08297600
H	0.73482000	0.94752700	-2.93983000
H	-0.37325200	0.80926700	-4.30827000
C	-2.66878900	0.17886800	-2.86497400
H	-2.76927800	0.11248500	-3.95449300
H	-3.28648800	-0.61045200	-2.43097400
H	-3.06419200	1.14734400	-2.55248900
C	-0.75221200	-1.43207400	-2.88920100
H	-1.32471100	-2.20297900	-2.36692300
H	-0.92313800	-1.56371700	-3.96370900
H	0.31261400	-1.59929500	-2.69751000
C	-4.25227900	0.30585900	0.71187300
C	-4.40978600	1.04579200	1.89587300

C	-5.04389700	0.64621500	-0.39528300
C	-5.27667100	2.13818500	1.94849800
H	-3.86286600	0.75042000	2.78673000
C	-5.91465900	1.73713400	-0.34289200
H	-4.99952100	0.04315600	-1.29438600
C	-6.02409500	2.49417800	0.82444800
H	-5.37864900	2.70008400	2.87207200
H	-6.51878400	1.98367800	-1.21096100
H	-6.70299000	3.34039200	0.86516600
C	3.78301700	-0.63134400	0.34203600
C	3.21645600	-1.73389100	0.24824200
C	3.15098800	-3.22786500	0.21218600
H	3.22947700	-3.55113300	-0.82970600
H	4.02476200	-3.61960100	0.75057200
O	1.93832200	-3.75955800	0.70691700
H	1.92747000	-3.66026800	1.66856400
C	4.49047400	0.59793600	0.47971000
C	4.68762900	1.15778600	1.76046400
C	5.03040900	1.23570800	-0.65786900
C	5.41394200	2.33607700	1.89376100
H	4.27547200	0.65967700	2.63203400
C	5.75662200	2.41215800	-0.50909300
H	4.88133200	0.79695800	-1.63913400
C	5.94735700	2.96244200	0.76263300
H	5.56910800	2.76557200	2.87815100
H	6.17736400	2.90034600	-1.38212500
H	6.51584200	3.88073000	0.87279300
<b>5</b>			
C	-3.26134400	0.49537000	0.50378500
C	-4.04386500	-0.46920000	-0.37864500
C	-4.76597300	-0.01914200	-1.49196700
C	-4.05828900	-1.83520700	-0.04948500
C	-5.48264700	-0.93390600	-2.26575000
H	-4.75484300	1.02696500	-1.76780800
C	-4.79236000	-2.73641700	-0.81725800
H	-3.49566000	-2.19847300	0.80687700
C	-5.50434400	-2.28803500	-1.93202000
H	-6.03326100	-0.57705900	-3.13049900
H	-4.80177900	-3.78772400	-0.54729000
H	-6.07067600	-2.99010900	-2.53558900
C	-3.17727400	1.97623000	0.15243400
O	-3.05253300	2.37584000	-0.98177000
O	-3.22092300	2.74296300	1.24891800
C	-3.07681100	4.17063700	1.03271500
H	-3.18259200	4.61917100	2.01846200
H	-2.09318100	4.38445100	0.61057700
H	-3.85512100	4.52592500	0.35605600

N	-3.63036500	0.33978600	1.83632500
N	-3.90240800	0.16464300	2.90843400
P	1.24078400	-0.59876300	0.12649700
C	1.33723500	-2.32978500	-0.82865400
C	1.93313900	-0.58947400	1.97591700
C	0.93811500	-1.39894200	2.82870300
H	0.89959000	-2.45226100	2.53617400
H	1.27152500	-1.36268000	3.87200100
H	-0.07606000	-0.98929800	2.78694400
C	3.33498000	-1.18860600	2.16500600
H	4.08759800	-0.72846700	1.53079800
H	3.63026400	-1.01696600	3.20688800
H	3.34755100	-2.26646800	2.00176500
C	1.91423300	0.88516800	2.41168300
H	0.92273000	1.33422600	2.29130300
H	2.18063700	0.94064500	3.47321000
H	2.63566000	1.48592800	1.85379400
C	2.58477600	-3.14950800	-0.46737200
H	2.52670500	-3.55034200	0.54713200
H	2.64092100	-4.00630900	-1.14900800
H	3.51306200	-2.58603200	-0.56422500
C	0.08163700	-3.14169400	-0.46322900
H	-0.83759400	-2.63802600	-0.77670200
H	0.12917800	-4.10615400	-0.98214700
H	0.01553500	-3.34958300	0.60857200
C	1.31816400	-2.01102700	-2.33194300
H	0.43844500	-1.42751400	-2.61999900
H	2.20739900	-1.46437900	-2.65437200
H	1.28397100	-2.95630000	-2.88511600
C	1.92104400	0.79832900	-0.97988600
C	3.26266800	1.21947300	-1.15565200
C	0.91157600	1.47975100	-1.68968100
C	3.51048000	2.32250100	-1.99568700
C	1.18480600	2.55160300	-2.53436700
H	-0.12304400	1.17097700	-1.58143900
C	2.49846600	2.98695700	-2.67999800
H	4.54022900	2.64320000	-2.11750400
H	0.37124300	3.04025800	-3.06102800
H	2.73788600	3.82804900	-3.32319100
C	4.49162100	0.61322900	-0.55599400
C	5.03938400	-0.57102900	-1.07097800
C	5.20959100	1.31394200	0.42736800
C	6.24560200	-1.07237800	-0.57606900
H	4.54037300	-1.08074100	-1.88929300
C	6.41438900	0.81308400	0.92255700
H	4.82038300	2.25614500	0.80298000
C	6.93074600	-0.38682200	0.42842300
H	6.65830900	-1.98787400	-0.98938900

H	6.95264400	1.36389900	1.68799700
H	7.87030700	-0.77460900	0.80969300
Au	-1.11381700	-0.06143100	0.40533800
TS <sub>5-6</sub>			
C	-3.14278800	0.43705500	0.35034200
C	-4.16838200	-0.41924800	-0.29983500
C	-5.37572500	0.12486200	-0.78188300
C	-3.94603500	-1.80468700	-0.42225300
C	-6.32070400	-0.69609600	-1.38901500
H	-5.56237100	1.19054100	-0.70880600
C	-4.90137800	-2.62445700	-1.01494600
H	-3.01894700	-2.22901200	-0.04831200
C	-6.08813100	-2.06991800	-1.50237700
H	-7.24091500	-0.26616200	-1.77101700
H	-4.72011100	-3.69072800	-1.10390200
H	-6.83065300	-2.70728300	-1.97256200
C	-3.21268600	1.92944400	0.11618400
O	-3.23370900	2.36813800	-1.01267100
O	-3.16419400	2.66237300	1.23575200
C	-3.10181400	4.09898400	1.04587700
H	-3.13344500	4.52113600	2.04842600
H	-2.17177600	4.36601600	0.54056600
H	-3.95288400	4.43665800	0.45264900
N	-3.50063700	0.29456300	2.02564500
N	-3.64579800	-0.06306500	3.06525300
P	1.29286900	-0.61817100	0.00798400
C	1.45852000	-2.21931200	-1.14516000
C	1.91179700	-0.84682500	1.86877000
C	0.89980500	-1.78452500	2.55439900
H	0.91123900	-2.79102500	2.12586300
H	1.17645200	-1.87771900	3.61071300
H	-0.12390400	-1.39985900	2.50882300
C	3.31831100	-1.43525900	2.05351500
H	4.09129400	-0.86510100	1.54607300
H	3.54466700	-1.41707900	3.12633900
H	3.37926200	-2.47485700	1.73111500
C	1.83614800	0.55481100	2.49868500
H	0.83955400	0.99733000	2.39697600
H	2.05861300	0.47220000	3.56857800
H	2.56402200	1.23982500	2.05779900
C	2.66054700	-3.10529100	-0.78621900
H	2.51732400	-3.61860200	0.16795300
H	2.75924500	-3.88009300	-1.55573100
H	3.60123300	-2.55526500	-0.74544200
C	0.16650600	-3.04110500	-0.98801500
H	-0.71099200	-2.48605100	-1.33268500
H	0.25138500	-3.94756800	-1.59876000

H	-0.00556800	-3.35644800	0.04529100
C	1.57075600	-1.72509300	-2.59606300
H	0.73201100	-1.08294800	-2.88113400
H	2.49483900	-1.17168200	-2.77805600
H	1.56318900	-2.59587900	-3.26137000
C	2.02031200	0.89759400	-0.89116300
C	3.36544200	1.33725900	-0.96076000
C	1.03861100	1.65540700	-1.56163600
C	3.64311200	2.52855000	-1.65920200
C	1.34136300	2.81586000	-2.26819100
H	0.00207600	1.33496300	-1.53203500
C	2.65774300	3.26533400	-2.30752400
H	4.67532000	2.86170600	-1.70037700
H	0.54897100	3.35978600	-2.77267000
H	2.92020800	4.17309200	-2.84193300
C	4.56971800	0.66953600	-0.37712300
C	5.14121500	-0.45961100	-0.98208300
C	5.24209300	1.26633200	0.70234600
C	6.32609400	-1.00994600	-0.48769000
H	4.67705400	-0.88709600	-1.86534700
C	6.42505900	0.71609300	1.19750700
H	4.83331600	2.16599900	1.15382300
C	6.96567500	-0.42917400	0.60878100
H	6.75796200	-1.88107000	-0.97139300
H	6.92744800	1.18609400	2.03760900
H	7.88853100	-0.85511700	0.99015400
Au	-1.09158900	-0.10911600	0.25747400
<b>6</b>			
C	-3.07314100	0.44840400	-0.21877500
C	-4.20182400	-0.39346100	-0.36067800
C	-5.53058700	0.13231500	-0.40217200
C	-4.02930700	-1.80809200	-0.44321900
C	-6.61772600	-0.71400900	-0.51877500
H	-5.68433000	1.20482900	-0.34921500
C	-5.12291700	-2.64851900	-0.55260000
H	-3.02040700	-2.20582000	-0.41104500
C	-6.41387800	-2.10124100	-0.59181400
H	-7.62441500	-0.31152600	-0.55355100
H	-4.98685600	-3.72313900	-0.60986100
H	-7.27156500	-2.76178900	-0.68095100
C	-3.28718000	1.92188300	-0.19093300
O	-3.22390900	2.55586000	-1.22595500
O	-3.48728000	2.41507400	1.02958000
C	-3.57329900	3.86250300	1.12853400
H	-3.71534400	4.06686400	2.18767000
H	-2.64940000	4.31558200	0.76467100
H	-4.41797700	4.23076700	0.54393100

N	-3.12162200	-0.45074800	3.43709100
N	-2.68957900	0.40521300	3.98641200
P	1.31182800	-0.58989400	-0.22129400
C	1.64009000	-1.96763200	-1.60605600
C	1.67071800	-1.15452400	1.63558900
C	0.57165000	-2.17102800	2.00105400
H	0.63363500	-3.08196500	1.39799300
H	0.70784200	-2.46546900	3.04799400
H	-0.43562100	-1.75477500	1.90013900
C	3.03754000	-1.79915400	1.90601900
H	3.87251500	-1.16857000	1.61385600
H	3.11412200	-1.96918700	2.98676700
H	3.14261600	-2.76941700	1.42068000
C	1.50939200	0.11848500	2.48500800
H	0.53873800	0.60056700	2.32716600
H	1.57868000	-0.15431400	3.54425300
H	2.29449800	0.84902600	2.27623400
C	2.76861500	-2.94252000	-1.24220500
H	2.48437300	-3.60578000	-0.42128400
H	2.96992700	-3.57801100	-2.11291700
H	3.69881200	-2.44051200	-0.97503500
C	0.33308500	-2.76169000	-1.78522300
H	-0.48256100	-2.12605300	-2.14322500
H	0.49843500	-3.54761600	-2.53150000
H	0.01270100	-3.24934500	-0.85971000
C	1.96637400	-1.22979600	-2.91386800
H	1.17943600	-0.52488400	-3.19841100
H	2.90693800	-0.67738200	-2.85747600
H	2.05670700	-1.96881800	-3.71802900
C	2.16320000	1.04171000	-0.71995400
C	3.50928400	1.44529700	-0.53671900
C	1.27995800	1.94397000	-1.34689800
C	3.88150700	2.73791900	-0.95440800
C	1.67741500	3.20777600	-1.77429600
H	0.24537400	1.65637300	-1.50459700
C	2.99148000	3.61476600	-1.56536600
H	4.91277300	3.04091800	-0.80328700
H	0.95900800	3.86279600	-2.25710000
H	3.32597100	4.59880800	-1.87888200
C	4.62499100	0.64495600	0.05671700
C	5.25816400	-0.37467100	-0.66887800
C	5.16211400	1.01711000	1.30047100
C	6.36729000	-1.04120300	-0.14270000
H	4.90567000	-0.62189500	-1.66516800
C	6.26934000	0.35091700	1.82714800
H	4.70678800	1.83265700	1.85531900
C	6.86975500	-0.68654800	1.11033200
H	6.84875200	-1.82445800	-0.72070900

H	6.66656700	0.64680900	2.79346100
H	7.73397000	-1.20237200	1.51728400
Au	-1.10415800	-0.07514900	-0.20875400
<b>1a</b>			
C	-2.50371700	-0.43403200	0.14599600
C	-3.45511700	0.31190500	-0.59498900
C	-4.85983500	0.15550100	-0.38657000
C	-3.01737000	1.23790800	-1.58788400
C	-5.76777500	0.88059300	-1.13676700
H	-5.21647000	-0.53751600	0.36791500
C	-3.93270600	1.95809200	-2.33647900
H	-1.95066300	1.36126100	-1.74044400
C	-5.30481800	1.77827700	-2.11166200
H	-6.83343100	0.75731500	-0.97569800
H	-3.59370200	2.65780700	-3.09302400
H	-6.02204900	2.34262400	-2.70070900
Au	-0.48123300	-0.38825500	-0.01162100
C	-3.00262600	-1.31603900	1.23790500
O	-3.08500200	-0.88723400	2.37244700
O	-3.28307800	-2.55789900	0.84291700
C	-3.68104200	-3.48482200	1.88763300
H	-3.85586100	-4.43006500	1.37783000
H	-2.88285300	-3.58186000	2.62590600
H	-4.59062600	-3.13342600	2.37783900
P	1.92187200	-0.70776100	-0.37830800
C	3.03577400	0.69487700	0.19924800
C	2.54655400	1.92967900	0.68751400
C	4.42668300	0.51675100	0.08441900
C	3.47549000	2.93955000	1.00255300
C	5.32843100	1.52267100	0.42191800
H	4.82138300	-0.41943300	-0.28719300
C	4.84755400	2.74893000	0.87539300
H	3.09707400	3.88583900	1.37631000
H	6.39499600	1.34699000	0.32313900
H	5.53316600	3.54880500	1.13722000
C	2.44261400	-2.33144900	0.61366800
C	2.17890100	-0.82582500	-2.32394200
C	2.60913300	-1.90638400	2.08315400
H	2.80225600	-2.79955200	2.68816100
H	3.44548400	-1.21807600	2.22614600
H	1.70122400	-1.43553800	2.47437500
C	3.73034200	-3.00161700	0.10919300
H	3.92712100	-3.87982000	0.73536300
H	3.64200400	-3.35690800	-0.92047000
H	4.60793500	-2.35708300	0.18652700
C	1.28284700	-3.34008500	0.51025500
H	1.09728300	-3.66600400	-0.51560200

H	1.54081500	-4.22862800	1.09804400
H	0.35135900	-2.93048700	0.91147100
C	1.40809700	-2.05198100	-2.83971600
H	1.86949000	-2.99274900	-2.52807800
H	0.36379000	-2.05002900	-2.51145200
H	1.41298900	-2.03565700	-3.93562300
C	3.64908500	-0.90335500	-2.76202600
H	3.67659000	-0.99497500	-3.85414400
H	4.20530600	-0.00148400	-2.49900800
H	4.17074300	-1.77016200	-2.35192600
C	1.55583700	0.45986800	-2.89824800
H	2.04373900	1.35897000	-2.51003800
H	1.67911100	0.45775300	-3.98733100
H	0.48502600	0.52373000	-2.68149100
C	1.11358400	2.27983100	0.93776600
C	0.50208800	3.30242000	0.19509600
C	0.40641700	1.72093600	2.01909600
C	-0.77903100	3.75374800	0.52144100
H	1.04547600	3.76054200	-0.62649900
C	-0.87422300	2.17885100	2.34941200
H	0.88405300	0.96775400	2.63866500
C	-1.46786600	3.19727700	1.60213800
H	-1.22726900	4.55848500	-0.05426900
H	-1.39766200	1.74368300	3.19472400
H	-2.45368800	3.56508800	1.87004300
<b>TS<sub>1a-2a</sub></b>			
C	-1.20730300	-2.18734500	-0.23762700
C	-2.48502500	-2.17201800	-0.87821800
C	-3.32159200	-3.32342000	-0.90096400
C	-2.95127200	-0.98933100	-1.51262300
C	-4.54872500	-3.29333700	-1.54277200
H	-3.00297100	-4.23164200	-0.40006900
C	-4.17811700	-0.96476100	-2.15608900
H	-2.32413900	-0.10578900	-1.47988500
C	-4.97606600	-2.11652400	-2.17267800
H	-5.17962500	-4.17584300	-1.55524500
H	-4.52145600	-0.05828700	-2.64362800
H	-5.93810100	-2.09707100	-2.67636800
Au	0.21130000	-0.71348600	-0.36686800
C	-0.70818300	-3.52331600	0.24199500
O	-0.79837600	-3.95820800	1.37771200
O	-0.11747300	-4.16955700	-0.76737500
C	0.43351600	-5.47587300	-0.46404600
H	0.82033800	-5.84777300	-1.41075300
H	1.23318400	-5.38494300	0.27280100
H	-0.34615900	-6.13367800	-0.07601600
P	1.80046800	1.05251200	-1.01820600

C	3.36731400	1.33076000	-0.00638900
C	3.63902300	0.69924000	1.22840400
C	4.28569300	2.27997800	-0.49274900
C	4.79682300	1.07850100	1.93501300
C	5.43622100	2.62427500	0.21131100
H	4.09747400	2.77541600	-1.43475800
C	5.68826100	2.02593000	1.44367600
H	4.99988500	0.59111600	2.88345800
H	6.12116100	3.35897900	-0.20019800
H	6.57474400	2.28541200	2.01403500
C	2.37283100	0.57633200	-2.85129200
C	0.80937600	2.75016700	-0.89426400
C	3.48351500	-0.47664200	-2.69459100
H	3.77016000	-0.83844400	-3.68863700
H	4.37696100	-0.06983300	-2.21512500
H	3.14152000	-1.34096000	-2.11553200
C	2.88007200	1.75924600	-3.69201900
H	3.14858500	1.38197900	-4.68581400
H	2.11636300	2.52742200	-3.83613300
H	3.77672900	2.22631600	-3.28147100
C	1.17322800	-0.06205000	-3.57710600
H	0.33546300	0.62950000	-3.69343800
H	1.49457900	-0.36183300	-4.58133000
H	0.81255900	-0.95624600	-3.06088500
C	-0.38273600	2.68701100	-1.86202100
H	-0.06986100	2.72972800	-2.90884500
H	-0.98157400	1.78388700	-1.71305900
H	-1.03348800	3.54892900	-1.67728400
C	1.64985700	4.00223600	-1.18751900
H	0.99186300	4.87609100	-1.11353800
H	2.45272600	4.13985700	-0.46085600
H	2.07995100	4.00554700	-2.19161400
C	0.30361500	2.81604400	0.55830100
H	1.13104400	2.82313700	1.27467600
H	-0.26283100	3.74459600	0.69367200
H	-0.36405600	1.98492200	0.80384600
C	2.83790000	-0.38827300	1.86992000
C	2.18947000	-0.15614700	3.09254600
C	2.88915600	-1.70153600	1.37354800
C	1.60269100	-1.20861700	3.80017100
H	2.16974600	0.84953700	3.50279900
C	2.30964800	-2.75265500	2.08610500
H	3.43000200	-1.90321900	0.45350000
C	1.66349100	-2.51086100	3.30039300
H	1.12366300	-1.01271100	4.75529200
H	2.38842700	-3.76682000	1.70708100
H	1.22590000	-3.33371200	3.85683300
C	-3.15383100	1.53823900	1.89948800

C	-2.63966500	0.51407200	2.29755800
C	-2.02399700	-0.69984500	2.82200200
H	-0.94534800	-0.54384300	2.95740500
H	-2.45170000	-0.93080500	3.80970500
O	-2.26677100	-1.80030000	1.93784400
H	-1.77173200	-2.58455800	2.24329600
C	-3.76525600	2.74483100	1.43630800
C	-4.80097100	2.69981100	0.48274700
C	-3.34478600	3.99476600	1.93179100
C	-5.39379300	3.87779200	0.03441000
H	-5.13621400	1.73684200	0.11028300
C	-3.94646100	5.16702600	1.47999600
H	-2.55639900	4.03295200	2.67682200
C	-4.96935600	5.11329100	0.52986100
H	-6.19518300	3.83238700	-0.69708300
H	-3.62025800	6.12476600	1.87432200
H	-5.43807500	6.02893100	0.18252000
<b>2a</b>			
C	-2.91933600	-0.81675200	0.19206200
C	-3.59860800	-2.15722700	0.28995100
C	-4.80223700	-2.29242600	1.01211500
C	-3.08948100	-3.28264500	-0.38374300
C	-5.46105800	-3.51841500	1.07268800
H	-5.21944400	-1.43562300	1.53412300
C	-3.75052600	-4.50873400	-0.32229500
H	-2.16374300	-3.18903700	-0.94331400
C	-4.93455700	-4.62907800	0.40823400
H	-6.38225800	-3.60814200	1.63977300
H	-3.33960400	-5.37003600	-0.83978400
H	-5.44594800	-5.58534600	0.46025600
Au	-0.85072900	-0.77545000	-0.27828000
C	-3.13396500	0.08435500	1.39708200
O	-3.64555800	1.18219100	1.39556700
O	-2.61750100	-0.51475400	2.48678600
C	-2.68048500	0.24934600	3.71020000
H	-3.71426900	0.51254800	3.94285600
H	-2.26607900	-0.40153000	4.47828000
H	-2.08748400	1.16198400	3.61714800
P	1.58492300	-0.81203900	-0.58891600
C	2.27271100	0.80398100	0.16187500
C	3.56535100	1.11517300	0.66084800
C	1.30049000	1.82631300	0.15507900
C	3.80215200	2.42785900	1.11458600
C	1.56475800	3.11949900	0.59862600
H	0.30127300	1.60532000	-0.20587300
C	2.83198000	3.42384500	1.08491700
H	4.79086800	2.65646400	1.49995100

H	0.78073300	3.86902400	0.56822700
H	3.06619600	4.42148500	1.44361500
C	2.15817900	-2.47081400	0.29870000
C	1.98860300	-0.74253900	-2.51024700
C	2.03353100	-2.20803300	1.80905400
H	2.25059500	-3.13848000	2.34630000
H	2.73517300	-1.45182700	2.15762400
H	1.01926200	-1.89609100	2.07965000
C	3.57011700	-2.94131100	-0.07756300
H	3.80030100	-3.84116600	0.50507900
H	3.63777700	-3.21875200	-1.13336100
H	4.33754000	-2.20195100	0.13953100
C	1.15037700	-3.57627400	-0.07700600
H	1.15348200	-3.81431700	-1.14212800
H	1.43343600	-4.48682200	0.46362200
H	0.13029800	-3.31792800	0.22101700
C	1.51812100	-2.04662000	-3.17291900
H	2.13211400	-2.90438600	-2.88864900
H	0.47194900	-2.27204600	-2.94183600
H	1.60023500	-1.93558800	-4.26032800
C	3.47815600	-0.50983400	-2.78579600
H	3.64067100	-0.51247100	-3.87025000
H	3.79826200	0.46403100	-2.40961800
H	4.11726400	-1.28046000	-2.35068100
C	1.18405200	0.43694400	-3.08444400
H	1.46003900	1.38826400	-2.62221500
H	1.39157500	0.51496700	-4.15808500
H	0.10673800	0.29196700	-2.95794300
C	4.75370900	0.20892500	0.81652700
C	5.04071700	-0.34579200	2.07503000
C	5.69704000	0.04902100	-0.20960500
C	6.19782800	-1.09831800	2.28071100
H	4.36036800	-0.17020000	2.90328200
C	6.85631900	-0.70255600	-0.00523000
H	5.53772000	0.53197000	-1.16647200
C	7.10445800	-1.28919500	1.23654300
H	6.39630600	-1.52289000	3.26029500
H	7.57258300	-0.81464500	-0.81381900
H	8.00704500	-1.87120800	1.39561600
C	-2.40993200	3.05760500	-1.19983800
C	-2.77728800	1.97602300	-1.60689600
C	-3.26155300	0.70486600	-2.07394200
H	-4.10113000	0.80607700	-2.76975300
H	-2.47754200	0.08193300	-2.51608900
O	-3.84634900	-0.07883600	-0.93519500
H	-4.41987200	-0.78723200	-1.28395700
C	-2.00365600	4.31383000	-0.65805700
C	-2.30353500	4.60852100	0.68750800

C	-1.31533200	5.25653900	-1.44468500
C	-1.91219400	5.82990900	1.23007500
H	-2.83877900	3.87523400	1.28233400
C	-0.93373500	6.47554000	-0.88934700
H	-1.09139100	5.02945400	-2.48198700
C	-1.22912100	6.76403600	0.44579600
H	-2.14604300	6.05663800	2.26578300
H	-0.40767200	7.20277000	-1.49998400
H	-0.93187000	7.71698600	0.87278300
<b>3a</b>			
C	-3.28665300	-1.20638800	-0.06035700
C	-4.22906300	-2.31302600	0.08015700
C	-3.83335900	-3.53851700	0.65932000
C	-5.54854100	-2.21072300	-0.41220700
C	-4.72671300	-4.60118800	0.74593700
H	-2.82492300	-3.64631800	1.03691800
C	-6.42755900	-3.29248500	-0.34413100
H	-5.92398500	-1.26672700	-0.79976000
C	-6.02434600	-4.49265500	0.23710000
H	-4.39898600	-5.53196100	1.19960600
H	-7.43663200	-3.18314100	-0.73017700
H	-6.71017300	-5.33162700	0.29744400
Au	0.61827800	0.19677500	-0.12034300
C	-2.12291400	-0.85367200	0.57228400
O	-1.45329300	0.21787500	0.26536200
O	-1.71937200	-1.66230000	1.58532500
C	-1.19260900	-1.02100100	2.76167900
H	-1.91774000	-0.30802600	3.16723700
H	-1.02406900	-1.82465500	3.47814800
H	-0.24943800	-0.51059000	2.55075100
P	2.95693100	0.25399600	-0.59723600
C	3.80634900	1.16111600	0.85288700
C	5.15060800	1.11036100	1.30598600
C	2.91769800	2.03875200	1.50826200
C	5.51903300	1.94228900	2.38205100
C	3.31183100	2.85949200	2.56082200
H	1.88182400	2.07689800	1.18720500
C	4.62932600	2.81066600	3.00480000
H	6.54686600	1.89281500	2.72738200
H	2.58860200	3.52030800	3.02846100
H	4.96360900	3.43400400	3.82835300
C	3.46464500	-1.62810000	-0.85566700
C	3.20045900	1.39599800	-2.17922300
C	3.46843400	-2.26338200	0.54482200
H	3.65508200	-3.33827700	0.44053200
H	4.24582800	-1.85230300	1.18721600
H	2.50082200	-2.13987400	1.04229200

C	4.80914000	-1.82058700	-1.57111700
H	5.02086700	-2.89514000	-1.61830100
H	4.77492300	-1.45525200	-2.60125000
H	5.63996000	-1.34166200	-1.05838600
C	2.35699700	-2.30637400	-1.68787800
H	2.28613300	-1.91540600	-2.70382700
H	2.60195300	-3.37213000	-1.76243300
H	1.37418300	-2.22242000	-1.21506100
C	2.60901800	0.69214400	-3.41046500
H	3.19200800	-0.18094000	-3.71343400
H	1.57069400	0.38471100	-3.25187800
H	2.62080800	1.39656000	-4.25012500
C	4.67659500	1.73674100	-2.41393000
H	4.75335600	2.35961900	-3.31290400
H	5.08425700	2.31363500	-1.58083200
H	5.29985100	0.85363100	-2.56862600
C	2.42108000	2.69542500	-1.91129600
H	2.79656000	3.22808100	-1.03357900
H	2.54006700	3.35759200	-2.77666800
H	1.35204800	2.50707000	-1.77314300
C	6.27301200	0.24206100	0.81282000
C	6.60489600	-0.92558900	1.51995100
C	7.12473500	0.65765300	-0.22174400
C	7.71204400	-1.69359400	1.15663500
H	6.00119400	-1.22312800	2.37242400
C	8.23468400	-0.10850400	-0.58467900
H	6.93332700	1.59379600	-0.73304400
C	8.52453900	-1.29266900	0.09470100
H	7.94649600	-2.59628700	1.71285500
H	8.88080600	0.23025200	-1.38912800
H	9.38889700	-1.88639500	-0.18655100
C	-6.44848500	1.55369400	-0.44957700
C	-5.28869400	1.32817600	-0.74019500
C	-3.91835900	1.13911200	-1.09764400
H	-3.65808400	1.53106800	-2.08326900
H	-3.18239200	1.45391600	-0.35873700
O	-3.53236200	-0.36836200	-1.25517100
H	-4.19516100	-0.83349600	-1.80466000
C	-7.80450200	1.80986300	-0.10141000
C	-8.21350300	1.74314300	1.24630700
C	-8.74529700	2.13423300	-1.10032100
C	-9.53987300	1.99490300	1.58190500
H	-7.48663300	1.49361800	2.01215400
C	-10.06814700	2.38732300	-0.75201600
H	-8.42730100	2.18703700	-2.13645700
C	-10.46656700	2.31735200	0.58613100
H	-9.85270800	1.94186100	2.61987100
H	-10.78992100	2.63918600	-1.52250600

H	-11.50019600	2.51501600	0.85320900
TS <sub>2a-7</sub>			
C	2.42070100	0.50818700	1.09833400
C	5.23783400	-0.02088300	1.45668400
C	5.04878600	0.68107600	2.46822300
C	4.69411800	1.44319900	3.51243900
H	4.67903000	2.52563900	3.43505800
H	4.49790400	1.00217700	4.48606300
C	5.70193300	-0.78672800	0.37769000
C	6.02001800	-0.16600900	-0.85801300
C	5.86678900	-2.19148400	0.50564000
C	6.50687900	-0.92767700	-1.91563900
H	5.90717200	0.90795900	-0.95349900
C	6.35085600	-2.93605200	-0.55881500
H	5.63464800	-2.66396700	1.45414800
C	6.67321500	-2.30735500	-1.77054000
H	6.76523200	-0.44442100	-2.85263800
H	6.49222700	-4.00686300	-0.44991200
H	7.06146100	-2.89539300	-2.59658900
C	2.38696300	-0.87681300	1.60810200
O	2.20575800	-1.06058300	2.81225100
O	2.50947200	-1.86469200	0.70366900
C	2.36550100	-3.20279000	1.22788600
H	1.33924000	-3.36676200	1.56514900
H	2.60682800	-3.86444700	0.39737300
H	3.04806800	-3.36343600	2.06348100
C	2.65203700	1.05573700	-0.24343300
C	2.71575900	2.47202400	-0.40277100
C	2.85133100	0.24440200	-1.40055200
C	2.93725600	3.03371100	-1.65264800
H	2.59719900	3.10372000	0.46922100
C	3.05545800	0.83552100	-2.64583900
H	2.84140700	-0.83264900	-1.30325000
C	3.09965000	2.22400200	-2.78509200
H	2.98814000	4.11438900	-1.74689100
H	3.19964400	0.19741300	-3.51252100
H	3.26924900	2.67278500	-3.75854800
O	2.30701500	1.40316700	2.11398200
H	2.19288700	0.84452400	2.91572300
Au	0.19576200	0.61538500	0.06573600
P	-2.19231000	0.60302600	-0.23561700
C	-2.67332500	-1.16683100	-0.76186200
C	-3.91386000	-1.84568600	-0.64488700
C	-1.60853800	-1.82958400	-1.40669600
C	-4.01058700	-3.14374500	-1.18464600
C	-1.73661300	-3.10709800	-1.94334500
H	-0.64910700	-1.32939000	-1.48905800

C	-2.95264500	-3.77387000	-1.83051600
H	-4.96012400	-3.66020500	-1.08607500
H	-0.88860100	-3.57199400	-2.43655700
H	-3.07951700	-4.77366100	-2.23403000
C	-2.89109000	1.23543900	1.49552900
C	-2.59329400	1.76515200	-1.77268800
C	-2.70952900	0.07105600	2.48209100
H	-3.01039000	0.41107400	3.47960600
H	-3.32490500	-0.79005700	2.22597300
H	-1.66359300	-0.24726100	2.54087300
C	-4.35101700	1.70697100	1.43650700
H	-4.65274900	2.00587500	2.44701400
H	-4.47015600	2.58395200	0.79410700
H	-5.03672900	0.93170500	1.10267100
C	-2.00348900	2.40732900	1.96022200
H	-2.06295600	3.27722200	1.30472200
H	-2.35575600	2.71794600	2.95051300
H	-0.95328000	2.11660800	2.05811700
C	-2.28213900	3.22255800	-1.40096400
H	-2.97953600	3.62534600	-0.66273400
H	-1.26099400	3.34308300	-1.02653600
H	-2.37686400	3.83611600	-2.30410700
C	-4.05490400	1.61966000	-2.21253000
H	-4.24061800	2.31189200	-3.04197300
H	-4.25833100	0.61020300	-2.57698100
H	-4.76340500	1.85542700	-1.41638700
C	-1.67097200	1.32405500	-2.92260200
H	-1.83955300	0.28317300	-3.21095600
H	-1.88712000	1.94827400	-3.79731400
H	-0.61309900	1.45126000	-2.67268800
C	-5.17453000	-1.37903000	0.02482600
C	-5.47108000	-1.82403800	1.32396900
C	-6.15849900	-0.66430100	-0.67457600
C	-6.68520400	-1.50224200	1.93231400
H	-4.75214300	-2.44237900	1.85368500
C	-7.37534400	-0.34448400	-0.06803300
H	-5.98429200	-0.37452400	-1.70423300
C	-7.63765100	-0.75150400	1.24092600
H	-6.89115600	-1.85120200	2.93973400
H	-8.12368500	0.21002300	-0.62643100
H	-8.58482600	-0.50435300	1.71037200
7			
C	-2.86178100	-0.54891700	-1.00860100
C	-4.34817200	-0.92147900	-1.33673600
C	-4.61565600	-1.29574800	-2.56684000
C	-4.91377900	-1.66222500	-3.78316400
H	-5.21630900	-0.93724200	-4.53520700

H	-4.87573400	-2.70567000	-4.08784700
C	-5.44435600	-0.87212400	-0.31270900
C	-6.14422300	0.32395400	-0.08833400
C	-5.82332600	-2.02070100	0.39768700
C	-7.18846800	0.37340400	0.83560600
H	-5.87882800	1.21205100	-0.65472400
C	-6.86695200	-1.97030300	1.32292100
H	-5.30511300	-2.95624400	0.21402400
C	-7.54933700	-0.77289800	1.54653900
H	-7.72692400	1.30358600	0.99129200
H	-7.15474400	-2.86925300	1.86015200
H	-8.36551600	-0.73633100	2.26181000
C	-2.15069000	-1.82477800	-0.48138300
O	-1.27738400	-2.36493300	-1.13518100
O	-2.60992100	-2.27710800	0.68207900
C	-2.00739700	-3.49985000	1.17501300
H	-0.96202500	-3.32031500	1.43432700
H	-2.58479400	-3.76748200	2.05825400
H	-2.06917200	-4.28116000	0.41614700
C	-2.75264100	0.63271000	-0.03414000
C	-2.29237100	1.88334500	-0.54429900
C	-3.15030600	0.56653600	1.30872200
C	-2.24577200	3.02244400	0.30069000
H	-2.19089000	2.00149400	-1.61906200
C	-3.09534400	1.70055400	2.12458300
H	-3.51838400	-0.36564600	1.71507000
C	-2.63682300	2.92610400	1.63620000
H	-1.94406000	3.97742800	-0.11843800
H	-3.42281000	1.62206000	3.15698500
H	-2.60648100	3.79906300	2.27991500
O	-2.18879100	-0.19890800	-2.19704300
H	-1.66660700	-0.98104900	-2.45099200
Au	-0.05969500	1.37955400	-0.20858300
P	2.28772600	0.83203500	-0.06829700
C	2.44703900	-0.60206800	1.18124500
C	3.46796000	-1.57874000	1.32061000
C	1.38270200	-0.61532700	2.10630000
C	3.35877500	-2.50333800	2.37869900
C	1.30855800	-1.53067600	3.15239900
H	0.58475000	0.11295100	2.00397200
C	2.30890200	-2.48849300	3.29034300
H	4.13986200	-3.25062600	2.47610100
H	0.47422300	-1.49017100	3.84599700
H	2.27593400	-3.21761800	4.09402400
C	2.79669500	0.43068600	-1.93023500
C	3.19999800	2.38329200	0.72917800
C	2.21457100	-0.95603800	-2.24592900
H	2.36428800	-1.15967800	-3.31255600



H	2.70944000	-1.74773900	-1.68623200
H	1.14028300	-1.00694100	-2.04359900
C	4.31070700	0.48031300	-2.17850900
H	4.49370200	0.20542700	-3.22366200
H	4.71339000	1.48666800	-2.03565500
H	4.86797200	-0.21286100	-1.55220200
C	2.10319000	1.46830000	-2.83574700
H	2.43447800	2.49106400	-2.65016400
H	2.35519500	1.22501500	-3.87424300
H	1.01331000	1.43215400	-2.74412000
C	3.15479500	3.55904900	-0.25854900
H	3.77941400	3.39092900	-1.13886600
H	2.13518200	3.78435600	-0.58684600
H	3.54170500	4.45040700	0.24829600
C	4.64843100	2.05180300	1.10656900
H	5.12078200	2.95633100	1.50691800
H	4.68681000	1.28973400	1.88802500
H	5.24329100	1.71444600	0.25608700
C	2.41964300	2.75464400	2.00209200
H	2.40112900	1.93739000	2.72808400
H	2.91636900	3.60813300	2.47759400
H	1.38898000	3.04722200	1.77897000
C	4.67520100	-1.80042300	0.45452600
C	4.65515100	-2.82556400	-0.50611300
C	5.89012600	-1.14432400	0.70283500
C	5.79589100	-3.13395800	-1.24844300
H	3.74342800	-3.39555100	-0.66004600
C	7.03329900	-1.45452400	-0.03737800
H	5.95189900	-0.40533300	1.49291300
C	6.98653900	-2.44070700	-1.02372400
H	5.75653700	-3.92502600	-1.99121500
H	7.96396900	-0.93476000	0.16982300
H	7.87621000	-2.68252000	-1.59696100
<b>8</b>			
C	2.35124500	-1.46487900	-0.33338900
C	1.83085700	-2.60749200	-0.82585500
H	1.77624800	-2.76539900	-1.90237000
H	1.74266500	-3.49084500	-0.19421900
C	3.06383600	-0.43965300	0.07156300
C	2.41564900	0.80183100	0.60126500
C	1.94210200	0.84641100	1.92128600
C	2.26826900	1.92876300	-0.22152300
C	1.33743700	2.00467100	2.41233500
H	2.07301700	-0.01758700	2.56439000
C	1.65620000	3.08166800	0.27214100
H	2.64377500	1.90418700	-1.23915500
C	1.19305700	3.12343200	1.58885300

H	0.98784900	2.03493100	3.44010000
H	1.54971600	3.94968600	-0.37113200
H	0.72798100	4.02610500	1.97345700
C	4.61236200	-0.60127800	-0.07194300
C	5.25541900	-0.99848500	1.28497300
O	6.05009600	-1.91452000	1.34266200
O	4.87007200	-0.26201300	2.32610700
C	5.51559500	-0.57276300	3.58749800
H	5.08182200	0.11645400	4.30980700
H	5.31604900	-1.60909100	3.86546400
H	6.59291800	-0.42070700	3.50231000
C	5.27002100	0.67554300	-0.63143900
C	5.61192400	0.70180500	-1.99043400
C	5.53271400	1.80169000	0.16171100
C	6.20553900	1.83547000	-2.54592000
H	5.42578800	-0.17551100	-2.59834800
C	6.13360300	2.93046300	-0.39749200
H	5.27198900	1.80255200	1.21338500
C	6.47018400	2.95245100	-1.75143400
H	6.47025800	1.84024600	-3.59913200
H	6.34032600	3.79236800	0.22985400
H	6.94045700	3.83089000	-2.18300100
O	4.82726200	-1.69652600	-0.93199800
P	-2.40471300	-0.84117500	-0.21019400
C	-2.85524200	-1.02304600	1.69712400
C	-3.33663600	-2.10659600	-1.39889000
C	-3.24274600	-3.52056700	-0.80680500
H	-3.83352900	-3.63173900	0.10513100
H	-3.64127600	-4.23038500	-1.54038900
H	-2.20903800	-3.81260700	-0.59559500
C	-4.80104400	-1.70813900	-1.61402000
H	-4.87495100	-0.74768200	-2.12864900
H	-5.27709100	-2.46046200	-2.25366900
H	-5.36974600	-1.65406800	-0.68423700
C	-2.60435100	-2.06947700	-2.75191500
H	-1.56804400	-2.41213100	-2.66729800
H	-3.12202400	-2.74170400	-3.44566300
H	-2.60607200	-1.07066600	-3.19604900
C	-4.35924600	-1.17595600	1.96609300
H	-4.75758100	-2.10291100	1.54460600
H	-4.50896100	-1.22651000	3.05085000
H	-4.94558900	-0.34015800	1.59004600
C	-2.11790200	-2.26686800	2.23390100
H	-1.03232700	-2.18088700	2.12384400
H	-2.33545600	-2.34782600	3.30503900
H	-2.44133600	-3.19692000	1.76425600
C	-2.27879300	0.21701300	2.39790400
H	-1.20880800	0.33590900	2.20071100

H	-2.78963500	1.13225400	2.10391400
H	-2.40849800	0.09598400	3.47972100
C	-2.63432900	0.88551700	-0.98462200
C	-3.68352800	1.82664700	-0.81435700
C	-1.60724700	1.18968800	-1.90136600
C	-3.64303400	3.00638000	-1.58321900
C	-1.59943900	2.35791900	-2.65755200
H	-0.78620000	0.49143600	-2.02850400
C	-2.63114400	3.27745900	-2.49824100
H	-4.44509800	3.72468500	-1.44579200
H	-0.78907300	2.54254700	-3.35574500
H	-2.64930200	4.19892100	-3.07188900
C	-4.85175700	1.76305700	0.12815500
C	-4.79117400	2.45625900	1.34878300
C	-6.07620500	1.19381000	-0.25267900
C	-5.89823100	2.51413200	2.19647000
H	-3.87526600	2.97082500	1.62484600
C	-7.18564600	1.25259400	0.59388600
H	-6.17290200	0.72364000	-1.22413300
C	-7.09658300	1.90131000	1.82632100
H	-5.82779600	3.05097500	3.13775400
H	-8.12387800	0.80457800	0.28048000
H	-7.96029800	1.94925600	2.48228800
Au	-0.03918500	-1.42676600	-0.37851800
H	5.57537600	-2.19068800	-0.54858300
<b>9</b>			
C	4.26080200	0.63599200	-0.33441500
C	2.93779600	-0.13304100	-0.10943200
C	1.85235500	0.64312100	-0.31235400
C	2.25289500	2.03053900	-0.67205000
H	1.85046000	2.81464800	-0.02744400
H	2.09515000	2.28672700	-1.72484100
C	2.95450100	-1.59272300	0.16190300
C	3.60281700	-2.13990500	1.28132000
C	2.28826800	-2.46181200	-0.71968700
C	3.57312700	-3.51499000	1.51531900
H	4.11559600	-1.49144300	1.98233400
C	2.26438600	-3.83653100	-0.48634500
H	1.79981700	-2.05110800	-1.59796100
C	2.90676800	-4.36768200	0.63367300
H	4.07212400	-3.91972900	2.39081600
H	1.75429700	-4.49312500	-1.18529100
H	2.89239500	-5.43811000	0.81552900
C	4.80241400	0.18822900	-1.70364500
O	5.28434100	-0.90069900	-1.89403200
O	4.60775400	1.10966100	-2.67928000
C	4.93733500	0.64837400	-4.01705400

H	4.35346600	-0.24107400	-4.25793700
H	4.67749900	1.47208300	-4.68064200
H	6.00023100	0.40901700	-4.08353000
C	5.28804100	0.63381200	0.79015000
C	6.56284300	0.07012800	0.65798600
C	4.92177900	1.22298400	2.01185600
C	7.45721000	0.10365300	1.73104100
H	6.85348600	-0.42086800	-0.26212900
C	5.81859600	1.25687100	3.07639300
H	3.93130900	1.65167600	2.12769600
C	7.09200100	0.69686100	2.93835100
H	8.44064200	-0.34197400	1.61785800
H	5.52235300	1.71543400	4.01486100
H	7.79025700	0.71930200	3.76933600
O	3.73967800	2.03306900	-0.42544700
H	4.31686300	2.72523600	-0.94610600
Au	-0.13731100	0.15428400	-0.15239200
P	-2.52280000	-0.42203800	0.04225200
C	-3.38189600	0.97779900	1.01880100
C	-4.73883900	1.39264700	1.05898300
C	-2.46412300	1.64198400	1.85950000
C	-5.09131700	2.43470500	1.93966800
C	-2.84066200	2.66000400	2.73099400
H	-1.41858400	1.35236800	1.82573200
C	-4.17161700	3.06230800	2.77275400
H	-6.13023000	2.74881500	1.95890500
H	-2.09460300	3.13354000	3.36195200
H	-4.49379500	3.85739100	3.43821500
C	-3.14746900	-0.67832500	-1.80309500
C	-2.67756600	-2.02722200	1.16692000
C	-3.22966300	0.72663000	-2.42399200
H	-3.48314700	0.62836900	-3.48612700
H	-3.99553500	1.34398900	-1.95660400
H	-2.26987700	1.24975700	-2.35575300
C	-4.47813400	-1.43095500	-1.93774200
H	-4.73796300	-1.48759800	-3.00174400
H	-4.40123700	-2.45852200	-1.57154900
H	-5.29979900	-0.93888800	-1.42241100
C	-2.05346000	-1.46550900	-2.55441600
H	-1.93929500	-2.48747100	-2.19048700
H	-2.34337400	-1.52230300	-3.61026700
H	-1.07998800	-0.96909000	-2.49854900
C	-2.08419700	-3.22948200	0.41535300
H	-2.70045600	-3.53820700	-0.43288800
H	-1.06653800	-3.03458300	0.06329900
H	-2.03570900	-4.07966300	1.10580900
C	-4.12505600	-2.31560700	1.58030700
H	-4.14325900	-3.22831500	2.18798700

H	-4.52756300	-1.50647800	2.19419500
H	-4.78875700	-2.47185100	0.72728500
C	-1.83762800	-1.76048100	2.42932500
H	-2.20620100	-0.90072500	2.99535800
H	-1.90118200	-2.63831600	3.08314500
H	-0.78265900	-1.59543900	2.19034100
C	-5.89325000	0.89124700	0.23853400
C	-6.29840800	1.61480200	-0.89543100
C	-6.70006100	-0.17170400	0.67108600
C	-7.43393500	1.24311600	-1.61642400
H	-5.72819600	2.48646500	-1.20337300
C	-7.83856200	-0.54329100	-0.04763100
H	-6.44950700	-0.69983400	1.58357700
C	-8.20221900	0.15456800	-1.20025100
H	-7.72455300	1.81274900	-2.49416800
H	-8.44839900	-1.37046200	0.30361200
H	-9.08843100	-0.13416800	-1.75712900
O	5.08271700	3.76065800	-1.63947100
H	5.76205500	4.23973000	-1.14469100
H	5.50925700	3.36597200	-2.41274200
<b>10</b>			
C	3.20452500	1.02722400	-0.77889800
C	2.85864000	-0.44909400	-0.47099700
C	2.21060500	-0.96323400	-1.58629200
C	2.21977000	0.06704600	-2.68725300
H	1.27235200	0.19520200	-3.21791900
H	2.99946900	-0.19400000	-3.41866600
C	3.43807600	-1.23325700	0.64089300
C	4.38250900	-0.66603900	1.51754000
C	3.09303800	-2.59193300	0.81274300
C	4.96589100	-1.43313400	2.52658000
H	4.67677700	0.37164000	1.41546600
C	3.67001300	-3.34658000	1.82753800
H	2.36844400	-3.05741700	0.15193800
C	4.61034600	-2.77100200	2.68951700
H	5.69826400	-0.97742100	3.18538300
H	3.38902100	-4.38851800	1.94815000
H	5.06058200	-3.36400300	3.47959000
C	4.74456800	1.12999500	-1.05658500
O	5.49918100	1.88907900	-0.49771300
O	5.10694800	0.27015100	-2.02320900
C	6.50235300	0.31278900	-2.40226400
H	7.13396700	0.09914700	-1.53784400
H	6.61933900	-0.45259400	-3.16779000
H	6.75398500	1.29855500	-2.79825300
C	2.76982400	2.11269900	0.20085100
C	2.85488000	3.44644400	-0.22832900

C	2.26481600	1.84649200	1.47791000
C	2.44250400	4.48608300	0.60124200
H	3.24330200	3.66808400	-1.21605100
C	1.85608200	2.89184400	2.31307700
H	2.20279500	0.82896000	1.84512300
C	1.94259500	4.21263900	1.87832000
H	2.52246200	5.51215100	0.25510200
H	1.47822600	2.66692700	3.30604400
H	1.63318600	5.02448700	2.52964300
O	2.52709900	1.29115100	-2.02190200
H	2.26909600	-4.81587700	-1.93760400
Au	0.38110100	-0.58624500	-0.28339700
P	-1.96013600	-0.53655000	0.39183500
C	-2.57995700	1.22324300	-0.00686700
C	-3.89051300	1.69091900	-0.28830700
C	-1.53114800	2.16491700	0.03948400
C	-4.06621000	3.07137300	-0.50735200
C	-1.73641100	3.52614400	-0.16641400
C	-0.51880000	1.83176300	0.24043700
C	-3.01935800	3.98523300	-0.44586700
H	-5.06908800	3.42191200	-0.73001100
H	-0.89226300	4.20593700	-0.11476900
H	-3.20824100	5.04009800	-0.61964600
C	-2.76995900	-2.00260900	-0.63978600
C	-2.08168400	-0.74843400	2.34480500
C	-2.81877900	-1.52318900	-2.09963800
H	-3.18947900	-2.34349300	-2.72514600
H	-3.48737400	-0.67450900	-2.23582300
H	-1.82404600	-1.24670900	-2.46535200
C	-4.15936100	-2.42407000	-0.13996300
H	-4.53574100	-3.21388300	-0.80052500
H	-4.11846900	-2.84312500	0.86908700
H	-4.88156500	-1.61117100	-0.15137500
C	-1.82267700	-3.21710700	-0.56032800
H	-1.72083900	-3.61483200	0.45010000
H	-2.25154100	-4.01211100	-1.18191000
H	-0.82226900	-2.99609700	-0.94345700
C	-1.67564300	-2.17729800	2.73631500
H	-2.40642400	-2.92470200	2.41863900
H	-0.69320400	-2.45059600	2.33918700
H	-1.61422000	-2.22997300	3.82933900
C	-3.49142200	-0.42783400	2.85585800
H	-3.51239300	-0.58068800	3.94130900
H	-3.75012300	0.61658900	2.66780100
H	-4.26079100	-1.06493100	2.41578900
C	-1.08492500	0.24767200	2.96092800
H	-1.30321900	1.28093600	2.67927300
H	-1.15466200	0.17815200	4.05258600

H	-0.05401000	0.01959100	2.67560800
C	-5.15811200	0.89631000	-0.42122900
C	-5.64281400	0.57396900	-1.69993800
C	-5.97507700	0.62580400	0.68690300
C	-6.87289400	-0.06565100	-1.86022300
H	-5.05929900	0.84384700	-2.57552800
C	-7.20747800	-0.01185900	0.52786700
H	-5.65891800	0.93473100	1.67630100
C	-7.65453400	-0.37101500	-0.74459900
H	-7.22579900	-0.31087100	-2.85749500
H	-7.82429900	-0.21244500	1.39885700
H	-8.61399800	-0.86387900	-0.86786900
O	1.58829900	-4.13318000	-1.99350600
H	0.99174700	-4.43866800	-2.68838200
H	2.10840000	-2.02519200	-1.80135000
<b>H<sub>2</sub>O</b>			
O	0.00000000	0.00000000	0.11884900
H	0.00000000	0.76007400	-0.47539600
H	0.00000000	-0.76007400	-0.47539600
<b>4a</b>			
C	-4.43216900	-0.17374300	-0.52199900
C	-5.31030500	-0.77701800	0.54885300
C	-4.72388700	-1.47933600	1.61198100
C	-6.70810300	-0.72680700	0.44637800
C	-5.52504000	-2.11270500	2.56063300
H	-3.64266400	-1.51854500	1.70057400
C	-7.50639400	-1.35883100	1.39798200
H	-7.18410100	-0.19560700	-0.37261300
C	-6.91628500	-2.05229300	2.45651400
H	-5.06260300	-2.64967000	3.38285300
H	-8.58720100	-1.31001500	1.31208700
H	-7.53893000	-2.54250700	3.19845500
C	-5.08788200	0.90420700	-1.40579200
O	-5.12623000	0.72724300	-2.62336000
O	-5.51649700	1.95995500	-0.76809800
C	-6.04885400	3.04914000	-1.57650300
H	-5.26897000	3.42562100	-2.23972900
H	-6.89834300	2.69324100	-2.16095900
H	-6.35317600	3.80728000	-0.85884800
C	-2.98956500	0.22553500	-0.16087900
C	-2.07420400	-0.58485800	-0.74028800
C	-2.72306000	-1.59889400	-1.60963300
H	-2.42924900	-1.56408600	-2.66197800
H	-2.67068900	-2.62706800	-1.24489500
O	-4.20860100	-1.25412400	-1.58330300
H	-4.49957200	-0.72983000	-2.41345600
C	-2.72083600	1.42327700	0.67581900

C	-1.64851300	2.26935600	0.33273200
C	-3.50015000	1.76343300	1.79594100
C	-1.34723900	3.39429500	1.09845900
H	-1.06078300	2.04660300	-0.55180200
C	-3.19640000	2.89022400	2.56026400
H	-4.33936300	1.14320400	2.08651900
C	-2.11824000	3.70797700	2.21948100
H	-0.51767500	4.03305800	0.80966300
H	-3.80623400	3.12652100	3.42718900
H	-1.88738900	4.58580400	2.81529900
P	2.40216700	-0.81458400	-0.16450900
C	3.05705000	-2.37815700	-1.15819900
C	2.62828100	-0.94408100	1.78440700
C	1.53271900	-1.89121500	2.31651200
H	1.65162400	-2.91896700	1.97004300
H	1.60138700	-1.90338400	3.41059800
H	0.52857600	-1.54898000	2.04862400
C	3.99766900	-1.46503900	2.24203000
H	4.82600400	-0.85525600	1.88863000
H	4.02096000	-1.45630400	3.33832100
H	4.16538800	-2.49878600	1.92682100
C	2.34666100	0.46374900	2.33690700
H	1.35639500	0.82280600	2.03784200
H	2.36896200	0.42226500	3.43220100
H	3.09164000	1.19140000	2.01814500
C	4.58683000	-2.42924400	-1.23499000
H	5.06294800	-2.45762500	-0.25290100
H	4.88332000	-3.33611300	-1.77566100
H	4.98018300	-1.57507400	-1.79084900
C	2.51008000	-3.65539000	-0.50138000
H	1.42257600	-3.62245700	-0.38062800
H	2.74612800	-4.50862000	-1.14792500
H	2.96538200	-3.85198300	0.47213800
C	2.48833000	-2.26060400	-2.58349500
H	1.39398900	-2.26287700	-2.58355800
H	2.83355400	-1.35595000	-3.09112700
H	2.83004900	-3.12130100	-3.17020200
C	3.21432800	0.70651000	-0.98656100
C	4.46067700	1.34202000	-0.74442900
C	2.40798500	1.20928700	-2.02926100
C	4.82090100	2.43205400	-1.56172900
C	2.79407100	2.27902000	-2.83194300
H	1.44305600	0.74783000	-2.21480300
C	4.01647000	2.89951300	-2.59537900
H	5.77280900	2.91580900	-1.36626900
H	2.13808800	2.62252200	-3.62603300
H	4.34197600	3.73981600	-3.20090300
C	5.47623800	1.03398400	0.31924600

C	6.51159300	0.11214800	0.10442400
C	5.51439600	1.81749500	1.48464800
C	7.51567800	-0.07004100	1.05793300
H	6.54644800	-0.45142500	-0.82045000
C	6.51539900	1.63487500	2.43971400
H	4.76322400	2.58761700	1.63412600
C	7.51391100	0.68140400	2.23394000
H	8.30751400	-0.78982100	0.87256200
H	6.52154300	2.24703800	3.33666000
H	8.29612300	0.54049300	2.97360100
Au	-0.02946400	-0.65797400	-0.51386900
<b>TS<sub>8-4a</sub></b>			
C	2.08817700	1.09233400	0.24037700
C	2.28972800	2.31022500	0.86929600
H	2.24633400	2.39687600	1.95334400
H	2.23414400	3.24891600	0.31655800
C	2.99767200	0.20819100	-0.16563400
C	2.69355900	-1.08785200	-0.82983200
C	2.12199000	-1.09246100	-2.11328900
C	2.91917800	-2.31318500	-0.18367100
C	1.78699800	-2.29377900	-2.73799100
H	1.95255700	-0.14851900	-2.62338100
C	2.57758800	-3.51325300	-0.80956400
H	3.34784300	-2.32765000	0.81204700
C	2.01440500	-3.50808700	-2.08668100
H	1.35351400	-2.28133100	-3.73378300
H	2.75125900	-4.45346300	-0.29491300
H	1.75489700	-4.44412400	-2.57194000
C	4.47186000	0.70148800	0.08300000
C	5.08652800	1.15948100	-1.26623500
O	5.44017600	2.31873300	-1.40880800
O	5.14790500	0.22985300	-2.20453200
C	5.72077800	0.63923400	-3.47465700
H	5.66865000	-0.24418200	-4.10766000
H	5.14002400	1.46046600	-3.89753900
H	6.75431200	0.95791400	-3.32985900
C	5.32042600	-0.32633100	0.84878200
C	5.32563200	-0.26724400	2.25039900
C	6.06103600	-1.32761200	0.20783200
C	6.05649600	-1.19210900	2.99443700
H	4.77459800	0.51614000	2.75753300
C	6.79766100	-2.24721400	0.95826000
H	6.06307700	-1.40284300	-0.87186700
C	6.79754800	-2.18548900	2.35086900
H	6.05376600	-1.12908500	4.07846500
H	7.37226400	-3.01296700	0.44601900
H	7.37230700	-2.90112200	2.93068600

O	4.40583000	1.90742500	0.84982900
P	-2.45858600	0.81282400	0.19010400
C	-2.93387900	0.93269700	-1.71577200
C	-3.20741600	2.24225400	1.31718900
C	-2.94963000	3.59968300	0.64582900
H	-3.54628800	3.73811700	-0.25880000
H	-3.23366600	4.39311500	1.34649300
H	-1.89346100	3.74264800	0.39641400
C	-4.70514800	2.04636500	1.57604800
H	-4.88877500	1.13350000	2.14681300
H	-5.07024200	2.88750600	2.17715400
H	-5.29497700	2.01269900	0.65812800
C	-2.45386600	2.18417400	2.65769700
H	-1.38164900	2.36401700	2.53077200
H	-2.85084000	2.96533600	3.31619000
H	-2.58651100	1.22482400	3.16486900
C	-4.41526600	1.23899300	-1.97629800
H	-4.69670400	2.22908300	-1.60737100
H	-4.58011600	1.24141700	-3.06018400
H	-5.08462400	0.50047000	-1.54092200
C	-2.07381400	2.05045500	-2.33976900
H	-1.00261500	1.85539000	-2.22871400
H	-2.29545300	2.08558800	-3.41269400
H	-2.29009000	3.03758700	-1.92871000
C	-2.51355200	-0.40508300	-2.34634000
H	-1.45516800	-0.62349800	-2.16844400
H	-3.10749200	-1.24058300	-1.97931900
H	-2.66239900	-0.34130000	-3.43053200
C	-2.87686100	-0.83658300	1.05199700
C	-4.02455000	-1.66531100	0.94236600
C	-1.86585300	-1.22002000	1.95792300
C	-4.08831700	-2.81863000	1.74909600
C	-1.96015300	-2.35889600	2.75215200
H	-0.97222500	-0.61007500	2.04378000
C	-3.08580500	-3.16932300	2.64687300
H	-4.96595700	-3.45038100	1.65540500
H	-1.15441400	-2.60744900	3.43574800
H	-3.18438500	-4.06719300	3.24902000
C	-5.20807200	-1.50733500	0.03058000
C	-5.27690300	-2.27036500	-1.14718100
C	-6.33651700	-0.76400000	0.40760400
C	-6.41016900	-2.23296600	-1.96070800
H	-4.44254400	-2.91140300	-1.41682500
C	-7.47258100	-0.72774900	-0.40422500
H	-6.33789600	-0.22822400	1.34948600
C	-7.50823600	-1.45156300	-1.59692700
H	-6.43939800	-2.82556700	-2.87021200
H	-8.33518200	-0.14535400	-0.09427700

H	-8.39245900	-1.42456600	-2.22628500
Au	-0.01528400	1.04652700	0.24742100
H	4.87691800	2.57433700	0.29658500
<b>TS<sub>9-10</sub></b>			
C	4.28391100	0.51152400	-0.69805100
C	3.07326300	-0.29839400	-0.13576500
C	1.92774800	0.18127900	-0.71087200
C	2.35127200	1.30415200	-1.64800300
H	2.29185200	2.28200800	-1.15331600
H	1.80194900	1.37459800	-2.59184400
C	3.23372400	-1.38238000	0.85355600
C	4.33180400	-1.40685000	1.73537800
C	2.29158800	-2.42847900	0.93822600
C	4.46265200	-2.42296800	2.68251000
H	5.08407500	-0.62837700	1.69540900
C	2.43256500	-3.44590700	1.87656700
H	1.44943000	-2.44565300	0.25342000
C	3.51716600	-3.44469700	2.75900200
H	5.31263900	-2.41403400	3.35770500
H	1.70100100	-4.24777500	1.91453700
H	3.62709700	-4.23920800	3.49065400
C	5.49439800	-0.37664400	-1.04990200
O	6.50291400	-0.46628200	-0.39696400
O	5.26478800	-1.08417700	-2.18003200
C	6.32031700	-1.99620100	-2.57250100
H	6.49678500	-2.72408900	-1.77898300
H	5.96272900	-2.48549300	-3.47721200
H	7.23882700	-1.44034800	-2.76755500
C	4.70198500	1.70882600	0.15566600
C	5.70190900	2.56418400	-0.33253000
C	4.07840300	2.01575000	1.36991000
C	6.07449200	3.69708300	0.38484400
H	6.18927800	2.34396400	-1.27729500
C	4.45572400	3.15208900	2.09111600
H	3.30316700	1.36777100	1.76517500
C	5.45263400	3.99349700	1.60133000
H	6.85218800	4.34788200	-0.00277500
H	3.96814300	3.37422900	3.03546900
H	5.74725200	4.87511200	2.16237600
O	3.73553900	0.99760500	-1.96362300
H	3.46040800	-0.52191400	-2.88041600
Au	-0.06116800	-0.13774200	-0.28772000
P	-2.44908200	-0.38304900	0.26714900
C	-3.23096600	1.35883700	0.18265300
C	-4.57824000	1.76642100	-0.00267200
C	-2.26076500	2.36088300	0.39548200
C	-4.86807900	3.14467000	0.04504900

C	-2.57601500	3.71554700	0.45074900
H	-1.22232800	2.07035700	0.52034900
C	-3.89704500	4.11358100	0.27366300
H	-5.89981100	3.44805600	-0.10266100
H	-1.79107000	4.44544800	0.62328800
H	-4.17250300	5.16320000	0.30599900
C	-3.17077700	-1.69960800	-1.00077200
C	-2.57257500	-0.93099700	2.15228200
C	-3.27031700	-0.97860900	-2.35536200
H	-3.57091100	-1.70410000	-3.12044700
H	-4.01100800	-0.18055400	-2.34603600
H	-2.30566500	-0.55448600	-2.65475800
C	-4.51598500	-2.31815900	-0.59597500
H	-4.82780100	-3.01446300	-1.38373600
H	-4.43507400	-2.89645300	0.32838500
H	-5.30537800	-1.57974500	-0.47632500
C	-2.12681600	-2.82761100	-1.13590700
H	-1.99306700	-3.39665800	-0.21476800
H	-2.47805700	-3.52503500	-1.90537500
H	-1.15025800	-2.44399400	-1.44838800
C	-2.04794800	-2.36791700	2.30160900
H	-2.71371500	-3.10744000	1.84968100
H	-1.04558200	-2.48671600	1.87855100
H	-1.98238900	-2.60292500	3.37024600
C	-4.00059200	-0.82290900	2.69685300
H	-4.00883000	-1.16554600	3.73836400
H	-4.34482900	0.21382600	2.69157500
H	-4.71510700	-1.43166800	2.13992600
C	-1.65968100	0.02280200	2.94451800
H	-1.98021100	1.06453500	2.85951700
H	-1.70402100	-0.25141000	4.00503300
H	-0.61612200	-0.04826600	2.62244300
C	-5.78223500	0.91501200	-0.29080600
C	-6.24337800	0.79589900	-1.61253100
C	-6.57625000	0.38909200	0.73931600
C	-7.42340900	0.10914000	-1.90200700
H	-5.68226300	1.26253900	-2.41711600
C	-7.75915000	-0.29554400	0.45166300
H	-6.28180200	0.53295300	1.77207800
C	-8.18003600	-0.44879700	-0.87015800
H	-7.75787600	0.02425000	-2.93168000
H	-8.35863400	-0.69557200	1.26406100
H	-9.10094500	-0.97910400	-1.09252400
O	2.69000900	-1.19272300	-2.98028100
H	2.08248300	-0.91216700	-3.68774400
H	2.23669900	-1.04121000	-2.05216800

**P<sub>4a</sub>**

C	0.67969700	-0.87280900	-0.39576400
C	-0.70499800	-0.59059300	-1.02821600
C	-0.80646700	-1.36056700	-2.12281200
C	0.41685300	-2.19652000	-2.31809400
H	0.86952800	-2.08197400	-3.31342500
H	0.20771300	-3.26775300	-2.16749500
C	-1.75511700	0.29089200	-0.47389300
C	-1.47300600	1.33169100	0.42924000
C	-3.09817000	0.10094300	-0.85685900
C	-2.48829700	2.16102100	0.90579800
H	-0.45648100	1.49587600	0.76114900
C	-4.10929500	0.93155600	-0.38324800
H	-3.35568200	-0.72100500	-1.51722100
C	-3.80895900	1.97147300	0.49999600
H	-2.24081000	2.96020400	1.59882700
H	-5.13547000	0.75944300	-0.69563100
H	-4.59724300	2.61857600	0.87370900
C	0.41884000	-1.70730700	0.88683100
O	0.45814000	-2.91448900	0.92687700
O	0.06158300	-0.93173400	1.93156100
C	-0.32603700	-1.64119700	3.12159600
H	0.50403900	-2.24509400	3.49626300
H	-0.60037100	-0.87350700	3.84457400
H	-1.17525800	-2.29712900	2.91569300
C	1.60219000	0.33288400	-0.19964700
C	2.54519200	0.38154200	0.83301700
C	1.60124700	1.35453300	-1.15913800
C	3.45470700	1.43765200	0.91626100
H	2.57471200	-0.40452000	1.57986300
C	2.50463100	2.41227200	-1.07501300
H	0.88597800	1.31658500	-1.97518600
C	3.43519500	2.45812500	-0.03428700
H	4.17972100	1.45900700	1.72493900
H	2.48374400	3.19937200	-1.82346700
H	4.14064200	3.28142800	0.03268800
O	1.33591700	-1.72437500	-1.33587300
H	-1.65912500	-1.40828800	-2.79041400
<b>P<sub>5a</sub></b>			
C	-1.24951200	-1.57974100	-1.81506800
C	-1.79950700	-2.37324500	-2.69392200
H	-1.73344300	-2.17068500	-3.76066600
H	-2.33320200	-3.27292600	-2.39500800
C	-0.72506500	-0.74484600	-0.94650800
C	-1.57593500	0.36540300	-0.40601900
C	-2.65717900	0.07771000	0.43983400
C	-1.35214800	1.69894200	-0.78286000
C	-3.49150100	1.09551000	0.90303800

H	-2.83773500	-0.95217200	0.73115400
C	-2.18636800	2.71635300	-0.31945600
H	-0.52702100	1.93576500	-1.44628000
C	-3.25727700	2.41886300	0.52575500
H	-4.32569500	0.85384100	1.55600000
H	-2.00175900	3.74245300	-0.62484400
H	-3.90687800	3.21243400	0.88426300
C	0.74775300	-0.97463100	-0.50574500
C	0.78162300	-1.88329300	0.74884600
O	1.51305500	-2.85303900	0.81317800
O	-0.05122000	-1.51277900	1.72716400
C	-0.01725300	-2.32772600	2.91686400
H	-0.75765800	-1.89295400	3.58704000
H	-0.27223600	-3.36161000	2.67488700
H	0.97725900	-2.29998200	3.36769200
C	1.52188100	0.33112900	-0.21925800
C	2.44484700	0.77732600	-1.17390000
C	1.33854500	1.08481000	0.94866300
C	3.16700500	1.95341100	-0.96737800
H	2.59129500	0.18760000	-2.07091800
C	2.06873900	2.25611200	1.15644800
H	0.62154600	0.76426800	1.69497900
C	2.98447300	2.69617100	0.20013200
H	3.87789800	2.28506400	-1.71920000
H	1.91662400	2.82597600	2.06884000
H	3.55144500	3.60827500	0.36387700
O	1.38779600	-1.70884600	-1.52733700
H	1.90377000	-2.39759500	-1.07265600
<b>II</b>			
C	2.95145700	-1.20606400	-0.42197800
C	3.19099100	-2.65610300	-0.04713700
C	4.23457100	-2.97218900	0.83429700
C	2.39678200	-3.69940500	-0.55425300
C	4.47704300	-4.29753300	1.20007100
H	4.87016400	-2.18319700	1.21781100
C	2.65198700	-5.02192000	-0.19516000
H	1.58092800	-3.48116300	-1.23445700
C	3.68958700	-5.32787300	0.68805800
H	5.29213600	-4.52115100	1.88181200
H	2.03272600	-5.81495500	-0.60381000
H	3.88137300	-6.35791400	0.97170700
Au	0.82561600	-0.75432500	0.02315500
C	2.92097400	-0.84480600	-1.82651100
O	3.37666400	0.32002400	-2.20999900
O	2.46975200	-1.64780100	-2.74428600
C	2.40804000	-1.18605200	-4.12440800
H	3.39929600	-0.87959500	-4.45910200

H	2.05636000	-2.04828800	-4.68608300
H	1.70393500	-0.35583700	-4.20184900
P	-1.52977900	-0.43962200	0.61419200
C	-2.21611200	0.91377200	-0.54593900
C	-3.54542700	1.18514700	-0.96301200
C	-1.19180100	1.77590700	-0.99115200
C	-3.76484600	2.30321700	-1.79280500
C	-1.43835100	2.88185200	-1.80004700
H	-0.16707700	1.57213400	-0.69701300
C	-2.74198000	3.14940700	-2.20670400
H	-4.78317400	2.50042100	-2.11267400
H	-0.61434100	3.51908900	-2.10608900
H	-2.96406900	4.00070800	-2.84283200
C	-2.33154200	-2.22965800	0.43029400
C	-1.61516300	0.29964800	2.43427200
C	-2.42670100	-2.50089300	-1.07993300
H	-2.78311500	-3.52643400	-1.23045000
H	-3.12491900	-1.83058500	-1.57912900
H	-1.44890600	-2.41424500	-1.56576300
C	-3.69544100	-2.38337200	1.11761400
H	-4.06614000	-3.39594700	0.91963000
H	-3.61539000	-2.27934300	2.20307000
H	-4.44098000	-1.68060600	0.75264300
C	-1.34780300	-3.24678500	1.04305900
H	-1.23027500	-3.13120400	2.12118300
H	-1.75092000	-4.25036000	0.86426200
H	-0.35713700	-3.20014200	0.58238000
C	-1.13002800	-0.76166800	3.43386900
H	-1.83491600	-1.58974300	3.53926600
H	-0.14969000	-1.16771500	3.16520000
H	-1.03399400	-0.29148200	4.41921300
C	-3.02916300	0.76965600	2.79501800
H	-3.02423700	1.13673800	3.82813900
H	-3.34222400	1.59796100	2.15548100
H	-3.77333400	-0.02561000	2.72730800
C	-0.66408600	1.50767800	2.46913800
H	-0.97095500	2.28771900	1.76735700
H	-0.68737000	1.94175600	3.47529500
H	0.36999900	1.23134800	2.24526500
C	-4.79508800	0.40522000	-0.66860700
C	-5.29582800	-0.48622900	-1.63203700
C	-5.58286300	0.67595600	0.46028600
C	-6.51229600	-1.14227500	-1.43838100
H	-4.73586500	-0.65161600	-2.54797700
C	-6.80208100	0.02258900	0.65370300
H	-5.25420000	1.41448700	1.18214400
C	-7.26457100	-0.89751100	-0.28831100
H	-6.87745500	-1.83241700	-2.19306100

H	-7.39645400	0.24531300	1.53484100
H	-8.21333400	-1.40336200	-0.13798400
C	2.87068200	2.92582000	0.86750000
C	3.13774500	1.76458100	1.10775300
C	3.55446400	0.39406400	1.38479600
H	4.47065100	0.39134600	1.98502000
H	2.78796100	-0.16576100	1.93177200
O	3.89273800	-0.31011200	0.16375900
H	3.78672100	0.71392000	-1.40147300
C	2.59799300	4.30294000	0.59685600
C	3.66357700	5.21634900	0.47234200
C	1.27521800	4.76661800	0.45805200
C	3.40717300	6.56011600	0.21382900
H	4.68331000	4.86235900	0.58381500
C	1.02885400	6.11260300	0.20005100
H	0.45146900	4.06755700	0.55762600
C	2.09188900	7.01118800	0.07728400
H	4.23412600	7.25728900	0.12148200
H	0.00619100	6.46332600	0.09903400
H	1.89575600	8.06035600	-0.12151200
TS <sub>2a-11</sub>			
C	2.34061800	1.88923800	0.35269000
C	2.23234600	3.36259500	0.00797400
C	3.14405100	3.98341200	-0.85646200
C	1.19328200	4.13133100	0.56060900
C	3.01571200	5.33969100	-1.16532300
C	3.96412700	3.41699800	-1.28194700
C	1.07962100	5.48726800	0.25987200
H	0.47715300	3.66880200	1.23183100
C	1.98681100	6.09768000	-0.60944500
H	3.73155600	5.80180400	-1.83845700
H	0.27478600	6.06641100	0.70270800
H	1.89120000	7.15196700	-0.84908700
Au	0.51963000	0.84135600	-0.09613700
C	2.69475200	1.57753800	1.77939300
O	3.68033200	0.82966700	1.97108600
O	1.96748700	2.08838500	2.73642300
C	2.34782400	1.76516900	4.10362100
H	3.37839900	2.07323200	4.28344200
H	1.65643900	2.32778900	4.72684100
H	2.24158100	0.69224400	4.27067300
P	-1.65213700	-0.16657000	-0.62716600
C	-2.21545000	-1.14154400	0.91562000
C	-3.51333800	-1.51444500	1.35290800
C	-1.10997000	-1.56959800	1.68055200
C	-3.62129100	-2.29174700	2.52339400
C	-1.24407800	-2.34956900	2.82552000



H	-0.11189300	-1.27975700	1.36791600
C	-2.51635300	-2.71486400	3.25404200
H	-4.61758400	-2.56702800	2.85472900
H	-0.36005600	-2.65834400	3.37515600
H	-2.65260200	-3.31683900	4.14717300
C	-2.77851600	1.36215200	-1.14601800
C	-1.40467700	-1.50220400	-2.04916200
C	-3.10101000	2.11896900	0.15294500
H	-3.64673100	3.03486000	-0.10197600
H	-3.72664700	1.53732700	0.82804300
H	-2.18950000	2.41224600	0.68415900
C	-4.05620400	0.97745100	-1.90448600
H	-4.61797900	1.89410600	-2.11915500
H	-3.83053100	0.50761400	-2.86574300
H	-4.70629100	0.31552200	-1.33653500
C	-1.92432400	2.28503800	-2.03989900
H	-1.63472500	1.81841800	-2.98249700
H	-2.52757700	3.16718700	-2.28349700
H	-1.01943100	2.63283500	-1.53241500
C	-1.00415900	-0.78795600	-3.34915700
H	-1.82595900	-0.21203100	-3.78116700
H	-0.14749700	-0.12183900	-3.20510800
H	-0.71499100	-1.54454800	-4.08758200
C	-2.66124100	-2.35225800	-2.26744800
H	-2.47174200	-3.05653400	-3.08624200
H	-2.89506000	-2.94052500	-1.37730000
H	-3.53690300	-1.75837200	-2.53479300
C	-0.25370500	-2.42005800	-1.59984000
H	-0.48950800	-2.94336300	-0.66897100
H	-0.09062400	-3.17850400	-2.37448100
H	0.68325100	-1.87159500	-1.46380600
C	-4.84138100	-1.15958000	0.74696000
C	-5.59525600	-0.11136900	1.30059900
C	-5.44011600	-1.96248800	-0.23537800
C	-6.87999700	0.17171200	0.83477000
H	-5.17746900	0.47421700	2.11446100
C	-6.72701700	-1.68245600	-0.70029800
H	-4.90887000	-2.82303800	-0.62484700
C	-7.44593400	-0.60724400	-0.17595400
H	-7.44248900	0.99118400	1.27207800
H	-7.17190500	-2.31548100	-1.46233000
H	-8.44697300	-0.39148200	-0.53656000
C	3.92570100	-2.11034600	-0.88709800
C	3.70750700	-0.94521800	-1.15392700
C	3.50930000	0.44638500	-1.48768900
H	4.30221400	0.82943400	-2.13570700
H	2.53685700	0.64493100	-1.94456700
O	3.57469700	1.31252400	-0.27932000

H	3.96200300	0.83226800	0.66630200
C	4.20768100	-3.47412400	-0.57664500
C	5.53539700	-3.94451000	-0.61862700
C	3.16966600	-4.36004600	-0.22688500
C	<b>5.81337400</b>	<b>-5.27410200</b>	<b>-0.31550600</b>
H	<b>6.33439700</b>	<b>-3.26202900</b>	<b>-0.88911800</b>
C	<b>3.45868800</b>	<b>-5.68761100</b>	<b>0.07463300</b>
H	<b>2.14717300</b>	<b>-3.99769800</b>	<b>-0.19730600</b>
C	<b>4.77816900</b>	<b>-6.14635300</b>	<b>0.03130800</b>
H	<b>6.83781100</b>	<b>-5.63119600</b>	<b>-0.34996400</b>
H	2.65557200	-6.36712300	0.34270600
H	4.99928800	-7.18289200	0.26675800
<b>12</b>			
C	4.22598900	-0.94110200	0.00639000
C	3.98960400	-2.38362400	0.15117100
C	4.37238200	-3.02449600	1.34728600
C	3.40099600	-3.16768000	-0.86242100
C	4.17114800	-4.39224000	1.52435500
H	4.85974600	-2.44774200	2.12645800
C	3.21506800	-4.53713600	-0.68144100
H	3.10854500	-2.70278100	-1.79547900
C	3.59108200	-5.15810900	0.51195300
H	4.48345900	-4.86225000	2.45242200
H	2.77318300	-5.12404500	-1.48211000
H	3.44247700	-6.22501800	0.64709300
Au	0.48182400	0.51696200	0.52317500
C	4.35496800	-0.19963200	-1.12506800
O	4.71804600	1.10914200	-1.09153900
O	4.11844600	-0.67776200	-2.35393000
C	5.03601300	-0.28133900	-3.39776800
H	6.05507300	-0.59071600	-3.14639200
H	4.69960500	-0.80562600	-4.29149500
H	5.00330500	0.79750500	-3.55853300
P	-1.60571600	-0.43672500	-0.27229000
C	-2.80554800	-0.43355500	1.21175500
C	-4.22449000	-0.44963100	1.23807600
C	-2.11768200	-0.46737800	2.44254600
C	-4.86276400	-0.49941700	2.49331600
C	-2.77340400	-0.53058900	3.66836800
H	-1.03301800	-0.44022600	2.44278600
C	-4.16430100	-0.54548300	3.69484000
H	-5.94807400	-0.50395500	2.50610400
H	-2.19678200	-0.55892100	4.58762500
H	-4.70306500	-0.58715900	4.63632000
C	-2.10744300	0.69159200	-1.80835500
C	-1.25754500	-2.32436700	-0.70465400
C	-2.60090200	2.02306100	-1.22059600

H	-2.81114100	2.71253300	-2.04627500
H	-3.51767500	1.90665500	-0.64457000
H	-1.84217500	2.48924400	-0.58329200
C	-3.16088800	0.05482500	-2.72542700
H	-3.38531900	0.76367800	-3.53100300
H	-2.79170600	-0.85994600	-3.19693800
H	-4.09312400	-0.16822400	-2.21151000
C	-0.82699300	0.96286900	-2.62324800
H	-0.40115900	0.06123600	-3.06483400
H	-1.09008300	1.64001600	-3.44396800
H	-0.05208600	1.45252100	-2.02546400
C	-0.37507200	-2.40497000	-1.95885000
H	-0.89959000	-2.08245800	-2.86131100
H	0.54595500	-1.82431300	-1.85444100
H	-0.08520400	-3.45113500	-2.10730900
C	-2.56208400	-3.10160300	-0.91281200
H	-2.31279800	-4.13871400	-1.16536900
H	-3.15983100	-3.12240600	0.00141800
H	-3.17179300	-2.69880900	-1.72404800
C	-0.49790200	-2.92018700	0.49377700
H	-1.07663100	-2.86346100	1.41972700
H	-0.30095400	-3.97857900	0.29009500
H	0.46990800	-2.43343900	0.64827200
C	-5.18118000	-0.38313900	0.08198600
C	-5.79302400	0.84077900	-0.23692800
C	-5.62886300	-1.54110300	-0.57144300
C	-6.77049400	0.91632400	-1.23015400
H	-5.51346000	1.73591500	0.31125600
C	-6.60902500	-1.46720900	-1.56376100
H	-5.22821000	-2.50759100	-0.28961200
C	-7.17367600	-0.23730000	-1.90500600
H	-7.22621300	1.87358400	-1.46491000
H	-6.94155200	-2.37519000	-2.05799700
H	-7.93763200	-0.18157300	-2.67436400
C	2.15316900	2.18980700	1.04697000
C	2.43287000	1.03643600	1.41911000
C	3.35538200	0.01917200	2.01626700
H	3.74009700	0.41214300	2.96273600
H	2.83498200	-0.92178400	2.21118500
O	4.49085900	-0.20175700	1.18047000
H	4.99293400	1.28592600	-0.17568100
C	1.94882500	3.52902000	0.60028900
C	1.18153600	4.43409700	1.36284700
C	2.56002100	3.95238300	-0.59988000
C	1.02987600	5.74519200	0.92445200
H	0.72000100	4.10095100	2.28681200
C	2.40255800	5.26905200	-1.02083100
H	3.15806800	3.24804000	-1.17001400

C	1.63799800	6.16268700	-0.26410300
H	0.44209900	6.44469700	1.51001500
H	2.87729600	5.60091100	-1.93864700
H	1.51813800	7.18832200	-0.59927600
<b>TS<sub>11-12</sub></b>			
C	3.67909200	0.28136200	-0.47456100
C	4.26022900	-0.40194200	0.71325300
C	5.22185000	0.26970900	1.48946700
C	3.91252100	-1.71597000	1.07350800
C	5.79919500	-0.34628100	2.59978700
H	5.54455700	1.26420700	1.20249400
C	4.50093600	-2.33004900	2.17726300
H	3.19045800	-2.26216900	0.48018100
C	5.43987200	-1.64686700	2.95316400
H	6.54222300	0.19147700	3.18117700
H	4.22156400	-3.34797200	2.43319000
H	5.89119900	-2.12595800	3.81628000
Au	1.08084300	0.31789400	-0.20035400
C	3.54124200	-0.31477000	-1.73566900
O	3.48454300	0.42548100	-2.84075200
O	3.52131500	-1.62411600	-1.90783500
C	3.51972600	-2.14661500	-3.25840400
H	4.39074800	-1.78516000	-3.80735600
H	3.56767900	-3.22712300	-3.13667400
H	2.60423500	-1.85843800	-3.77868900
P	-0.95256300	-1.08336200	-0.15773000
C	-2.00900200	-0.46460600	1.31261700
C	-3.40820500	-0.52589900	1.54179100
C	-1.19458600	0.07612200	2.32982300
C	-3.90112300	-0.05102600	2.77424100
C	-1.70527200	0.52464200	3.54465500
H	-0.12388300	0.14599900	2.16502500
C	-3.07721100	0.46049400	3.77063000
H	-4.97302300	-0.09697400	2.93923600
H	-1.03242800	0.91969600	4.29983100
H	-3.50487500	0.80543200	4.70705700
C	-1.73236500	-0.83920000	-1.95125800
C	-0.51816800	-2.95005600	0.28072200
C	-2.30195900	0.58737100	-1.98919700
H	-2.65015700	0.79799800	-3.00729000
H	-3.14947000	0.71279200	-1.31779200
H	-1.54103000	1.33182000	-1.73542400
C	-2.79652000	-1.87775600	-2.33388900
H	-3.18938800	-1.61781700	-3.32409500
H	-2.37414000	-2.88349400	-2.41224100
H	-3.63655900	-1.90345600	-1.64279400
C	-0.57502000	-0.91569400	-2.96732600

H	-0.09420700	-1.89522000	-2.98988600
H	-0.98821800	-0.72778700	-3.96515000
H	0.18831600	-0.15577100	-2.77327700
C	0.34700800	-3.53550000	-0.84551200
H	-0.22242100	-3.69518600	-1.76474000
H	1.21166100	-2.90316800	-1.06952000
H	0.72286500	-4.51391300	-0.52444200
C	-1.77058600	-3.80783000	0.49723900
H	-1.45769500	-4.83683000	0.71113700
H	-2.34036800	-3.45569600	1.35924600
H	-2.43006000	-3.83499300	-0.37166200
C	0.29058200	-2.91932500	1.58844800
H	-0.29772400	-2.53522500	2.42542900
H	0.58806700	-3.94470800	1.83758700
H	1.19750000	-2.31684600	1.49886100
C	-4.48723000	-1.00726400	0.61347000
C	-5.21823600	-0.07389300	-0.14030100
C	-4.91978500	-2.34182800	0.61692000
C	-6.30082600	-0.47464700	-0.92453000
H	-4.94683500	0.97692000	-0.09525600
C	-6.00491400	-2.74423400	-0.16502700
H	-4.42210400	-3.06761400	1.24925900
C	-6.69084400	-1.81470500	-0.94802900
H	-6.84760700	0.26292000	-1.50445600
H	-6.32196100	-3.78275000	-0.14873200
H	-7.53562900	-2.12776100	-1.55386100
C	0.73252000	3.11451300	-0.01173600
C	1.80836100	2.49585900	0.00167100
C	3.28389100	2.56054000	0.19365000
H	3.66199100	3.55030700	-0.07454400
H	3.51944200	2.36539200	1.24603200
O	3.99121600	1.64435700	-0.64564200
H	3.66301500	1.34351800	-2.55238300
C	-0.50199900	3.80845800	-0.06218100
C	-1.33451100	3.88068900	1.07711800
C	-0.89041200	4.46832200	-1.25051800
C	-2.52427900	4.59783500	1.02199700
H	-1.03908700	3.36924200	1.98672100
C	-2.08313000	5.18175700	-1.29186200
H	-0.24575900	4.41804800	-2.12204200
C	-2.89942000	5.24857500	-0.15813500
H	-3.16047300	4.65400100	1.89956100
H	-2.37604000	5.69094400	-2.20448900
H	-3.82770200	5.81062800	-0.19353800
<b>13</b>			
C	-4.40913900	-0.53322000	-0.33531800
C	-5.31047000	-0.56611400	0.90422200

C	-5.52831600	-1.79197900	1.54674800
C	-5.89765700	0.59678400	1.42345700
C	-6.31557700	-1.85096700	2.69668300
H	-5.09103300	-2.69591500	1.14069900
C	-6.68759400	0.52903600	2.57201700
H	-5.73449300	1.55749900	0.95009200
C	-6.89873000	-0.69261500	3.21203500
H	-6.47644200	-2.80701700	3.18530600
H	-7.13650000	1.43600700	2.96519400
H	-7.51503100	-0.74185600	4.10433100
C	-5.07907300	0.18121900	-1.50538600
O	-5.26759600	-0.50517000	-2.57486000
O	-5.40310700	1.41689400	-1.45806800
C	-6.00032400	2.05651500	-2.63788800
H	-5.30130100	1.98974200	-3.47150600
H	-6.93992400	1.55756000	-2.87535200
H	-6.16132100	3.08753500	-2.33487100
C	-2.96726700	0.03322200	-0.16652800
C	-2.06401100	-0.90648300	-0.50922700
C	-2.77083100	-2.15359800	-0.93006300
H	-2.53858600	-2.46884300	-1.95384000
H	-2.58394800	-2.99871600	-0.25886600
O	-4.21509900	-1.85234900	-0.86944000
H	-4.91687200	-1.41640400	-2.28751500
C	-2.70874700	1.41941700	0.30127500
C	-2.28094500	2.40037000	-0.60922700
C	-2.85077000	1.77310300	1.65352200
C	-2.00506000	3.69974800	-0.18279900
H	-2.15011000	2.13294800	-1.65460200
C	-2.57406100	3.07332200	2.07914000
H	-3.16281400	1.02390400	2.37335100
C	-2.15436100	4.04000400	1.16320500
H	-1.66933500	4.44411800	-0.89897400
H	-2.67986800	3.32852000	3.12937400
H	-1.93881000	5.05041600	1.49735000
P	2.44003800	-0.80436000	-0.21974000
C	3.15780600	-2.04836600	-1.56144900
C	2.82013900	-1.32468100	1.63732500
C	1.84646100	-2.46390700	2.00573800
H	2.01844900	-3.37518200	1.43072500
H	1.99992200	-2.70879700	3.06326100
H	0.80086300	-2.16770000	1.87901500
C	4.25688200	-1.79943000	1.89667800
H	5.00512000	-1.04597400	1.66052600
H	4.35342200	-2.04043600	2.96220600
H	4.49148300	-2.71160400	1.34049400
C	2.46769500	-0.10182200	2.50112200
H	1.43604400	0.22430800	2.33282100

H	2.56301900	-0.37820200	3.55772100
H	3.13287900	0.74068100	2.31764700
C	4.67607400	-1.92169400	-1.72519500
H	5.21928500	-2.11138100	-0.79769700
H	5.01528000	-2.65330200	-2.46840000
H	4.94850200	-0.92997100	-2.09350700
C	2.77829300	-3.48543500	-1.17139400
H	1.70340500	-3.59313600	-0.99495500
H	3.04709600	-4.15405400	-1.99753900
H	3.31591700	-3.83278600	-0.28602100
C	2.47831000	-1.69345200	-2.89666400
H	1.39169100	-1.81370000	-2.84341800
H	2.69896800	-0.66983800	-3.21155400
H	2.85708600	-2.36842000	-3.67331100
C	3.06788800	0.92351700	-0.74004900
C	4.27760100	1.60574600	-0.44437800
C	2.15018900	1.55217700	-1.60718900
C	4.49731300	2.86122600	-1.04504200
C	2.39774000	2.78787300	-2.19813200
H	1.20785500	1.05776400	-1.82081500
C	3.58730100	3.45109600	-1.91575700
H	5.42243500	3.37812700	-0.80969400
H	1.66031600	3.22466100	-2.86470100
H	3.80614600	4.41818000	-2.35817100
C	5.38341300	1.18820300	0.48356900
C	6.48128200	0.43987200	0.03334600
C	5.42617400	1.71326900	1.78588400
C	7.55627100	0.16575900	0.88185700
H	6.50731900	0.08579100	-0.99043900
C	6.49832500	1.43835700	2.63583400
H	4.62042300	2.35631800	2.12795700
C	7.56272600	0.65336900	2.18946400
H	8.39523600	-0.41738700	0.51366800
H	6.50693800	1.84919400	3.64107000
H	8.39959900	0.44135000	2.84789100
Au	-0.01559700	-0.82519300	-0.40618400
<b>TS</b> <sub>12-13</sub>			
C	-4.77290500	-0.47859900	-0.86209500
C	-5.26181000	-1.17043900	0.34004400
C	-5.30405500	-2.57865400	0.33385600
C	-5.70084700	-0.48949500	1.49270600
C	-5.75443800	-3.28210500	1.44840000
H	-5.01515100	-3.11584600	-0.56308500
C	-6.15368700	-1.20222900	2.60140900
H	-5.69156400	0.59213000	1.51899100
C	-6.17806200	-2.59829300	2.58943200
H	-5.78684900	-4.36712000	1.41930100

H	-6.49218200	-0.66099000	3.48005700
H	-6.53350300	-3.14710200	3.45598000
C	-5.15908900	0.77682800	-1.33237400
O	-4.82981800	1.19133800	-2.55414600
O	-5.87831600	1.60869400	-0.60814600
C	-6.35826400	2.83246500	-1.21653100
H	-5.52953800	3.42232700	-1.60913000
H	-7.06429600	2.60050700	-2.01641800
H	-6.85731400	3.36320700	-0.40831500
C	-2.64778500	0.50825600	-0.21829200
C	-2.05138000	-0.47759400	-0.78690700
C	-2.75464000	-1.58853000	-1.50250000
H	-2.28594300	-1.86081200	-2.44974100
H	-2.77708500	-2.47482400	-0.85690600
O	-4.11573800	-1.19577700	-1.83860900
H	-4.37667900	0.43734800	-2.97817500
C	-2.79480400	1.66824300	0.58550000
C	-2.80848500	2.95509600	-0.00275700
C	-2.94707700	1.54779500	1.98711100
C	-2.94409900	4.08583000	0.79418700
H	-2.69825400	3.04489100	-1.07894400
C	-3.08778300	2.68734900	2.77268900
H	-2.94765700	0.56067600	2.43602800
C	-3.08399200	3.95421200	2.18080300
H	-2.93722000	5.07213900	0.34060000
H	-3.19481900	2.59079200	3.84853600
H	-3.18722200	4.84022200	2.79981500
P	2.44156100	-0.79605900	-0.16463800
C	3.11290400	-2.36095400	-1.14507700
C	2.61942900	-0.92058500	1.78862700
C	1.53034400	-1.88704600	2.29848400
H	1.69349300	-2.91720400	1.97931600
H	1.55847000	-1.87435000	3.39409300
H	0.52612500	-1.58252600	1.98829300
C	3.98773100	-1.41841200	2.27527700
H	4.80939400	-0.78336700	1.95311400
H	3.97970600	-1.42444600	3.37172600
H	4.18772600	-2.44432400	1.95196000
C	2.30749300	0.48375800	2.33360800
H	1.32317900	0.83323500	2.00402000
H	2.29679900	0.43932100	3.42888200
H	3.05525100	1.21930900	2.03944600
C	4.64546500	-2.38622500	-1.19957700
H	5.10597300	-2.43270100	-0.21086600
H	4.96332200	-3.27345900	-1.75974300
H	5.03343400	-1.51041800	-1.72399600
C	2.57718400	-3.64248400	-0.48806600
H	1.48690800	-3.63433500	-0.39227100

H	2.84705200	-4.49552500	-1.12113500
H	3.01374100	-3.81940000	0.49762800
C	2.56085200	-2.25424100	-2.57841600
H	1.46631300	-2.25417800	-2.59559300
H	2.91539300	-1.35642800	-3.09206100
H	2.90717800	-3.12177400	-3.15185200
C	3.26174300	0.71817100	-0.99098300
C	4.49669700	1.36509500	-0.72359800
C	2.48393300	1.19580700	-2.06645200
C	4.87494700	2.44206100	-1.55002800
C	2.88823900	2.25248200	-2.87677700
H	1.52909700	0.72416600	-2.27498600
C	4.09917300	2.88525000	-2.61545500
H	5.81794800	2.93483100	-1.33523900
H	2.25503600	2.57627800	-3.69702200
H	4.43739200	3.71666000	-3.22619500
C	5.48095800	1.08350400	0.37590900
C	6.52793800	0.16429300	0.21173000
C	5.47503600	1.88696700	1.52827700
C	7.49956100	0.00374900	1.20218200
H	6.59768000	-0.41447600	-0.70181200
C	6.44351000	1.72572000	2.51988300
H	4.71491600	2.65489000	1.63911900
C	7.45352400	0.77474800	2.36460600
H	8.30059700	-0.71485600	1.05629300
H	6.41585400	2.35276100	3.40607500
H	8.21002800	0.65016300	3.13329500
Au	0.03182400	-0.60011800	-0.53968800
<b>TS<sub>13-4a</sub></b>			
C	-4.41960600	-0.19969800	-0.52290400
C	-5.30443900	-0.80606000	0.54773200
C	-4.71861100	-1.50945100	1.60909700
C	-6.70108400	-0.76482800	0.43939600
C	-5.52038200	-2.15368300	2.55017200
H	-3.63750400	-1.54220000	1.70129800
C	-7.50101400	-1.40644000	1.38395700
H	-7.17877300	-0.23658700	-0.38160900
C	-6.91159600	-2.10189100	2.44108100
H	-5.05784200	-2.69284800	3.37095600
H	-8.58170800	-1.36475300	1.29227300
H	-7.53422300	-2.60069700	3.17724300
C	-5.07022900	0.89771900	-1.37000600
O	-5.07585400	0.67357900	-2.60972000
O	-5.51215800	1.97210700	-0.81899900
C	-6.01666000	3.03938100	-1.68592100
H	-5.20807600	3.38951200	-2.32806900
H	-6.84532500	2.65882700	-2.28365600

H	-6.34357300	3.81784400	-1.00152500
C	-2.98704000	0.24080300	-0.14369600
C	-2.07086100	-0.55386700	-0.74599900
C	-2.74802700	-1.54636500	-1.63092500
H	-2.43691800	-1.49783400	-2.67906300
H	-2.66794200	-2.58115700	-1.28519200
O	-4.19791800	-1.19986500	-1.59835200
H	-4.59722400	-0.41193300	-2.49119300
C	-2.74252000	1.42521900	0.71623400
C	-1.65530900	2.27262300	0.42468000
C	-3.56403700	1.75859600	1.80853000
C	-1.38107500	3.38851100	1.21293700
H	-1.03202400	2.05515800	-0.43654600
C	-3.28824900	2.87768700	2.59491000
H	-4.41415300	1.13652900	2.06113900
C	-2.19512000	3.69503100	2.30546700
H	-0.53781300	4.02636000	0.96435100
H	-3.93112000	3.10711200	3.43960000
H	-1.98494700	4.56600200	2.91874400
P	2.40306300	-0.80936200	-0.17339800
C	3.05014100	-2.36649400	-1.18226700
C	2.63118600	-0.95965000	1.77337500
C	1.53084400	-1.90589100	2.29739700
H	1.64214600	-2.93030500	1.93883600
H	1.60215200	-1.93109700	3.39113100
H	0.52833600	-1.55422700	2.03584900
C	3.99817900	-1.49271800	2.22393300
H	4.82922600	-0.88405600	1.87498300
H	4.02345100	-1.49523300	3.32024000
H	4.15956000	-2.52406900	1.89780600
C	2.35761300	0.44383600	2.34080800
H	1.36971000	0.81152600	2.04433100
H	2.37847100	0.39045900	3.43563200
H	3.10721400	1.17048800	2.03064900
C	4.57956500	-2.42444700	-1.26105500
H	5.05641000	-2.46694300	-0.27977200
H	4.87113700	-3.32633000	-1.81269200
H	4.97672600	-1.56566500	-1.80706000
C	2.49735400	-3.64721900	-0.53709900
H	1.41022000	-3.60977200	-0.41471000
H	2.72810500	-4.49540800	-1.19215900
H	2.95303300	-3.85547400	0.43385600
C	2.48054100	-2.23282400	-2.60585900
H	1.38625600	-2.22936800	-2.60487900
H	2.83027200	-1.32539100	-3.10546400
H	2.81719600	-3.08991500	-3.20075000
C	3.22545900	0.71485400	-0.98007800
C	4.47507800	1.34173200	-0.73214600

C	2.42163600	1.23225000	-2.01758100
C	4.84070200	2.43814000	-1.53848800
C	2.81306700	2.30789500	-2.80973200
H	1.45423600	0.77752500	-2.20693600
C	4.03853900	2.91996100	-2.56728300
H	5.79510300	2.91508700	-1.33842100
H	2.15878700	2.66243700	-3.60040300
H	4.36827000	3.76461900	-3.16443700
C	5.48970200	1.01789600	0.32779300
C	6.52015900	0.09291800	0.10317000
C	5.53245400	1.78925300	1.50107500
C	7.52370800	-0.10411500	1.05428200
H	6.55123700	-0.46178800	-0.82717300
C	6.53285700	1.59177800	2.45378800
H	4.78522500	2.56155800	1.65879800
C	7.52635600	0.63531800	2.23788100
H	8.31158400	-0.82624700	0.86130400
H	6.54242200	2.19461200	3.35701200
H	8.30803700	0.48269000	2.97578600
Au	-0.02948800	-0.63404800	-0.51927200
<b>TS<sub>1a-14</sub></b>			
C	-2.07541300	-0.72100400	0.29140900
C	-2.58361300	-1.69788100	-0.66347500
C	-3.56886500	-2.66282100	-0.32576500
C	-2.07746200	-1.69943000	-1.98729000
C	-4.00038700	-3.59068100	-1.26679500
H	-3.97465100	-2.68253600	0.67726500
C	-2.53057800	-2.61279900	-2.92934800
H	-1.31912900	-0.97001000	-2.25374300
C	-3.49088400	-3.56540900	-2.56976300
H	-4.74285700	-4.33196800	-0.98829400
H	-2.13170200	-2.59522400	-3.93869100
H	-3.84041000	-4.28663900	-3.30263900
Au	-0.10797700	-0.03836300	0.10713700
C	-2.36558000	-0.91048100	1.75606500
O	-2.25098100	-2.00263000	2.27944000
O	-2.58426100	0.22115400	2.45666800
C	-2.68696100	0.03192300	3.88567000
H	-1.74530800	-0.34529400	4.29015400
H	-2.90960200	1.01769400	4.29268200
H	-3.48367200	-0.67665600	4.12295700
P	2.22981400	0.74492800	0.08912900
C	3.63929800	-0.51209800	0.07555000
C	3.46493700	-1.91064900	-0.04325700
C	4.95020000	0.00256000	0.09448800
C	4.61282400	-2.72063700	-0.14951200
C	6.07029800	-0.81860800	-0.00041900

H	5.11045000	1.06766100	0.17800300
C	5.89967700	-2.19492300	-0.12797700
H	4.47243500	-3.79347400	-0.23589700
H	7.06341900	-0.38078600	0.02059500
H	6.75819700	-2.85477800	-0.20651600
C	2.48214300	1.79422900	-1.56149000
C	2.41659900	1.77382100	1.75809300
C	2.66751900	0.75923200	-2.68588600
H	2.69538300	1.28447200	-3.64763600
H	3.60008800	0.19988400	-2.58206200
H	1.83922600	0.04353100	-2.71946700
C	3.67283800	2.76384200	-1.53995300
H	3.70646000	3.28911000	-2.50213300
H	3.57795000	3.52610300	-0.76200100
H	4.63153400	2.25573700	-1.42462800
C	1.19301600	2.59100900	-1.82099500
H	1.01450100	3.36479100	-1.07132300
H	1.27970200	3.08933100	-2.79375800
H	0.31366400	1.94189300	-1.85206400
C	1.41302000	2.93721100	1.71115900
H	1.71566700	3.71308300	1.00245000
H	0.40570900	2.60041900	1.44884100
H	1.36632500	3.40198700	2.70319000
C	3.82252000	2.32010100	2.05051100
H	3.76812300	2.92604000	2.96273300
H	4.54344600	1.52246400	2.23715100
H	4.20618800	2.96541600	1.25732000
C	2.02691900	0.79623000	2.88283400
H	2.69870800	-0.06691700	2.92033500
H	2.10119800	1.31518700	3.84580800
H	1.00038200	0.43425000	2.77114500
C	2.16792900	-2.65243900	-0.06555700
C	1.39300300	-2.80629400	1.09511000
C	1.80187900	-3.36441900	-1.21917800
C	0.28239700	-3.65322100	1.10252600
H	1.68654500	-2.29470200	2.00683100
C	0.68661400	-4.20356600	-1.21400200
H	2.40870900	-3.27313700	-2.11575500
C	-0.07202500	-4.35346200	-0.05170100
H	-0.30654600	-3.76003900	2.00641000
H	0.42218300	-4.75256100	-2.11305700
H	-0.93166600	-5.01624000	-0.04249300
C	-3.12341400	1.86298700	-0.35801400
C	-3.70127400	0.80476200	-0.08302500
C	-5.02250600	0.12244900	0.07771200
H	-5.80371200	0.87390600	-0.10174600
H	-5.12134400	-0.65007200	-0.68962300
O	-5.19698200	-0.52945400	1.31769600

H	-5.16123800	0.13788900	2.01594400
C	-2.49575200	3.08696000	-0.66318200
C	-2.13187500	3.97866800	0.37361600
C	-2.32176800	3.47752900	-2.01204100
C	-1.60508300	5.22622100	0.06184500
H	-2.28163200	3.67897700	1.40539100
C	-1.80252500	4.73184100	-2.30957500
H	-2.61568300	2.79649500	-2.80392600
C	-1.44373000	5.60493400	-1.27629900
H	-1.33262700	5.91258900	0.85723900
H	-1.68244600	5.03585200	-3.34444600
H	-1.04484400	6.58638300	-1.51423800
<b>14</b>			
C	-2.92588700	-0.84951900	0.63487800
C	-3.22123900	-1.94988800	-0.31977400
C	-2.99211300	-3.30860800	-0.00613000
C	-3.79167600	-1.64352200	-1.57741600
C	-3.34210000	-4.31098800	-0.90803600
H	-2.55471000	-3.57317000	0.94747800
C	-4.13076800	-2.64903900	-2.47387500
H	-3.95832100	-0.60719200	-1.85146100
C	-3.90922300	-3.99051300	-2.14270700
H	-3.17232100	-5.34937900	-0.64072900
H	-4.57255300	-2.38984100	-3.43108700
H	-4.17909400	-4.77633400	-2.84132400
Au	-0.86964600	-0.11118600	0.02412200
C	-2.63935300	-1.21661500	2.08309000
O	-1.85270400	-2.07259500	2.44455900
O	-3.36462200	-0.47043200	2.92609400
C	-3.16386900	-0.72795600	4.33636200
H	-2.12857300	-0.51666900	4.61158900
H	-3.84712400	-0.05485200	4.85092900
H	-3.39594800	-1.76935700	4.56591800
P	1.58638100	-0.44953900	-0.46960900
C	2.51419500	1.14676400	0.01285200
C	3.87994300	1.35253600	0.34489500
C	1.66539100	2.27129700	-0.02550200
C	4.30478100	2.66909900	0.61171100
C	2.11412100	3.56372900	0.23117700
H	0.61707400	2.13746800	-0.26397700
C	3.45146300	3.76594400	0.55466200
H	5.34839400	2.81804400	0.87017200
H	1.41472000	4.39206500	0.18422800
H	3.83025200	4.76109300	0.76633600
C	2.07342100	-2.06584300	0.55079100
C	1.76188800	-0.63505900	-2.41902600
C	2.16462000	-1.63256700	2.02285000

H	2.33830200	-2.52384100	2.63667900
H	2.98452000	-0.93972600	2.20438800
H	1.23129400	-1.17564000	2.36676500
C	3.37007200	-2.73395300	0.07319800
H	3.57299400	-3.59006900	0.72748800
H	3.27613800	-3.12484900	-0.94387200
H	4.23286300	-2.07324200	0.11654900
C	0.90990600	-3.06751700	0.41796900
H	0.73519100	-3.38994900	-0.60948900
H	1.17062700	-3.95886400	1.00066900
H	-0.02146600	-2.67550500	0.83494600
C	1.09169600	-1.94426900	-2.86294400
H	1.64753700	-2.82785300	-2.54077800
H	0.06188300	-2.02537600	-2.50078700
H	1.05789800	-1.96343700	-3.95828800
C	3.22539100	-0.59880500	-2.87311200
H	3.25995200	-0.73010000	-3.96114900
H	3.68355800	0.36593600	-2.64503300
H	3.82903600	-1.38888800	-2.42320800
C	1.01330500	0.55511200	-3.04408500
H	1.42867400	1.51650400	-2.73048100
H	1.10535700	0.49310100	-4.13466500
H	-0.05280500	0.53859000	-2.79684400
C	4.97341400	0.33285600	0.49360500
C	5.34224700	-0.10134300	1.77792500
C	5.76913900	-0.05776100	-0.59388600
C	6.42724100	-0.95962400	1.96084800
H	4.78457800	0.25076000	2.64096100
C	6.85769700	-0.91372700	-0.41184700
H	5.55315400	0.32548200	-1.58418300
C	7.18223800	-1.37772500	0.86369100
H	6.69000800	-1.28863900	2.96176500
H	7.46063200	-1.20441900	-1.26703600
H	8.02972600	-2.04153100	1.00435000
C	-2.55041000	1.23776500	0.05209900
C	-3.57883100	0.49318300	0.42276700
C	-5.03707600	0.83140100	0.61543900
H	-5.65417100	0.15757300	0.00006600
H	-5.29781800	0.62466100	1.65863400
O	-5.32584600	2.19279800	0.38186300
H	-5.33852800	2.35048700	-0.57068900
C	-2.22142400	2.61520400	-0.27927500
C	-2.15849800	3.58250300	0.74608700
C	-1.97266200	3.00634400	-1.61166500
C	-1.88778700	4.91187400	0.43538300
H	-2.34851400	3.28265400	1.77106200
C	-1.69964000	4.33802100	-1.91223800
H	-2.01040400	2.26308200	-2.40233200

C	-1.65665100	5.29278200	-0.89097900
H	-1.86426400	5.65464300	1.22674800
H	-1.52567600	4.63431600	-2.94202900
H	-1.44811700	6.33143000	-1.12856900
<b>TS</b> <sub>14-15</sub>			
C	-3.04954700	-0.58840700	0.71200300
C	-3.10853000	-1.80594800	-0.20496000
C	-3.04789200	-3.11782600	0.29598100
C	-3.33310400	-1.62815200	-1.58262900
C	-3.19644800	-4.20872300	-0.56260300
H	-2.87970200	-3.28799400	1.35100100
C	-3.47415700	-2.72174900	-2.43619900
H	-3.41175800	-0.62444500	-1.98888400
C	-3.40444700	-4.02054200	-1.92931100
H	-3.15262100	-5.21328300	-0.15249900
H	-3.64761000	-2.55582200	-3.49533600
H	-3.52000900	-4.87402400	-2.58996800
Au	-0.74159500	-0.15432400	-0.07994200
C	-2.54923400	-0.76416400	2.14348400
O	-1.83121000	-1.66200500	2.54046700
O	-3.01880100	0.21003000	2.94422800
C	-2.59708200	0.14621300	4.32510200
H	-1.50788700	0.18546900	4.39102900
H	-3.04549500	1.01534800	4.80352500
H	-2.95355600	-0.77661800	4.78679200
P	1.61380100	-0.42789900	-0.45952600
C	2.47233200	1.21861500	-0.02109400
C	3.82669000	1.47036100	0.32449000
C	1.59631200	2.31789400	-0.12636100
C	4.21784800	2.80791700	0.53126300
C	2.01361800	3.63025800	0.07448300
H	0.55384200	2.14493900	-0.36878600
C	3.34103600	3.87993700	0.40622100
H	5.25296400	2.99297900	0.80010500
H	1.29673100	4.43883100	-0.02260700
H	3.69344300	4.89300800	0.57383000
C	2.09541700	-1.99048000	0.64917600
C	1.83541600	-0.69052700	-2.39666500
C	2.12255900	-1.49035700	2.10207400
H	2.31119800	-2.34751000	2.75840700
H	2.90798700	-0.75740700	2.27906700
H	1.15937100	-1.06023600	2.39337200
C	3.42772500	-2.63264400	0.23693400
H	3.64765300	-3.43913700	0.94585200
H	3.36967300	-3.08734400	-0.75616800
H	4.26441300	-1.93832200	0.25846800
C	0.96914700	-3.03384800	0.52106800

H	0.83854400	-3.40376200	-0.49642600
H	1.24432100	-3.88995800	1.14817200
H	0.01235500	-2.65632900	0.88820700
C	1.19743200	-2.02877800	-2.79960700
H	1.76180300	-2.88713300	-2.42770200
H	0.16066500	-2.11437100	-2.45953700
H	1.19337700	-2.09268400	-3.89371200
C	3.31397000	-0.65317400	-2.80085300
H	3.38512000	-0.83892300	-3.87888400
H	3.74993500	0.32913400	-2.60793800
H	3.91349400	-1.40972100	-2.29230500
C	1.09557400	0.46318600	-3.09451500
H	1.49076200	1.44173600	-2.80912100
H	1.22755000	0.35445000	-4.17721600
H	0.02273000	0.44672500	-2.88203800
C	4.93813700	0.48428800	0.54788400
C	5.27176300	0.10620700	1.85926800
C	5.78114700	0.07603500	-0.49670600
C	6.37034800	-0.71668800	2.11071800
H	4.67636400	0.47540600	2.68922400
C	6.88272400	-0.74524700	-0.24609300
H	5.59122400	0.41794500	-1.50741100
C	7.17312000	-1.15471900	1.05606100
H	6.60590100	-1.00251500	3.13144600
H	7.52205400	-1.05132800	-1.06882200
H	8.03082600	-1.79142100	1.24992200
C	-3.22229700	1.00374000	0.08738400
C	-4.21595200	0.36373200	0.58649400
C	-5.66677900	0.33583300	0.94541000
H	-6.13006500	-0.54327600	0.47253600
H	-5.73785300	0.18879900	2.02897500
O	-6.32808600	1.54021900	0.64015800
H	-6.55404000	1.54372700	-0.29875000
C	-2.63888500	2.24337500	-0.42485900
C	-2.35189600	3.28075000	0.48120100
C	-2.44982900	2.45232100	-1.80292400
C	-1.88080300	4.50518100	0.00975600
H	-2.51867900	3.12296400	1.54157200
C	-1.97719700	3.67970100	-2.26395800
H	-2.69378400	1.66342100	-2.50745700
C	-1.69002100	4.70659000	-1.36026400
H	-1.67813000	5.30760300	0.71252400
H	-1.84637000	3.83954800	-3.32968400
H	-1.33225800	5.66474000	-1.72441300
<b>15</b>			
C	-3.50875800	-0.24505400	0.93180600
C	-3.02960300	-1.43737800	0.13748400



C	-3.10784200	-2.73150100	0.67333200
C	-2.58778700	-1.29338600	-1.20829600
C	-2.81435800	-3.85304500	-0.10430700
H	-3.42589700	-2.86129100	1.70288700
C	-2.29488200	-2.44448400	-1.99123700
H	-2.70357100	-0.32948200	-1.69988000
C	-2.40536500	-3.71942900	-1.43527200
H	-2.91446000	-4.84330100	0.33021500
H	-2.02816700	-2.32094200	-3.03640400
H	-2.19379200	-4.59727400	-2.03673800
Au	-0.32441200	-1.09223100	-0.70008900
C	-2.81314900	-0.07851000	2.26436400
O	-1.74833000	-0.60101900	2.54944800
O	-3.48822800	0.73515600	3.08877400
C	-2.86888000	1.00519800	4.36214700
H	-1.91123000	1.51108500	4.21942700
H	-3.56631700	1.65119700	4.89328200
H	-2.70618900	0.07584400	4.91225100
P	2.03228600	-0.75736100	-0.27253800
C	2.47051200	0.99456000	-0.89171500
C	3.55132200	1.84261500	-0.53383200
C	1.58218200	1.43782300	-1.89333100
C	3.67584700	3.07561800	-1.20495900
C	1.73752900	2.65477200	-2.55125000
H	0.74128000	0.80933600	-2.16838700
C	2.79813700	3.48558400	-2.20241500
H	4.50149400	3.72091200	-0.92228500
H	1.03055200	2.94375400	-3.32276200
H	2.94232700	4.44223100	-2.69492200
C	2.25905000	-1.09637500	1.65616200
C	2.98770000	-2.01286000	-1.45141700
C	1.70456000	0.13875300	2.38299200
H	1.77643100	-0.03901400	3.46221900
H	2.26950000	1.04202100	2.15830500
H	0.64828600	0.29969900	2.15161700
C	3.71198800	-1.38864900	2.05799900
H	3.73835500	-1.53715800	3.14366300
H	4.08526500	-2.30882000	1.60053100
H	4.39578500	-0.57652400	1.82000000
C	1.37655800	-2.30681500	2.02148800
H	1.67644700	-3.22548700	1.51472200
H	1.48372200	-2.47743500	3.09889900
H	0.31820500	-2.11412900	1.82896700
C	2.73333800	-3.44995800	-0.97220000
H	3.22122600	-3.66564700	-0.01898500
H	1.66564800	-3.67161400	-0.87867600
H	3.15029100	-4.14021900	-1.71442900
C	4.49148700	-1.71602100	-1.48928600

H	4.97850300	-2.46306300	-2.12684600
H	4.68846300	-0.73485400	-1.92708600
H	4.96040200	-1.76225100	-0.50508200
C	2.40735300	-1.83545300	-2.86521300
H	2.53692100	-0.81703300	-3.24061300
H	2.93961300	-2.50945500	-3.54617500
H	1.34354600	-2.08937300	-2.90471900
C	4.60440600	1.62481800	0.51534000
C	4.46890700	2.24213800	1.76995100
C	5.81517600	0.98150900	0.21759600
C	5.48350000	2.15580300	2.72421400
H	3.56962800	2.80924200	1.99181700
C	6.83237100	0.89665600	1.17090500
H	5.97501800	0.56458400	-0.76981600
C	6.66489700	1.47242900	2.43113600
H	5.35535000	2.63514600	3.69009500
H	7.76159700	0.39348000	0.92070300
H	7.45709900	1.40853400	3.17070500
C	-4.04934200	0.99881600	0.23869500
C	-4.94729200	0.21858900	0.75942500
C	-6.36060100	-0.07985500	1.11281800
H	-6.57534000	-1.14574900	0.94086900
H	-6.49638700	0.09960000	2.18630100
O	-7.27114900	0.77050000	0.43999500
H	-7.32677400	0.48539800	-0.48141500
C	-3.66761100	2.22296400	-0.42909200
C	-4.67125500	3.11660100	-0.85008100
C	-2.31720900	2.54523900	-0.64612000
C	-4.32212300	4.30412300	-1.48536300
C	-5.71114000	2.86793700	-0.65931200
C	-1.97578500	3.73913900	-1.27988000
H	-1.54172600	1.86418100	-0.30557200
C	-2.97601600	4.61727100	-1.70350100
H	-5.09856500	4.99133300	-1.80715400
H	-0.92975700	3.98371300	-1.43835700
H	-2.70946400	5.54696900	-2.19698500
TS <sub>2a-16</sub>			
C	2.14797800	0.09067200	0.56560600
C	2.62308600	-1.21546100	-0.00074700
C	2.41613600	-1.54698700	-1.35442500
C	3.21994500	-2.16860100	0.84211000
C	2.82327000	-2.78458100	-1.84817200
H	1.95487700	-0.83338400	-2.02501600
C	3.63247100	-3.40157600	0.33755500
H	3.36515200	-1.94201100	1.89054000
C	3.43674300	-3.71626300	-1.00801600
H	2.66436900	-3.01788900	-2.89666300

H	4.10180400	-4.11945800	1.00343100
H	3.75391500	-4.67872600	-1.39737300
Au	-0.08509800	-0.06060500	0.61144600
C	2.36130500	1.42878000	-0.14330500
O	2.20246200	2.49029500	0.42910200
O	2.67414200	1.30677800	-1.43311300
C	2.86032500	2.54899000	-2.15248100
H	3.68433200	3.11229100	-1.71165300
H	3.09517900	2.25522600	-3.17392000
H	1.94816200	3.14791800	-2.11672800
P	-2.52481500	-0.35468200	0.49761100
C	-3.26034000	1.34193200	0.03711800
C	-4.50293100	1.66222700	-0.56977500
C	-2.41333600	2.40217400	0.42278900
C	-4.82019800	3.02323900	-0.74767700
C	-2.75813500	3.73895000	0.24584200
H	-1.45175200	2.17962200	0.87349300
C	-3.97676900	4.05400600	-0.34677800
H	-5.76925400	3.26173400	-1.21730400
H	-2.07196300	4.51773600	0.56327500
H	-4.26936300	5.08773700	-0.50239100
C	-2.77678500	-1.80653500	-0.80868100
C	-3.13193600	-0.76758800	2.32297200
C	-2.50724200	-1.18952600	-2.19046500
H	-2.53426600	-1.98758000	-2.94114700
H	-3.25392500	-0.44719700	-2.46769500
H	-1.51660800	-0.72398700	-2.23836300
C	-4.15991100	-2.46931600	-0.74223500
H	-4.21634300	-3.22414200	-1.53530000
H	-4.31297600	-2.99009100	0.20707700
H	-4.97812300	-1.76841500	-0.89262500
C	-1.69682600	-2.87385600	-0.53637600
H	-1.79772800	-3.34764000	0.44082400
H	-1.80533000	-3.65843500	-1.29382000
H	-0.68145600	-2.47472000	-0.62380800
C	-2.59761600	-2.14842400	2.73255200
H	-3.07526200	-2.96121500	2.18052400
H	-1.51286200	-2.22765200	2.60915300
H	-2.81958100	-2.30315600	3.79448400
C	-4.66030900	-0.72705500	2.43033900
H	-4.94608200	-0.98764600	3.45606400
H	-5.04166800	0.27652600	2.22973600
H	-5.15266200	-1.43212700	1.75777100
C	-2.53237900	0.30773700	3.24627500
H	-2.86183200	1.31497700	2.97849200
H	-2.86788900	0.11086000	4.27089400
H	-1.43812100	0.28640100	3.24396900
C	-5.54908000	0.72513300	-1.10177300

C	-5.61401600	0.47623100	-2.48310500
C	-6.58176900	0.23475900	-0.28850900
C	-6.63902300	-0.30080700	-3.02439900
H	-4.86561600	0.91133100	-3.13937900
C	-7.61013200	-0.54038500	-0.82946800
H	-6.59798700	0.47839400	0.76726300
C	-7.63508500	-0.82128900	-2.19631200
H	-6.66662200	-0.48562700	-4.09407600
H	-8.40018100	-0.91035800	-0.18276600
H	-8.43634400	-1.42162300	-2.61607100
C	5.76371000	0.77806600	0.78103700
C	4.81001200	0.90182900	1.52321200
C	3.68196700	1.07274200	2.41056800
H	3.88497300	0.71950000	3.42513000
H	3.34627200	2.11130700	2.43492200
O	2.52328900	0.22659400	2.01212500
H	1.23819400	0.41938900	1.70458900
C	6.88534300	0.61069100	-0.08450800
C	7.58551800	1.73256300	-0.57022800
C	7.30286500	-0.68220000	-0.45783900
C	8.68366000	1.55913300	-1.40787800
H	7.26621100	2.72780300	-0.27808200
C	8.39730700	-0.84343700	-1.30249000
H	6.76019800	-1.54425000	-0.08382400
C	9.09021900	0.27387000	-1.77642800
H	9.22412000	2.42665800	-1.77376000
H	8.71452100	-1.84161100	-1.58826600
H	9.94707800	0.14322800	-2.43033400
<b>P<sub>1a</sub></b>			
C	1.33382300	0.22749200	0.32665700
C	2.43805900	-0.75579600	-0.02371600
C	3.49486700	-0.96254400	0.87139000
C	2.42816600	-1.43348100	-1.24658200
C	4.52388400	-1.84613800	0.54670100
H	3.49445200	-0.43690500	1.82028000
C	3.46160100	-2.31330200	-1.57221400
H	1.60957500	-1.27445400	-1.94329200
C	4.51111900	-2.52198700	-0.67574900
H	5.33756700	-2.00636300	1.24845900
H	3.44268900	-2.83958100	-2.52234900
H	5.31342000	-3.21002500	-0.92684700
C	1.82827100	1.65880200	0.04522100
O	2.20966400	2.44713400	0.88135800
O	1.79470100	1.91318600	-1.27786300
C	2.30407400	3.19897200	-1.67268800
H	3.35134800	3.30297600	-1.37856400
H	2.20576900	3.23435200	-2.75738100

H	1.72476100	4.00033300	-1.20750600
C	-2.41457200	0.20469200	0.94099100
C	-1.37446100	0.48589200	1.49925200
C	-0.10694200	0.82627000	2.15474900
H	0.09715000	1.89975700	2.04969800
H	-0.16695700	0.60699600	3.22573500
O	1.00730600	0.05961700	1.69044600
H	0.46094600	0.04619000	-0.31522200
C	-3.64781000	-0.12791400	0.29880600
C	-4.20829100	0.73288200	-0.66488000
C	-4.32123900	-1.32266800	0.61982300
C	-5.40993900	0.40484500	-1.28759000
H	-3.69181000	1.65419200	-0.91454100
C	-5.52211400	-1.64368400	-0.00806900
H	-3.89110500	-1.98792400	1.36150700
C	-6.07006300	-0.78268300	-0.96220500
H	-5.83270400	1.07694200	-2.02877300
H	-6.03211600	-2.56792300	0.24768100
H	-7.00695300	-1.03596500	-1.44979900
<b>P<sub>2a</sub></b>			
C	0.54435300	-0.50157400	0.08491800
C	1.47674200	0.64643000	-0.23237400
C	2.21311100	0.65436400	-1.42382900
C	1.58794900	1.74649600	0.63148300
C	3.03590400	1.73611900	-1.74499000
H	2.13610800	-0.19284700	-2.09919900
C	2.40959500	2.82662400	0.31221800
H	1.03885200	1.75026500	1.56867800
C	3.13713000	2.82614600	-0.88002500
H	3.60050200	1.72389800	-2.67354000
H	2.48038000	3.67014500	0.99375800
H	3.77657500	3.66803200	-1.13077900
C	0.75030100	-1.28611400	1.36542400
O	0.09945400	-2.26922900	1.66536400
O	1.75293700	-0.80953600	2.13386900
C	2.00954600	-1.55273100	3.33511800
H	2.27001000	-2.58774200	3.09966200
H	2.84520500	-1.04800500	3.82014300
H	1.13084300	-1.55367700	3.98539900
C	-0.89312600	-0.48258900	-0.43082000
C	-0.09504900	-1.31427600	-1.02798100
C	0.13663600	-2.49588700	-1.88857800
H	0.25568700	-3.36432400	-1.22093500
H	-0.75566700	-2.67240100	-2.50883600
O	1.29828100	-2.29844700	-2.68928400
H	1.54988600	-3.15221500	-3.06252900
C	-2.18552900	0.11790600	-0.19385500

C	-2.35101300	1.07672000	0.81935100
C	-3.29542800	-0.24460000	-0.98053000
C	-3.59833000	1.65524200	1.04502000
H	-1.49482000	1.36508700	1.42053500
C	-4.53830500	0.33788700	-0.75295100
H	-3.17255900	-0.98383300	-1.76641200
C	-4.69399900	1.28852500	0.26086500
H	-3.71522700	2.39479500	1.83176500
H	-5.38867000	0.05100300	-1.36482000
H	-5.66540700	1.74138700	0.43673100
<b>Ab</b>			
C	0.07695300	0.37962800	0.00008000
C	-1.37153700	0.08039100	-0.00005800
C	-1.83759900	-1.24707800	-0.00034400
C	-2.31626000	1.12441600	0.00009300
C	-3.20738200	-1.50800400	-0.00047400
H	-1.12433700	-2.05992200	-0.00046200
C	-3.68113600	0.85067400	-0.00003900
H	-1.99022700	2.16048400	0.00031600
C	-4.13759400	-0.46855300	-0.00032400
H	-3.54575300	-2.54041600	-0.00069600
H	-4.38869300	1.67490400	0.00008200
H	-5.20238200	-0.68138600	-0.00042800
C	1.18342400	-0.59185600	-0.00003100
O	1.05515900	-1.80215000	-0.00023700
O	2.38662400	0.03234800	0.00013100
C	3.54423300	-0.83512000	0.00003700
H	3.50160100	-1.48062400	0.88278400
H	3.50168700	-1.48032000	-0.88293600
N	0.44572700	1.64474600	0.00032200
N	0.73720100	2.74524400	0.00055600
C	4.77433800	0.05217500	0.00025000
H	4.79616600	0.69152400	0.88737300
H	5.67628000	-0.56762300	0.00018500
H	4.79625000	0.69183100	-0.88665000
<b>Db</b>			
C	-0.82812000	-0.61521100	0.16080300
C	-1.88207600	0.21021300	0.22869500
C	-3.29917600	-0.25471400	0.36501700
H	-3.34414600	-1.35273000	0.28342800
H	-3.67202000	0.01107900	1.37027700
O	-4.08517000	0.38323800	-0.63995800
H	-5.01439100	0.21600100	-0.43826400
C	0.59398100	-0.25055000	0.07295600
C	1.05477600	1.07883100	0.12082800
C	1.54871100	-1.27327700	-0.06599700
C	2.41272100	1.36789900	0.02552200

H	0.34575100	1.89275700	0.23686800
C	2.90968000	-0.98528300	-0.16010300
H	1.21305600	-2.30689200	-0.10289500
C	3.34838500	0.33822800	-0.11559600
H	2.74524700	2.40154100	0.06438600
H	3.62618300	-1.79477400	-0.26795400
H	4.40752900	0.56776200	-0.18764600
H	-1.02216100	-1.68850100	0.16808500
H	-1.75699200	1.29104000	0.20062900
<b>AuL<sub>2</sub></b>			
P	-0.07410000	0.15473500	-0.14188200
C	1.29812000	0.38760100	-1.46302400
C	1.50644700	1.84456000	-1.92373200
C	2.61992100	-0.28284500	-1.04780600
H	0.87565500	-0.17624500	-2.30578100
C	2.53493000	1.88648500	-3.07249800
H	1.86804600	2.45666100	-1.09054000
H	0.56298900	2.28131400	-2.26522200
C	3.63989700	-0.21712700	-2.19969100
H	3.03490800	0.22626600	-0.16882200
H	2.44505000	-1.32698800	-0.76106200
C	3.86084100	1.22384200	-2.67923900
H	2.69523800	2.92955300	-3.36505000
H	2.11376900	1.37713900	-3.94979300
H	4.58341900	-0.66423100	-1.86983500
H	3.27777500	-0.83148100	-3.03514300
H	4.55216200	1.23521200	-3.52807300
H	4.33921700	1.80689400	-1.88030300
C	-1.69457200	0.97084700	-0.75803500
C	-2.94442900	0.22142300	-0.25411800
C	-1.77947600	2.47480900	-0.41252900
H	-1.62962400	0.85531400	-1.84807000
C	-4.22814100	0.84679600	-0.82833700
H	-2.97811600	0.25975200	0.84360600
H	-2.88911100	-0.83739000	-0.53448000
C	-3.06560300	3.08611100	-1.00262100
H	-1.79489600	2.59845200	0.67770700
H	-0.90786000	3.01873100	-0.78734300
C	-4.31907700	2.34696200	-0.51995300
H	-5.09658900	0.31582800	-0.42485300
H	-4.24488800	0.69323600	-1.91577600
H	-3.11098400	4.14541700	-0.72823900
H	-3.01206500	3.04918200	-2.09893600
H	-5.21169400	2.77364900	-0.98865100
H	-4.43527200	2.49235800	0.56276500
C	0.34495000	0.76569300	1.62801300
C	1.03779000	-0.31041800	2.48623300

C	1.14573400	2.08559400	1.64186900
H	-0.65259300	0.95187800	2.04817800
C	1.22992300	0.19323400	3.92827800
H	2.01352400	-0.56077200	2.05048000
H	0.44261600	-1.23157400	2.49026700
C	1.32596500	2.57963100	3.09101900
H	2.13341800	1.91569800	1.19686300
H	0.64964600	2.85582200	1.04535300
C	1.99887100	1.52056300	3.97255100
H	1.75144000	-0.57448100	4.50931500
H	0.24445600	0.32350500	4.39579100
H	1.91384900	3.50364200	3.07886300
H	0.34385700	2.84001100	3.50813900
H	2.06954700	1.87941300	5.00440200
H	3.02912200	1.35856200	3.62730300
Au	-0.44224100	-2.20258100	-0.03649500
<b>17</b>			
C	3.27403300	-0.74681600	-0.76099000
C	2.85007800	-1.97035600	-0.26535300
C	2.62283200	-3.15771400	-1.17768500
H	2.30062200	-2.81396700	-2.17353200
H	1.83029000	-3.80046100	-0.76937700
O	3.86829800	-3.83450300	-1.23085800
H	3.72503400	-4.72995600	-1.56450800
C	3.93160000	0.35007500	-0.04305100
C	4.25387500	0.28780900	1.32778000
C	4.28838100	1.49948900	-0.77353100
C	4.90750300	1.34879900	1.94325100
H	4.00787200	-0.59535100	1.90888400
C	4.94503600	2.56041400	-0.15406900
H	4.05801800	1.55081100	-1.83457400
C	5.25343900	2.48765100	1.20546000
H	5.15975000	1.28779000	2.99717600
H	5.22172800	3.43693400	-0.73114000
H	5.77005300	3.31022700	1.69020500
H	3.22664000	-0.61993300	-1.84332400
H	3.05707600	-2.22809100	0.77204100
P	-1.31074600	0.10180000	0.19212700
C	-1.15646000	1.93531300	0.74058500
C	-2.42277500	2.57547300	1.33914400
C	-0.54703300	2.80842000	-0.37274100
H	-0.41316200	1.85219900	1.54602200
C	-2.10995900	3.99503200	1.85198900
H	-3.21353600	2.63026900	0.58258200
H	-2.80754700	1.96857800	2.16497600
C	-0.25158000	4.22640700	0.14770700
H	-1.24784500	2.87424800	-1.21478300

H	0.37250000	2.35034900	-0.75705800
C	-1.50130200	4.87826200	0.75457600
H	-3.02709500	4.44613500	2.24588500
H	-1.40938400	3.92506700	2.69558600
H	0.14331400	4.83888900	-0.67028400
H	0.53950500	4.17209900	0.90837000
H	-1.25311200	5.86507400	1.15958700
H	-2.24679400	5.04472700	-0.03535700
C	-2.12943100	-0.86778100	1.63160600
C	-1.62204300	-2.32374600	1.68147900
C	-3.67067700	-0.83146800	1.63515100
H	-1.76151400	-0.34307700	2.52421700
C	-2.19527400	-3.07302700	2.89715900
H	-1.91783300	-2.84426700	0.75921100
H	-0.52593900	-2.34227100	1.71641800
C	-4.23215000	-1.57396000	2.86247000
H	-4.04745500	-1.31743600	0.72601200
H	-4.04002000	0.19770700	1.62423000
C	-3.72817900	-3.02132000	2.92853400
H	-1.84476700	-4.11085700	2.88275900
H	-1.79580000	-2.62064500	3.81522400
H	-5.32668800	-1.54841800	2.82844500
H	-3.93592700	-1.03861800	3.77494300
H	-4.10383800	-3.51202300	3.83257300
H	-4.13066100	-3.58675200	2.07659900
C	-2.35547700	-0.15203100	-1.39728400
C	-1.48901200	-0.07839900	-2.67131700
C	-3.59460800	0.75739700	-1.52812600
H	-2.69840000	-1.19005400	-1.28462600
C	-2.31232700	-0.44614200	-3.91791600
H	-1.08764500	0.93715200	-2.78508500
H	-0.62755900	-0.75092000	-2.58131500
C	-4.41516300	0.37548300	-2.77445000
H	-3.27113200	1.80129400	-1.62180900
H	-4.22567600	0.69702500	-0.63779500
C	-3.56684800	0.42831800	-4.05129800
H	-1.68248600	-0.35404000	-4.80957500
H	-2.60864200	-1.50228400	-3.85238300
H	-5.27714300	1.04636300	-2.85715500
H	-4.82026200	-0.63730900	-2.64301800
H	-4.16058700	0.10789800	-4.91391100
H	-3.26791500	1.46746500	-4.24702200
Au	0.93569500	-0.73167100	-0.16194700
<b>18</b>			
C	2.89417800	0.08865800	-0.43588500
C	3.41124000	-1.33339700	-0.25719100
C	4.42449100	-1.62913800	0.66462200

C	2.89267700	-2.35607900	-1.06821400
C	4.89645300	-2.93753400	0.77711300
H	4.82689700	-0.85593200	1.30619800
C	3.38396300	-3.65572500	-0.96270000
H	2.10313800	-2.13674700	-1.78242800
C	4.38555500	-3.95042500	-0.03545200
H	5.67475800	-3.15981400	1.50032900
H	2.97929000	-4.43648300	-1.59897400
H	4.76408800	-4.96374100	0.05381800
C	3.28179300	1.17208100	0.56936600
O	3.34950000	0.95584800	1.75678800
O	3.48235300	2.34826600	-0.03576300
C	3.81011000	3.49411300	0.82044600
H	3.44463300	4.35039800	0.25171800
H	3.24277400	3.39667100	1.74792500
N	3.15956200	0.52474700	-1.73481700
N	3.33538400	0.83469500	-2.79593500
C	5.30395000	3.57402400	1.07550900
H	5.86162200	3.62457800	0.13637200
H	5.52273700	4.47932400	1.65027400
H	5.65025300	2.71442700	1.65454000
P	-1.69511100	0.15347900	0.12288200
C	-1.97808200	-0.67987200	1.82922500
C	-3.37805700	-0.50482200	2.44547300
C	-1.53388300	-2.15547400	1.82846000
H	-1.26691700	-0.11826900	2.45153000
C	-3.41503200	-1.09806000	3.86720400
H	-4.12951800	-1.00705600	1.82648900
H	-3.65015400	0.55439000	2.48861900
C	-1.58756000	-2.73828800	3.25257100
H	-2.19462200	-2.74138000	1.17657500
H	-0.51933900	-2.24810400	1.42267300
C	-2.97629900	-2.56833600	3.88317400
H	-4.42617200	-0.99266900	4.27515700
H	-2.75260800	-0.51187500	4.51883400
H	-1.30460300	-3.79615100	3.22224800
H	-0.83758000	-2.23175600	3.87546700
H	-2.97352600	-2.95021400	4.90958400
H	-3.70625300	-3.17325000	3.32744400
C	-2.29206500	1.97203600	0.26695200
C	-1.47044700	2.90067900	-0.64971200
C	-3.80212900	2.17781500	0.02715700
H	-2.06124200	2.22343100	1.31148400
C	-1.86838200	4.37334200	-0.45290000
H	-1.63553200	2.61591200	-1.69884600
H	-0.39986800	2.77188200	-0.45327800
C	-4.19207400	3.65282200	0.23823000
H	-4.04886500	1.88911300	-1.00282800

H	-4.39891700	1.54259300	0.68729200
C	-3.37352700	4.59090500	-0.65748800
H	-1.29190500	5.00091700	-1.14158100
H	-1.58942300	4.68556500	0.56315500
H	-5.26348700	3.77289000	0.04431700
H	-4.03425800	3.91958600	1.29230200
H	-3.63600400	5.63429200	-0.45291200
H	-3.62984700	4.40535300	-1.70987200
C	-2.62719800	-0.68220800	-1.33207300
C	-1.77005900	-1.76794100	-2.01365200
C	-4.02668400	-1.22621900	-0.98314300
H	-2.74462100	0.14920200	-2.04124400
C	-2.47719300	-2.32724300	-3.26077900
H	-1.57798700	-2.58304700	-1.30372800
H	-0.79338900	-1.35403200	-2.29112800
C	-4.72534700	-1.77397900	-2.24165900
H	-3.92914300	-2.03655600	-0.25066400
H	-4.64694900	-0.45245800	-0.52322500
C	-3.88172600	-2.85205000	-2.93360400
H	-1.86311800	-3.12061300	-3.70120000
H	-2.55068600	-1.53351300	-4.01717000
H	-5.70698200	-2.17276400	-1.96355700
H	-4.91151800	-0.94741500	-2.94110600
H	-4.37909500	-3.19470700	-3.84708200
H	-3.79914100	-3.72767700	-2.27503200
Au	0.68402900	0.12539800	-0.25520200
<b>TS<sub>18-19</sub></b>			
C	2.79129300	0.00262200	-0.22948500
C	3.50833700	-1.29640100	-0.14433400
C	4.83756700	-1.36475200	0.31896000
C	2.86431100	-2.48155800	-0.54850400
C	5.49336900	-2.58923100	0.39063600
H	5.34813100	-0.46541600	0.64585800
C	3.52840700	-3.70310700	-0.48745900
H	1.83976700	-2.43464000	-0.90581400
C	4.84268400	-3.75809600	-0.01589700
H	6.51255100	-2.63357200	0.76059400
H	3.02223200	-4.61083000	-0.79977600
H	5.35934100	-4.71141400	0.03796200
C	3.30006000	1.14556800	0.62305400
O	3.43204800	0.98904500	1.81717900
O	3.48274600	2.28736800	-0.05022400
C	3.86411300	3.46648500	0.73400800
H	3.48342200	4.30097400	1.14314700
H	3.33928300	3.42072500	1.69020600
N	3.11577600	0.54111700	-1.82741600
N	3.16969800	0.67408300	-2.92693900

C	5.36883100	3.53948800	0.91872500
H	5.88516700	3.53142700	-0.04523400
H	5.62392900	4.47152300	1.43259100
H	5.73025600	2.70853900	1.52953900
P	-1.74141600	0.14289600	0.12131900
C	-2.12610700	-0.76022700	1.77152200
C	-3.53678400	-0.55659400	2.35283900
C	-1.74955700	-2.25287700	1.70076000
H	-1.41292700	-0.26855500	2.44839400
C	-3.65140900	-1.23003000	3.73439300
H	-4.28811400	-0.98482900	1.68025400
H	-3.76181900	0.50987400	2.45134500
C	-1.87753700	-2.91447000	3.08481300
H	-2.41408300	-2.76805900	0.99505800
H	-0.72717200	-2.36968500	1.32120900
C	-3.27931300	-2.71746500	3.67779000
H	-4.67089200	-1.10200300	4.11422600
H	-2.98775400	-0.71428500	4.44193100
H	-1.64033000	-3.98087200	3.00192200
H	-1.12926000	-2.47894800	3.76116200
H	-3.33063400	-3.15800700	4.67918900
H	-4.01461400	-3.25496500	3.06279800
C	-2.29300400	1.96926700	0.32787600
C	-1.41962700	2.91135300	-0.52535700
C	-3.78791100	2.23670600	0.06244000
H	-2.07984700	2.16989000	1.38718600
C	-1.77503800	4.38605600	-0.26839100
H	-1.56648300	2.68017000	-1.59034900
H	-0.35881100	2.74008800	-0.30974000
C	-4.13592700	3.71134000	0.33929600
H	-4.01602000	2.01079600	-0.98713600
H	-4.42164600	1.58813300	0.67290600
C	-3.26755200	4.66342000	-0.49243300
H	-1.16401700	5.02619400	-0.91457600
H	-1.50823700	4.64054300	0.76682500
H	-5.19823000	3.87712200	0.12949600
H	-3.99257900	3.92059100	1.40832000
H	-3.50019100	5.70434100	-0.24375300
H	-3.50645000	4.53622900	-1.55748400
C	-2.64901300	-0.59730700	-1.40014800
C	-1.80824800	-1.69305500	-2.08644200
C	-4.08598400	-1.09368700	-1.14332100
H	-2.69835900	0.26311900	-2.08238600
C	-2.47318600	-2.16258100	-3.39237300
H	-1.69533500	-2.54774000	-1.40634800
H	-0.79929000	-1.31762900	-2.29445900
C	-4.74404100	-1.55075800	-2.45888100
H	-4.05973600	-1.94018600	-0.44654900

H	-4.69481400	-0.31507100	-0.67666700
C	-3.91546400	-2.63375400	-3.16147000
H	-1.87370700	-2.96368400	-3.83907800
H	-2.47125600	-1.33277400	-4.11283400
H	-5.75551300	-1.91546600	-2.24930200
H	-4.85647200	-0.68439600	-3.12524500
H	-4.38000300	-2.90774200	-4.11467100
H	-3.90825100	-3.54365900	-2.54524100
Au	0.66587000	0.05550500	-0.16564700
<b>19</b>			
C	2.72432700	-0.16508800	0.34369100
C	3.54711000	-1.27853100	0.04597200
C	4.95947800	-1.24957800	0.26341100
C	2.97020700	-2.46443300	-0.50017300
C	5.74121300	-2.34705700	-0.04764100
H	5.41872200	-0.36222400	0.68532100
C	3.76054700	-3.55530700	-0.81642000
H	1.89803500	-2.48601800	-0.66557200
C	5.14309700	-3.49652300	-0.58778400
H	6.81206000	-2.32306200	0.12376500
H	3.31704900	-4.45246000	-1.23485200
H	5.76207900	-4.35523900	-0.83141400
C	3.35255200	1.03205100	0.96766100
O	3.39527300	1.10644300	2.18113400
O	3.76652200	1.94230000	0.09148500
C	4.28714900	3.20597800	0.63002200
H	4.07333500	3.92758600	-0.15940300
H	3.71387400	3.45632600	1.52487200
N	2.10438400	0.63068400	-3.46613800
N	1.44234200	1.51247100	-3.53886400
C	5.77337200	3.10377500	0.92121500
H	6.32760300	2.79562600	0.03018200
H	6.14911200	4.08357500	1.23212900
H	5.96723100	2.39721700	1.73255400
P	-1.74286600	0.14556000	0.17402900
C	-2.33501900	-0.77844800	1.74895000
C	-3.79285700	-0.55146100	2.19056800
C	-1.98831200	-2.27837600	1.67828600
H	-1.68518700	-0.32391800	2.51035500
C	-4.05940600	-1.25388200	3.53609700
H	-4.48338100	-0.94321400	1.43546400
H	-4.00147000	0.51819900	2.29365700
C	-2.26900500	-2.96947700	3.02387000
H	-2.58765300	-2.76031400	0.89517900
H	-0.93541300	-2.41086300	1.40020200
C	-3.71792000	-2.74909900	3.47999400
H	-5.10828400	-1.10914500	3.81720700

H	-3.45774400	-0.77146900	4.31873400
H	-2.05121700	-4.03983000	2.93738900
H	-1.58167900	-2.57012100	3.78235100
H	-3.87976300	-3.21005300	4.46027900
H	-4.40032100	-3.25374900	2.78185200
C	-2.26511500	1.98359600	0.35180600
C	-1.27374900	2.90539900	-0.38792200
C	-3.71366900	2.29272200	-0.07567700
H	-2.16797700	2.16713100	1.43090400
C	-1.61778200	4.38872900	-0.16905800
H	-1.30077900	2.68184100	-1.46407600
H	-0.24937300	2.70605500	-0.05222000
C	-4.04985200	3.77760400	0.15759200
H	-3.83357400	2.06696400	-1.14337700
H	-4.42732500	1.66432700	0.46494200
C	-3.06565200	4.70350100	-0.56824800
H	-0.91782200	5.01188700	-0.73680600
H	-1.46971300	4.63739100	0.89102000
H	-5.07603400	3.97152500	-0.17329200
H	-4.02483000	3.98771000	1.23571100
H	-3.29919000	5.75101100	-0.34964400
H	-3.18044200	4.57807300	-1.65391900
C	-2.50539000	-0.53415400	-1.45178200
C	-1.61366700	-1.62061400	-2.08668500
C	-3.96601800	-1.01554200	-1.35224200
H	-2.47610000	0.34753700	-2.10740400
C	-2.15483300	-2.04586600	-3.46303700
H	-1.57488700	-2.49477500	-1.42272600
H	-0.58590800	-1.25219900	-2.18686300
C	-4.49862600	-1.42985000	-2.73659800
H	-4.02082500	-1.87954000	-0.67838100
H	-4.60711100	-0.23924400	-0.92690400
C	-3.61708400	-2.50497700	-3.38504600
H	-1.52310600	-2.84179900	-3.87337800
H	-2.07569700	-1.19668900	-4.15601900
H	-5.52910900	-1.78762100	-2.63514300
H	-4.53900500	-0.54573600	-3.38781600
H	-3.99035500	-2.74935800	-4.38526800
H	-3.67749300	-3.42974900	-2.79437400
Au	0.69329900	-0.04009600	0.19004400
<b>20</b>			
C	2.80518200	-0.07003300	0.08791700
C	3.63296500	-1.20005900	-0.12221400
C	5.05423700	-1.12513900	0.00909100
C	3.05186700	-2.45133500	-0.48845400
C	5.84067900	-2.24075000	-0.21325900
H	5.51785800	-0.18579100	0.28998700

C	3.84628500	-3.56140000	-0.71525200
H	1.97268300	-2.50843800	-0.58630500
C	5.23793000	-3.45564900	-0.57551200
H	6.91873100	-2.18055700	-0.10904700
H	3.39930900	-4.50918900	-0.99556600
H	5.86039900	-4.32865400	-0.74948200
C	3.44005900	1.19574500	0.54801900
O	3.50012300	1.41720700	1.74278500
O	3.84183500	1.99083200	-0.43842200
C	4.36181800	3.31352400	-0.06637800
H	4.12731500	3.93352600	-0.93253100
H	3.80349500	3.66605100	0.80311100
C	5.85393200	3.25596700	0.20630100
H	6.39539900	2.85250100	-0.65399600
H	6.22576300	4.26764900	0.39632900
H	6.06881600	2.64817700	1.08921600
P	-1.67063100	0.16959300	0.08151600
C	-2.20026900	-0.72418200	1.69538500
C	-3.64772800	-0.51139800	2.17606500
C	-1.83093200	-2.21962200	1.65311200
H	-1.53563800	-0.23947700	2.42478300
C	-3.85713800	-1.17749000	3.54994700
H	-4.35394300	-0.94062200	1.45650300
H	-3.87490900	0.55667500	2.25284600
C	-2.05387300	-2.87665000	3.02625400
H	-2.44885500	-2.73212700	0.90457700
H	-0.78603600	-2.34326000	1.34256700
C	-3.49021400	-2.66768700	3.52586000
H	-4.89880700	-1.04298000	3.86125100
H	-3.23927400	-0.66156700	4.29775800
H	-1.82030500	-3.94529800	2.96266300
H	-1.34855300	-2.44402700	3.74915300
H	-3.61003600	-3.10207200	4.52413100
H	-4.18662100	-3.20450200	2.86663200
C	-2.21188100	2.00418700	0.23767200
C	-1.24871900	2.92422800	-0.54030600
C	-3.67362500	2.28698500	-0.16315500
H	-2.09315700	2.20884500	1.31077900
C	-1.60761000	4.40692200	-0.34318200
H	-1.29522900	2.67911400	-1.61126100
H	-0.21541400	2.74447400	-0.22163900
C	-4.02400500	3.77218000	0.04603000
H	-3.81466700	2.03613700	-1.22268200
H	-4.36682000	1.66164400	0.40699600
C	-3.06718600	4.69515900	-0.71899200
H	-0.92744700	5.02802000	-0.93669900
H	-1.44158800	4.67798200	0.70865200
H	-5.05924300	3.94601300	-0.26736400

H	-3.97970400	4.00535000	1.11874400
H	-3.30999200	5.74391700	-0.51715800
H	-3.20245600	4.54569100	-1.79928200
C	-2.47498400	-0.55619400	-1.50324100
C	-1.58835700	-1.64335100	-2.14380600
C	-3.92442900	-1.05570900	-1.34652100
H	-2.48033800	0.31116900	-2.17797400
C	-2.16608100	-2.10211700	-3.49428000
H	-1.51868800	-2.50384000	-1.46464300
H	-0.56893300	-1.26415700	-2.28275100
C	-4.49455200	-1.50260900	-2.70566700
H	-3.94462100	-1.90720700	-0.65514700
H	-4.56252100	-0.28018300	-0.91512200
C	-3.61927600	-2.57767900	-3.36280000
H	-1.53699300	-2.89800300	-3.90862600
H	-2.11856000	-1.26575400	-4.20541400
H	-5.51661300	-1.87138600	-2.56586900
H	-4.56616900	-0.63061900	-3.37038000
H	-4.02001200	-2.84343800	-4.34683700
H	-3.65036200	-3.49326700	-2.75567700
Au	0.76787300	0.01506600	0.01614300
TS <sub>20-21</sub>			
C	0.38644500	3.07574000	-1.96558000
C	-0.95530200	3.06791200	-1.91484500
C	-1.78439300	2.10245200	-2.69062200
H	-1.17586200	1.27568600	-3.07691300
H	-2.27020000	2.60395400	-3.54091300
O	-2.86645800	1.58902600	-1.86320800
H	-3.40751000	0.99637800	-2.40670300
C	1.29329100	4.01890800	-1.29633400
C	2.65028900	4.03592200	-1.66499500
C	0.86436700	4.90596700	-0.29010200
C	3.54934600	4.91585900	-1.06298400
H	2.99738000	3.36162000	-2.44452000
C	1.76261000	5.78222800	0.31278100
H	-0.17332300	4.90093700	0.02923200
C	3.10797300	5.79337100	-0.07151700
H	4.59050700	4.92050500	-1.37175300
H	1.41381200	6.46169600	1.08499000
H	3.80366800	6.48182400	0.39849100
H	0.88132500	2.32689300	-2.58636500
H	-1.51034500	3.80117700	-1.33927900
C	-2.78625100	0.42885500	-0.01995200
C	-3.97068000	-0.33400300	-0.36070000
C	-5.27111400	0.21274700	-0.20756900
C	-3.84894200	-1.65375000	-0.86137500
C	-6.39478100	-0.53635400	-0.52820000



H	-5.38684700	1.22695800	0.16024800
C	-4.97653700	-2.40322900	-1.17186600
H	-2.85513300	-2.07370300	-0.98131500
C	-6.24901100	-1.84498200	-1.00543600
H	-7.38505100	-0.10977200	-0.40611100
H	-4.87175800	-3.41841800	-1.54070600
H	-7.13061200	-2.43056900	-1.24863200
C	-2.96372500	1.62209100	0.89392400
O	-2.72357700	2.78228900	0.65222200
O	-3.37270100	1.14342000	2.08632100
C	-3.44855400	2.09289600	3.19475800
H	-4.22285000	1.67650300	3.84137300
H	-3.77800800	3.05574300	2.80005900
C	-2.11483500	2.20617200	3.91202000
H	-1.78210300	1.23011700	4.27680700
H	-2.22007700	2.87432900	4.77270400
H	-1.34990900	2.62309900	3.25142500
P	1.35476500	-1.29577100	0.29832800
C	1.09335800	-2.99807000	1.14737600
C	2.33872000	-3.67470300	1.74933700
C	0.30494200	-3.96596700	0.24471200
H	0.43573200	-2.71219300	1.98089800
C	1.94350800	-4.95605700	2.50836100
H	3.05067000	-3.93234500	0.95693700
H	2.85274000	-2.99283300	2.43374600
C	-0.07528500	-5.24598000	1.00975500
H	0.91433300	-4.23745000	-0.62708300
H	-0.59716400	-3.47410600	-0.13869400
C	1.15808700	-5.92767900	1.61800300
H	2.84639400	-5.43740300	2.89991000
H	1.33228200	-4.68432600	3.38013300
H	-0.60072400	-5.93248500	0.33629200
H	-0.78292600	-4.98907100	1.81037800
H	0.85728800	-6.80973100	2.19352700
H	1.80910600	-6.28977300	0.80998600
C	2.41508000	-0.23617300	1.49909000
C	2.07520500	1.26007700	1.35510100
C	3.93709600	-0.45738300	1.39488100
H	2.07710700	-0.57433800	2.48889900
C	2.83850300	2.11270300	2.38318100
H	2.33453700	1.60112300	0.34410100
H	0.99664000	1.41564900	1.46753200
C	4.69004900	0.39143100	2.43626200
H	4.27739100	-0.16853300	0.39197600
H	4.19454100	-1.51208200	1.52705000
C	4.35328700	1.88135200	2.30329300
H	2.60186800	3.16912100	2.21822700
H	2.48417600	1.86129100	3.39301800

H	5.76762100	0.22735500	2.32430300
H	4.42511800	0.04321200	3.44428500
H	4.86662500	2.45680600	3.08139500
H	4.72576500	2.25608300	1.33990300
C	2.28430200	-1.42481200	-1.37703200
C	1.30601300	-1.60514800	-2.55618600
C	3.41026400	-2.47569100	-1.44392200
H	2.73759900	-0.42743100	-1.46774100
C	2.04559000	-1.53982100	-3.90439900
H	0.79852600	-2.57478500	-2.46624100
H	0.52384200	-0.83771800	-2.51705500
C	4.15096200	-2.39569900	-2.79182500
H	2.97850500	-3.47830300	-1.33593900
H	4.12153400	-2.34580200	-0.62476200
C	3.19110500	-2.55907500	-3.97684900
H	1.33337000	-1.70382200	-4.72115600
H	2.45090800	-0.52731000	-4.04167700
H	4.93260700	-3.16267800	-2.82239700
H	4.66292600	-1.42616100	-2.86505500
H	3.73292900	-2.45155200	-4.92266700
H	2.77416800	-3.57578800	-3.96994400
Au	-0.86795700	-0.31989300	0.02208800
<b>21</b>			
C	2.90425900	-1.31752200	-1.70486800
C	3.33558400	-0.05239400	-1.85455400
C	2.51235400	0.97754200	-2.52369900
H	1.49693700	0.64027400	-2.74383700
H	2.98852700	1.38583300	-3.42140600
O	2.39789100	2.21634200	-1.66244000
H	2.09414600	2.97057600	-2.19972800
C	3.64955900	-2.43623300	-1.11893400
C	4.79053400	-2.24671000	-0.31571100
C	3.20417400	-3.74925600	-1.35546300
C	5.46617000	-3.33950700	0.21925700
H	5.13495000	-1.24140300	-0.09282500
C	3.88561800	-4.84311500	-0.82406300
H	2.32538800	-3.91000600	-1.97547700
C	5.01957400	-4.64054000	-0.03530500
H	6.34246600	-3.17881800	0.83994800
H	3.53451900	-5.85037200	-1.02668400
H	5.55175400	-5.48973700	0.38232500
H	1.90787100	-1.56601700	-2.07156800
H	4.32730500	0.25507700	-1.54259600
C	1.53435100	2.30728800	-0.30035800
C	1.09585500	3.75266900	-0.34081800
C	2.02851900	4.77720400	-0.07853300
C	-0.21682900	4.11320300	-0.69139900

C	1.65198900	6.11636800	-0.14912800
H	3.05179700	4.52130400	0.18340200
C	-0.59252800	5.45478900	-0.76042200
H	-0.94230400	3.33158300	-0.89599000
C	0.33975500	6.45738500	-0.48756100
H	2.38027200	6.89319800	0.06196400
H	-1.61259800	5.71643400	-1.02421000
H	0.04595400	7.50134100	-0.53819500
C	2.59267000	2.04080100	0.75850100
O	3.74384600	1.71739000	0.55179600
O	2.04981700	2.21420700	1.97563500
C	2.92566700	2.01671200	3.12370300
H	2.49192800	2.65317700	3.89695800
H	3.92204300	2.38165500	2.86615300
C	2.96089100	0.55844900	3.54830400
H	1.95497000	0.19261900	3.77482100
H	3.57175000	0.45560100	4.45091100
H	3.40179800	-0.06493000	2.76632800
P	-1.76909600	-0.78705400	0.22179300
C	-3.13197200	0.12582100	1.22107900
C	-4.17618200	-0.75434200	1.93225100
C	-3.80290500	1.23861400	0.39309000
H	-2.52384900	0.61253300	1.99685900
C	-5.10445100	0.11078700	2.80617100
H	-4.77878000	-1.29764100	1.19521700
H	-3.68472700	-1.50322500	2.56109100
C	-4.73658900	2.09022200	1.27185400
H	-4.38786700	0.79172800	-0.42094800
H	-3.04249900	1.87568800	-0.07366900
C	-5.77827100	1.22498000	1.99442400
H	-5.85728200	-0.52942400	3.27907100
H	-4.51765300	0.55651000	3.62137700
H	-5.22925900	2.84869900	0.65316200
H	-4.13484200	2.63330100	2.01379300
H	-6.39880400	1.84735500	2.64816900
H	-6.45641200	0.77712000	1.25472600
C	-1.13350100	-2.20594500	1.35107500
C	0.35629400	-2.49956800	1.08681100
C	-1.95500100	-3.50863800	1.29881300
H	-1.22435500	-1.77315900	2.35729100
C	0.90690100	-3.54695400	2.06941800
H	0.47794800	-2.87203500	0.06003300
H	0.94321700	-1.57751700	1.15484000
C	-1.40647400	-4.54584000	2.29635200
H	-1.90215900	-3.93000900	0.28632900
H	-3.01069100	-3.31823600	1.50900200
C	0.07896800	-4.83847000	2.05022300
H	1.95349000	-3.75708900	1.82432100

H	0.89882700	-3.12422600	3.08384300
H	-1.99771400	-5.46548500	2.22421600
H	-1.54172300	-4.16794000	3.31919400
H	0.45600300	-5.54228700	2.80025100
H	0.19552800	-5.33059600	1.07435600
C	-2.42467100	-1.55920800	-1.40914200
C	-2.31408000	-0.56676300	-2.58539200
C	-3.83770600	-2.17410900	-1.35465900
H	-1.70525600	-2.37105400	-1.58776300
C	-2.66845700	-1.24704200	-3.91899600
H	-2.99481100	0.27790200	-2.41634700
H	-1.30235800	-0.14710100	-2.63016200
C	-4.18175100	-2.86166300	-2.68958500
H	-4.57274500	-1.38254600	-1.16410900
C	-3.92565700	-2.89350700	-0.53682800
C	-4.05920300	-1.89499500	-3.87476700
H	-2.61313800	-0.51305400	-4.73102000
H	-1.91527300	-2.01633000	-4.14100800
H	-5.19498600	-3.27467700	-2.63448200
H	-3.50547000	-3.71456700	-2.84011200
H	-4.26255700	-2.41903400	-4.81488100
H	-4.82281500	-1.11011900	-3.78375700
Au	0.01643700	0.83077000	-0.16920200
TS <sub>21-22</sub>			
C	4.70465100	-1.23306600	0.02435300
C	4.20210200	-0.22840200	-0.71683200
C	2.75433200	0.10734900	-0.71702100
H	2.15052500	-0.61972400	-0.16598000
H	2.34479700	0.23668900	-1.72207500
O	2.58259000	1.42824100	-0.06707500
H	2.80816100	1.53437200	1.07893300
C	6.09409900	-1.69234600	0.09703300
C	7.12903400	-1.13637800	-0.67971200
C	6.41055800	-2.73639800	0.98454200
C	8.43198000	-1.60803200	-0.56437600
H	6.91517200	-0.33569100	-1.38088200
C	7.71634500	-3.20878100	1.10025900
C	5.62215200	-3.17764100	1.58929400
C	8.73102200	-2.64505500	0.32592200
H	9.21880700	-1.16995300	-1.17086700
H	7.94103400	-4.01496900	1.79176600
H	9.74958300	-3.01103200	0.41156200
H	4.00871900	-1.79331600	0.65107700
H	4.83804800	0.37272400	-1.36136300
C	1.23915700	2.07201300	0.01511100
C	1.11302200	3.16239400	-1.03305300
C	2.22561100	3.59785200	-1.76660600

C	-0.12799600	3.77950900	-1.25701800
C	2.09461100	4.61896600	-2.70995600
H	3.19513600	3.14343300	-1.59839600
C	-0.24990700	4.81168300	-2.18616100
H	-1.00052400	3.45005800	-0.70096200
C	0.86009900	5.23193200	-2.92176500
H	2.96589900	4.93930700	-3.27340500
H	-1.21721800	5.27960100	-2.34296100
H	0.76192200	6.02711600	-3.65414900
C	1.34706900	2.55910700	1.43028700
O	2.31582600	2.11063300	2.10089800
O	0.46858000	3.40330400	1.88592200
C	0.60542100	3.88256600	3.27243100
H	0.10976800	4.85315400	3.24652100
H	1.66833100	4.01705000	3.47912500
C	-0.05437200	2.92623100	4.24711500
H	-1.10677600	2.77133300	3.99409300
H	-0.00534400	3.35465100	5.25304900
H	0.45924700	1.96179500	4.26527900
P	-2.27064500	-0.87777100	-0.17326600
C	-2.12306100	-1.73770000	-1.88352700
C	-3.35618200	-2.50572500	-2.39404400
C	-0.84640000	-2.59668300	-1.96598200
H	-1.97945700	-0.86737100	-2.53969700
C	-3.11484300	-3.02029700	-3.82666800
H	-3.57228800	-3.35672400	-1.73783100
H	-4.24040300	-1.86067900	-2.38694900
C	-0.62203900	-3.11192800	-3.39843600
H	-0.93449000	-3.45446700	-1.28674000
H	0.02225600	-2.01561000	-1.63316000
C	-1.84563800	-3.87730200	-3.92065200
H	-3.98969800	-3.59021700	-4.15830700
H	-3.02615700	-2.16176400	-4.50673100
H	0.26945900	-3.74863200	-3.42286300
H	-0.41578800	-2.25821200	-4.05890100
H	-1.67946100	-4.19448000	-4.95577400
H	-1.98018300	-4.79522300	-3.33129200
C	-3.92920500	0.08682500	-0.16117100
C	-3.84142800	1.31668000	0.76667500
C	-5.18014200	-0.74889100	0.17420700
H	-4.01315300	0.44441600	-1.19718600
C	-5.11986200	2.16978300	0.69090500
H	-3.69045400	0.97906600	1.80249700
H	-2.96880900	1.92636100	0.50610200
C	-6.45443200	0.11104100	0.07776000
H	-5.09574500	-1.13877600	1.19701100
H	-5.26838100	-1.61343300	-0.48913600
C	-6.37742100	1.34305100	0.98838600

H	-5.03874100	3.01118200	1.38834000
H	-5.19862100	2.60592000	-0.31470100
H	-7.32509000	-0.50250500	0.33432000
H	-6.59518600	0.43182300	-0.96365500
H	-7.27410500	1.96048200	0.86819300
H	-6.36047200	1.01837700	2.03824600
C	-2.29575300	-2.10854400	1.29834300
C	-0.87621600	-2.37476000	1.84084600
C	-3.04214700	-3.43516300	1.05382400
H	-2.84281200	-1.54163100	2.06501200
C	-0.92427700	-3.22635400	3.12125400
H	-0.28483600	-2.89838100	1.07746600
H	-0.36653000	-1.42505100	2.03901100
C	-3.08739100	-4.28073700	2.34051700
H	-2.52420600	-4.00559400	0.27303400
H	-4.05830300	-3.25432600	0.69412400
C	-1.68281000	-4.54172700	2.89988200
H	0.09624600	-3.42478300	3.46827600
H	-1.41773200	-2.65009200	3.91629200
H	-3.60019600	-5.22661500	2.13396700
H	-3.69141100	-3.75789500	3.09497800
H	-1.74696600	-5.10474000	3.83726700
H	-1.12160300	-5.17121600	2.19527000
Au	-0.39792300	0.67233800	-0.01234400
<b>22</b>			
C	4.58037100	-1.07214900	-0.07151000
C	4.23553600	0.15753800	-0.48806300
C	2.81792100	0.56475800	-0.71175300
H	2.12900600	-0.27633700	-0.55958300
H	2.66542200	0.96314400	-1.72287900
O	2.49178800	1.61907900	0.23185500
H	2.38167500	1.76373000	2.01577900
C	5.92891200	-1.60740700	0.15136600
C	7.10233200	-0.88220800	-0.12986000
C	6.05877200	-2.90679700	0.67256600
C	8.35483900	-1.43771900	0.11072400
H	7.03731100	0.11860000	-0.54563800
C	7.31327600	-3.46392500	0.91397700
H	5.16284000	-3.48285300	0.89148400
C	8.46635400	-2.72992800	0.63450000
H	9.24939400	-0.86456000	-0.11397300
H	7.39022200	-4.46901900	1.31759800
H	9.44602800	-3.16022100	0.81860400
H	3.77448300	-1.78075700	0.12751400
H	4.98918800	0.91317100	-0.69854400
C	1.20483900	2.23373000	0.11859400
C	1.09307800	3.23402100	-1.01951900

C	2.26368200	3.80105300	-1.54583300
C	-0.14559400	3.63734500	-1.53753400
C	2.19342600	4.74400700	-2.57156100
H	3.22726800	3.50566300	-1.14477800
C	-0.21347000	4.59178300	-2.55301600
H	-1.06024600	3.20250100	-1.14506400
C	0.95589400	5.14428800	-3.07776500
H	3.10902400	5.17081900	-2.96998000
H	-1.18144900	4.89469500	-2.94093400
H	0.90312400	5.87819700	-3.87593100
C	0.95884600	2.75584900	1.45392900
O	1.68752400	2.32446800	2.45114300
O	0.05886500	3.65944300	1.68296400
C	-0.15459000	4.17308500	3.04950100
H	-0.59445300	5.15336100	2.86700700
H	0.82096400	4.29310400	3.52284100
C	-1.07874000	3.26989000	3.84295200
H	-2.03466600	3.13754800	3.32949100
H	-1.27558600	3.73632300	4.81332000
H	-0.62628500	2.29193200	4.02500100
P	-2.12779900	-0.97781100	-0.19440300
C	-1.87351500	-1.72954800	-1.94198200
C	-3.02304300	-2.57892200	-2.51576100
C	-0.52340500	-2.46534600	-2.04268200
H	-1.80002000	-0.81626900	-2.54954300
C	-2.71389000	-2.98715200	-3.96949700
H	-3.16502300	-3.48146700	-1.91041100
H	-3.96497700	-2.02179300	-2.49035400
C	-0.22898400	-2.87458600	-3.49650400
H	-0.54617500	-3.36598700	-1.41539800
H	0.28388200	-1.83061300	-1.65841400
C	-1.36886200	-3.71616800	-4.08684300
H	-3.52677100	-3.61609300	-4.34871700
H	-2.69694100	-2.08675400	-4.59907500
H	0.71715400	-3.42569400	-3.53682200
H	-0.09034000	-1.96922100	-4.10362000
H	-1.15883900	-3.95432300	-5.13507800
H	-1.42609300	-4.67616400	-3.55488200
C	-3.86910900	-0.17222100	-0.16903900
C	-3.90706900	1.02326800	0.80440100
C	-5.03377000	-1.13950600	0.12287800
H	-3.97863000	0.21393400	-1.19202600
C	-5.26402300	1.74699400	0.75259800
H	-3.72570600	0.66232300	1.82733200
H	-3.09858900	1.72517500	0.57040700
C	-6.38730200	-0.40733300	0.05331400
H	-4.91248000	-1.56011900	1.12966200
H	-5.03329600	-1.98101600	-0.57519200

C	-6.43344500	0.78822500	1.01253500
H	-5.26939500	2.56643800	1.48033800
H	-5.38409900	2.20868700	-0.23730500
H	-7.19262400	-1.11427000	0.28093700
H	-6.55792100	-0.06060200	-0.97515600
H	-7.38674400	1.31824300	0.91322400
H	-6.38395500	0.42526100	2.04864300
C	-2.05631500	-2.27313300	1.21993900
C	-0.62753300	-2.43069300	1.77882100
C	-2.66860600	-3.65202300	0.90152000
H	-2.66884700	-1.79620100	1.99836300
C	-0.61913200	-3.33645000	3.02226600
H	0.02163600	-2.86573400	1.00704800
H	-0.20913900	-1.44810400	2.02510200
C	-2.66247800	-4.54988200	2.15299400
H	-2.08146000	-4.13772900	0.11239800
H	-3.68927500	-3.55326400	0.52347400
C	-1.25152900	-4.70524000	2.73506500
H	0.40966500	-3.45578700	3.38036800
H	-1.17488500	-2.84040500	3.83036400
H	-3.08315100	-5.52881000	1.89808900
H	-3.32645100	-4.11388500	2.91226000
H	-1.28255400	-5.30756700	3.64934400
H	-0.62212500	-5.25401900	2.02066300
Au	-0.40556400	0.72798800	0.06578100

TS<sub>22-23</sub>

C	1.14793300	-3.00574400	0.85819900
C	-0.08516000	-3.23434500	0.30155400
C	-1.28670400	-3.51429000	1.16965400
H	-1.19969000	-3.00927800	2.13928600
H	-1.37765200	-4.59097000	1.35348400
O	-2.52422100	-3.16285100	0.53539100
H	-2.84259000	-3.54077900	-1.29516500
C	2.46487600	-3.17196800	0.24693000
C	2.65131400	-3.59629900	-1.08450600
C	3.60379300	-2.93942000	1.04222500
C	3.93154600	-3.77269400	-1.59753300
H	1.79368800	-3.79907300	-1.71857300
C	4.88606700	-3.11979600	0.52804000
H	3.47614200	-2.62582100	2.07519400
C	5.05360400	-3.53589200	-0.79409900
H	4.05950800	-4.10646500	-2.62267700
H	5.75176700	-2.94411000	1.15899100
H	6.05089400	-3.68536600	-1.19621700
H	1.16700700	-2.74985400	1.91817900
H	-0.14537000	-3.61133800	-0.71921400
C	-2.69650400	-1.79902800	0.20292600

C	-3.22074600	-0.91813200	1.28560200
C	-3.56356500	-1.48687900	2.52527400
C	-3.40639800	0.46756000	1.11391600
C	-4.06242300	-0.69556000	3.56055100
H	-3.47095800	-2.55736800	2.66681800
C	-3.91747900	1.24905700	2.14837000
H	-3.16270100	0.92868300	0.16493300
C	-4.24024600	0.67606900	3.38104700
H	-4.32625100	-1.16040700	4.50593900
H	-4.06782400	2.31317600	1.98878100
H	-4.63471200	1.28918500	4.18524900
C	-3.08913100	-1.72084700	-1.14404000
O	-3.03326100	-2.80503700	-1.91503700
O	-3.56508000	-0.62462700	-1.69785000
C	-4.18969100	-0.69503500	-3.02448800
H	-4.84713100	0.17528500	-3.02716500
H	-4.79614000	-1.60134400	-3.07169600
C	-3.17061600	-0.63411800	-4.14788600
H	-2.55944200	0.26944000	-4.07763100
H	-3.70160500	-0.61055500	-5.10496600
H	-2.51849900	-1.51019300	-4.14373300
P	0.62093900	1.43271600	-0.04210200
C	0.87709400	1.82288800	1.82558200
C	1.12666100	3.29186800	2.21542300
C	1.93016600	0.88859300	2.45278400
H	-0.10494400	1.53733900	2.22753500
C	1.17369100	3.44177600	3.74875000
H	2.07281300	3.64355500	1.78839100
H	0.33428400	3.93366700	1.81909800
C	1.97366900	1.05384000	3.98200600
H	2.92063500	1.11882900	2.04033700
H	1.71446200	-0.15361500	2.19172900
C	2.21712500	2.51445900	4.38457800
H	1.38151900	4.48690400	4.00335300
H	0.18177600	3.21126300	4.16159600
H	2.75344300	0.40585300	4.39851800
H	1.02032100	0.71156600	4.40842100
H	2.19797200	2.61496500	5.47515600
H	3.22230300	2.81903600	4.06099300
C	-0.58580900	2.75276900	-0.74071100
C	-1.32738800	2.21255000	-1.97893800
C	0.05177900	4.11962300	-1.06344000
H	-1.31366500	2.88275400	0.07194400
C	-2.38462900	3.21352400	-2.47762100
H	-0.59930600	2.02579100	-2.78212500
H	-1.79712800	1.25100400	-1.75149000
C	-1.01396200	5.12196300	-1.54400800
H	0.79828600	3.99285400	-1.85774900

H	0.57649000	4.53018700	-0.19771100
C	-1.77835400	4.59359900	-2.76418900
H	-2.87105300	2.81675200	-3.37661300
H	-3.17104400	3.31186900	-1.71595300
H	-0.53262500	6.07810700	-1.77723100
H	-1.71970800	5.32011000	-0.72533400
H	-2.56306400	5.29955400	-3.05691600
H	-1.09105700	4.51853000	-3.61843000
C	2.22549600	1.57350300	-1.08968200
C	2.91967500	0.21011600	-1.25610200
C	3.23474200	2.64873700	-0.63607700
H	1.83050600	1.86965800	-2.07190000
C	4.09956100	0.30501000	-2.23758000
H	3.28372100	-0.13986900	-0.28193500
H	2.19993400	-0.53871200	-1.60388000
C	4.40909900	2.74150500	-1.62882400
H	3.62815200	2.38685900	0.35367700
H	2.75731500	3.62728800	-0.53956600
C	5.10372400	1.38690700	-1.81701600
H	4.59116600	-0.67123500	-2.30705800
H	3.71540300	0.53562900	-3.24141600
H	5.12251800	3.49435800	-1.27544200
H	4.03438300	3.09912200	-2.59797200
H	5.90439700	1.47229800	-2.55982000
H	5.58305700	1.09070600	-0.87338500
Au	-0.34709100	-0.82128700	-0.05566000
<b>23</b>			
C	0.25562300	-2.93532800	1.64973600
C	-1.04596600	-2.68639700	1.24580700
C	-2.11403800	-2.23283500	2.22921500
H	-1.77254800	-1.38088700	2.82958100
H	-2.33407100	-3.05986900	2.91506900
O	-3.36496200	-1.94581800	1.60670200
C	-3.90343800	-3.04607100	-0.03296400
H	1.25984600	-3.78997700	0.99730600
C	1.03857300	-4.43593100	-0.23503500
C	2.48664800	-3.99031500	1.65633800
C	2.01957000	-5.25250100	-0.78630100
H	0.09800100	-4.30622700	-0.76181200
C	3.46617200	-4.81339300	1.10371500
H	2.66513200	-3.50490700	2.61247500
C	3.23573100	-5.44407400	-0.11975200
H	1.83585800	-5.74941200	-1.73375400
H	4.40371100	-4.96548600	1.62901500
H	3.99533100	-6.08798100	-0.55192100
H	0.53562200	-2.59436600	2.64793100
H	-1.42457500	-3.15801900	0.34075100

C	-3.38551800	-0.87018500	0.69814600
C	-3.41188400	0.49266400	1.24553700
C	-3.65405300	0.67479900	2.62231300
C	-3.24309900	1.64320500	0.44564100
C	-3.72348300	1.95230000	3.17690000
H	-3.83130100	-0.19241300	3.24903200
C	-3.33324400	2.91713500	1.00499200
H	-3.07210500	1.53023600	-0.61764300
C	-3.56662300	3.08298200	2.37323700
H	-3.92439300	2.06249100	4.23862400
H	-3.22784000	3.78836100	0.36391600
H	-3.64157300	4.07737100	2.80239500
C	-3.60378900	-1.28081300	-0.58333500
O	-3.76200200	-2.59541600	-0.88412400
O	-3.67240300	-0.45709800	-1.63503500
C	-4.75797800	-0.68318800	-2.59263100
H	-5.06618300	0.32341500	-2.88524700
H	-5.59031300	-1.16472600	-2.07257000
C	-4.30013400	-1.49309600	-3.79161700
H	-3.45027200	-1.01197800	-4.28394800
H	-5.11756800	-1.56047000	-4.51722400
H	-4.01461400	-2.50502300	-3.49719800
P	1.08704400	1.18470200	-0.40259200
C	0.64715600	2.55727900	0.86102500
C	0.85911500	4.00908800	0.39170200
C	1.30529900	2.30296100	2.23087700
H	-0.43371400	2.39932100	0.97190500
C	0.33522800	4.99430300	1.45505200
H	1.92304200	4.20328600	0.21512400
H	0.33735500	4.18713400	-0.55414300
C	0.78027000	3.29966100	3.28000600
H	2.39417100	2.41249800	2.14683600
H	1.11293500	1.27484300	2.56186600
C	0.98088900	4.75212500	2.82562800
H	0.51897600	6.02047300	1.11805700
H	-0.75353500	4.88037800	1.54148900
H	1.28564700	3.12184200	4.23591400
H	-0.28895500	3.11286200	3.44742100
H	0.56243000	5.44131100	3.56708900
H	2.05611800	4.97203100	2.76788800
C	0.27003400	1.65121700	-2.07477900
C	-0.12410300	0.38919200	-2.86908200
C	1.10544100	2.60874100	-2.94851300
H	-0.64887700	2.16657700	-1.76382800
C	-0.84957800	0.75440000	-4.17576300
H	0.77944000	-0.19149800	-3.10407200
H	-0.76967700	-0.25289700	-2.25964900
C	0.35240900	2.97492800	-4.24047300

H	2.05126900	2.12246100	-3.22022300
H	1.36123800	3.52028500	-2.40108000
C	-0.03429100	1.72478100	-5.03971500
H	-1.07153100	-0.16240300	-4.73360600
H	-1.81663800	1.21215600	-3.92643800
H	0.97688700	3.64182300	-4.84497000
H	-0.55281700	3.54242900	-3.98409300
H	-0.60250500	2.00543900	-5.93310700
H	0.87674400	1.22269700	-5.39396600
C	2.97512400	0.96646700	-0.68989700
C	3.59553300	-0.05275600	0.28674600
C	3.79190500	2.27448100	-0.70260700
H	3.00791700	0.52670700	-1.69654000
C	5.06900300	-0.32419300	-0.06524200
H	3.53062700	0.33553800	1.31190800
H	3.03039600	-0.99104200	0.26562600
C	5.26254200	1.99132900	-1.06356700
H	3.75355400	2.73649100	0.29106100
H	3.37196600	2.99686100	-1.40693800
C	5.89406400	0.96879400	-0.11047900
H	5.49242100	-1.02639100	0.66160100
H	5.11657300	-0.82195200	-1.04382100
H	5.82496600	2.93130000	-1.04781400
H	5.31470600	1.61411100	-2.09426200
H	6.92307400	0.75084400	-0.41588100
H	5.95237700	1.39963900	0.89869600
Au	0.14277800	-0.87050900	0.45999000
TS <sub>23-24</sub>			
C	-2.43515500	-0.05459000	0.06055000
C	-1.55601400	0.37362100	1.14896100
C	-1.91122800	1.78924500	1.51382600
H	-1.70189600	2.50893700	0.71671600
H	-1.47329300	2.14036000	2.44843300
O	-3.37899600	1.79593100	1.73465400
H	-4.13446100	0.50124800	2.86691100
C	-2.75128600	-1.47036500	-0.21644100
C	-2.65823400	-2.47772300	0.76404600
C	-3.12858700	-1.84286300	-1.52140400
C	-2.92008200	-3.80791600	0.44354700
H	-2.36574500	-2.22644300	1.77828400
C	-3.39880100	-3.17276500	-1.83906900
H	-3.19186900	-1.08030000	-2.29274100
C	-3.29281400	-4.16071600	-0.85716700
H	-2.83032900	-4.57314700	1.20881800
H	-3.68019400	-3.43945500	-2.85327800
H	-3.49218700	-5.19910000	-1.10398200
H	-2.38751900	0.54955800	-0.84303200

H	-1.62858800	-0.27559700	2.02811600
C	-4.05546600	1.15912800	0.69429800
C	-4.44963600	1.99878300	-0.47393900
C	-4.26169700	3.38875400	-0.40791500
C	-4.98780300	1.44084100	-1.64663100
C	-4.60314300	4.20044200	-1.48960700
H	-3.86853000	3.82986300	0.50121900
C	-5.33328600	2.25914500	-2.72110400
H	-5.14314200	0.37057700	-1.71734200
C	-5.13985200	3.64036300	-2.64946500
H	-4.45710100	5.27415600	-1.41971500
H	-5.75354900	1.81457400	-3.61834200
H	-5.40842200	4.27378500	-3.48916300
C	-4.94312800	0.19380900	1.25818200
O	-4.79641100	-0.14345000	2.52024000
O	-5.86371800	-0.39367400	0.56016000
C	-6.86345300	-1.26590400	1.20970200
H	-7.73247600	-1.14996100	0.56156700
H	-7.08465000	-0.84962900	2.19376300
C	-6.38897100	-2.70235800	1.27817100
H	-6.11285300	-3.07280100	0.28819700
H	-7.20591700	-3.32103300	1.66309400
H	-5.53267700	-2.80903800	1.94669600
P	2.80335100	-0.00109800	-0.20788700
C	3.44488100	1.76806900	-0.58263600
C	4.75970700	1.88201000	-1.37647100
C	3.47430900	2.63833300	0.68885800
H	2.63656800	2.14855500	-1.22338100
C	5.06232100	3.35552900	-1.71038800
H	5.59000100	1.46722800	-0.79358600
H	4.70096000	1.30759100	-2.30646300
C	3.78979400	4.10500100	0.34511600
H	4.24108200	2.26106600	1.37751400
H	2.51440100	2.57211200	1.21472200
C	5.09609200	4.23110400	-0.45149800
H	6.01517200	3.41723700	-2.24772500
H	4.29217400	3.73381100	-2.39699800
H	3.84333900	4.69341500	1.26796900
H	2.96126100	4.52191500	-0.24449100
H	5.27435600	5.27737900	-0.72280500
H	5.94013800	3.92567200	0.18267200
C	2.92947600	-0.99542400	-1.84609700
C	1.83166500	-2.07640500	-1.91865600
C	4.31120900	-1.61259700	-2.13843100
H	2.71431300	-0.23801800	-2.61309600
C	1.84609600	-2.79901400	-3.27688800
H	1.98972900	-2.81109000	-1.11586300
H	0.84747200	-1.62875300	-1.74159100

C	4.31961600	-2.32581400	-3.50355000
H	4.55509700	-2.34407000	-1.35696700
H	5.09629700	-0.85192200	-2.11818000
C	3.22421500	-3.39560100	-3.59162000
H	1.07785100	-3.58051400	-3.28220900
H	1.57029600	-2.08393200	-4.06476400
H	5.30634800	-2.77092300	-3.67338100
H	4.17225900	-1.58264300	-4.29945900
H	3.22143000	-3.85516900	-4.58607200
H	3.44394800	-4.20025200	-2.87603200
C	3.84751000	-0.91932300	1.11691000
C	3.28289800	-0.69682600	2.53532300
C	5.36544600	-0.65327100	1.08908900
H	3.67731100	-1.97296100	0.85319900
C	4.01505900	-1.57533700	3.56406500
C	3.39568800	0.35942200	2.81313800
H	2.20846300	-0.91199600	2.55190800
C	6.09295900	-1.53702300	2.11985700
H	5.55339400	0.40023200	1.32938700
H	5.77933300	-0.83123100	0.09336900
C	5.53153500	-1.34189300	3.53452700
H	3.61532900	-1.37693400	4.56494200
H	3.80478600	-2.63208600	3.34708000
H	7.16513800	-1.31209700	2.09750300
H	5.99009200	-2.59113500	1.82698100
H	6.03312600	-2.01582500	4.23755900
H	5.74854900	-0.31930000	3.87354000
Au	0.47589300	0.19319000	0.49226500
<b>24</b>			
C	-2.57144200	0.18016900	-0.04412200
C	-1.51985900	0.60805900	0.99243000
C	-1.91537500	2.03322500	1.27007500
H	-1.65505200	2.73189400	0.46983400
H	-1.58581300	2.43540800	2.22929500
O	-3.40716700	2.00925400	1.32354900
H	-4.16572100	1.32425000	2.56516700
C	-2.71468200	-1.30995000	-0.28567100
C	-2.70498500	-2.24207600	0.76371700
C	-2.81416000	-1.79360800	-1.59896400
C	-2.80038800	-3.61098700	0.50792900
H	-2.59948600	-1.90667000	1.79211800
C	-2.91497100	-3.16193900	-1.85860800
H	-2.80314300	-1.09036500	-2.42737000
C	-2.91043500	-4.07621400	-0.80468400
H	-2.77534000	-4.31566900	1.33434400
H	-2.98848200	-3.51139300	-2.88414300
H	-2.98088100	-5.14132000	-1.00300900

H	-2.34862700	0.65382100	-1.00449500
H	-1.66448700	0.03194800	1.91660900
C	-3.89592000	0.99460200	0.42998500
C	-4.69786800	1.60430900	-0.72455300
C	-4.86276600	2.99256100	-0.79739400
C	-5.25556500	0.78895800	-1.72086400
C	-5.56483900	3.55941300	-1.86295200
H	-4.44167600	3.62326600	-0.02373100
C	-5.95927900	1.36233000	-2.77954800
H	-5.14209300	-0.28831400	-1.67604200
C	-6.11515900	2.74815600	-2.85489600
H	-5.68317700	4.63754600	-1.91152700
H	-6.38526700	0.72349900	-3.54726100
H	-6.66326200	3.19086000	-3.68079000
C	-4.82548600	0.20769900	1.33962100
O	-4.82220400	0.53919500	2.58164800
O	-5.59601100	-0.70482400	0.89617000
C	-6.59816700	-1.36228600	1.78487200
H	-7.36243400	-1.67157200	1.07298200
H	-6.99507600	-0.59235700	2.44810300
C	-5.98707200	-2.53075600	2.52792100
H	-5.52463600	-3.23747500	1.83580600
H	-6.78729100	-3.04676400	3.06773200
H	-5.24497300	-2.20146800	3.25902500
P	2.83903000	0.03866900	-0.20867400
C	3.55964500	1.77471400	-0.59647800
C	4.89388700	1.83314800	-1.36302000
C	3.59426900	2.66096600	0.66422900
H	2.77970500	2.17714900	-1.25872400
C	5.25710400	3.29035300	-1.70770400
H	5.69691700	1.39602000	-0.75845600
H	4.83361100	1.24964900	-2.28720600
C	3.96887800	4.11098000	0.31040500
H	4.33329300	2.26598700	1.37311700
H	2.62249600	2.63454500	1.17118900
C	5.29559100	4.18033900	-0.45882500
H	6.22285200	3.31180400	-2.22503100
H	4.51577900	3.68776800	-2.41502600
H	4.02391900	4.70941200	1.22689200
H	3.16881100	4.54965000	-0.30240100
H	5.51801400	5.21605000	-0.73845800
H	6.11397300	3.85218600	0.19738300
C	2.97835000	-0.98655500	-1.82692300
C	1.84974600	-2.03522600	-1.90549700
C	4.34467700	-1.65160600	-2.08237600
H	2.80156100	-0.23729900	-2.61173500
C	1.86791000	-2.78003400	-3.25143600
H	1.96984000	-2.76150900	-1.08846000

H	0.87663000	-1.55607800	-1.75354500
C	4.35847200	-2.38629500	-3.43585600
H	4.54927600	-2.37804200	-1.28504900
H	5.15364700	-0.91656800	-2.05703100
C	3.23256700	-3.42373200	-3.52992300
H	1.07580900	-3.53755600	-3.25978600
H	1.62995500	-2.06985100	-4.05609600
H	5.33411800	-2.86404200	-3.57991800
H	4.24898500	-1.65161300	-4.24577500
H	3.23535300	-3.89928900	-4.51699500
H	3.41341700	-4.22272400	-2.79723600
C	3.82917600	-0.89210100	1.14917500
C	3.24942900	-0.61926100	2.55254200
C	5.35703000	-0.69004500	1.14486800
H	3.62049300	-1.94349300	0.90394000
C	3.92773300	-1.50426200	3.61223700
H	3.39884700	0.43741400	2.81102400
H	2.16728300	-0.79058100	2.55237100
C	6.03033200	-1.58110200	2.20556900
H	5.58538200	0.35944200	1.36730800
H	5.78104000	-0.90568400	0.16094800
C	5.45310200	-1.33457700	3.60558100
H	3.52000500	-1.26868000	4.60196000
H	3.67754000	-2.55605300	3.41365200
H	7.11127600	-1.40103400	2.19856700
H	5.88902700	-2.63605000	1.93199500
H	5.91408300	-2.01399400	4.33103300
H	5.70647300	-0.31499600	3.92838500
Au	0.49124300	0.33741400	0.42694300
TS <sub>24-25</sub>			
C	-2.55870100	0.18102800	0.02977200
C	-1.55501200	0.01686000	1.18602800
C	-1.98523800	1.08969000	2.13938000
C	-1.73033400	2.10548800	1.83317800
H	-1.73017100	0.93690500	3.18866600
O	-3.50835300	1.06617600	2.08270600
H	-4.05155900	0.12282800	2.70008000
C	-2.61718800	-0.95018000	-0.97968500
C	-2.54797700	-2.29847300	-0.59687800
C	-2.70005700	-0.65233200	-2.34790000
C	-2.57300000	-3.31587000	-1.55173700
H	-2.45405400	-2.56546100	0.45192800
C	-2.72907000	-1.66800800	-3.30579100
H	-2.73575200	0.38599200	-2.66656100
C	-2.66817600	-3.00446700	-2.91014900
H	-2.50586500	-4.35275200	-1.23478900
H	-2.79151100	-1.41266300	-4.35937100



H	-2.68475500	-3.79656300	-3.65249800
H	-2.32866800	1.10063100	-0.51749900
H	-1.70804500	-0.95613800	1.67090400
C	-3.93265200	0.55767100	0.77318200
C	-4.79347700	1.58609200	0.04828400
C	-4.97229600	2.86705100	0.58553400
C	-5.38752100	1.26423200	-1.18177600
C	-5.72757400	3.81671100	-0.10470500
H	-4.52838500	3.11967900	1.54105400
C	-6.14335100	2.21802200	-1.86292700
H	-5.26135500	0.27660200	-1.60979800
C	-6.31500300	3.49638200	-1.32837300
H	-5.85888300	4.80651000	0.32153600
H	-6.59885300	1.95885800	-2.81377600
H	-6.90485500	4.23572900	-1.86112600
C	-4.77207900	-0.63599400	1.24974000
O	-4.74136300	-0.82677800	2.49613800
O	-5.46802200	-1.32524900	0.42095300
C	-6.37466400	-2.38645700	0.93202900
H	-7.14139100	-2.43084900	0.15916700
H	-6.80652200	-2.02345600	1.86594500
C	-5.63913500	-3.70009800	1.09588100
H	-5.15917300	-3.99967500	0.16162800
H	-6.36553100	-4.47022800	1.37355400
H	-4.88901400	-3.64322800	1.88843600
P	2.86681100	0.25177500	0.11198600
C	3.81808600	-0.60018700	1.54592000
C	5.33453500	-0.34973600	1.63824100
C	3.48681800	-2.10365900	1.62103900
H	3.35035000	-0.11709300	2.41591600
C	5.91279500	-0.99195600	2.91369400
H	5.84200600	-0.76948800	0.76222600
H	5.54685400	0.72400300	1.64853900
C	4.07943000	-2.73649300	2.89236800
H	3.89813800	-2.61722400	0.74244200
H	2.40075700	-2.25251000	1.59596400
C	5.59106300	-2.48963600	2.99615300
H	6.99600600	-0.82921800	2.94325500
H	5.49709200	-0.48107500	3.79345000
H	3.86372900	-3.81095500	2.90125500
H	3.57893800	-2.30978300	3.77288800
H	5.98038700	-2.90970000	3.93010800
H	6.10300300	-3.01780300	2.17948400
C	3.45140700	2.07985800	0.06800000
C	2.33839900	2.99469700	-0.48414000
C	4.77466000	2.33744400	-0.67885200
H	3.59525600	2.32142000	1.13069100
C	2.74321300	4.47755100	-0.41729100

H	2.12941900	2.72204500	-1.52891100
H	1.40835700	2.83248400	0.07183300
C	5.17860000	3.82091300	-0.59370300
H	4.65317000	2.06584000	-1.73544500
H	5.57997400	1.71368000	-0.28184000
C	4.07487200	4.73942500	-1.13296300
H	1.94682400	5.09400300	-0.84987900
H	2.83144700	4.77651200	0.63667800
H	6.11184100	3.97584000	-1.14671100
H	5.39055300	4.07774500	0.45353100
H	4.36583600	5.78973900	-1.02153200
H	3.94990900	4.56238700	-2.21046300
C	3.25777500	-0.51262000	-1.60583400
C	2.26051000	-1.63492300	-1.96126400
C	4.70765600	-0.98425300	-1.83254700
C	3.06227900	0.33111800	-2.28355800
C	2.46504500	-2.11821400	-3.40736600
H	2.39930800	-2.47924000	-1.27296700
H	1.23165300	-1.28528200	-1.82287000
C	4.90515400	-1.46033100	-3.28413500
H	4.92973900	-1.81667900	-1.15380000
H	5.42383300	-0.18998100	-1.60640700
C	3.91084200	-2.56655700	-3.66063800
H	1.76577500	-2.93429200	-3.62223500
H	2.21175300	-1.30045600	-4.09692900
H	5.93578600	-1.80858900	-3.41588300
H	4.77595500	-0.60588400	-3.96314600
H	4.04191600	-2.85306800	-4.71001500
H	4.12340900	-3.46424800	-3.06316600
Au	0.48431700	0.12757800	0.65530600
<b>25</b>			
C	-2.56898200	0.20382700	0.05692800
C	-1.55813400	0.05012700	1.20880300
C	-1.93585700	1.13984600	2.13809500
H	-1.73502600	2.15434800	1.79714100
H	-1.69306300	1.01911900	3.19363800
O	-3.52385600	1.12623400	2.09510100
H	-3.89513600	0.40765200	2.72828800
C	-2.59254000	-0.92660200	-0.95592900
C	-2.51504500	-2.27416600	-0.57371900
C	-2.64060300	-0.62445900	-2.32453500
C	-2.49575000	-3.28823900	-1.53189900
H	-2.45626300	-2.54366800	0.47676200
C	-2.62556300	-1.63734200	-3.28571300
H	-2.68543300	0.41418600	-2.64115000
C	-2.55483200	-2.97373800	-2.89171400
H	-2.42655500	-4.32508000	-1.21569500

H	-2.66299900	-1.37967400	-4.33988700
H	-2.53881100	-3.76379400	-3.63624500
H	-2.34840000	1.12731500	-0.48807300
H	-1.70318700	-0.91293000	1.71260800
C	-3.95678300	0.54414300	0.78654700
C	-4.82582200	1.55741400	0.05542600
C	-5.04747600	2.83757700	0.58008100
C	-5.38947900	1.21566700	-1.18413500
C	-5.81630100	3.76310800	-0.12810700
H	-4.63015500	3.11453100	1.54074700
C	-6.15763300	2.14573800	-1.88339100
H	-5.23407600	0.22812000	-1.60080700
C	-6.37322700	3.42183300	-1.35981300
H	-5.98140600	4.75069200	0.29140300
H	-6.58982300	1.86854700	-2.83999400
H	-6.97327000	4.14241600	-1.90665300
C	-4.75922400	-0.67077000	1.30271700
O	-4.73297500	-0.90561200	2.51367300
O	-5.44068400	-1.32947800	0.40872100
C	-6.34179100	-2.40303700	0.87167000
H	-7.09824800	-2.43914500	0.08749400
H	-6.79457500	-2.07256600	1.80809600
C	-5.60861100	-3.72131200	1.02208500
H	-5.11368500	-4.00354600	0.08998800
H	-6.33541700	-4.49938100	1.27570900
H	-4.86989200	-3.67475800	1.82586500
P	2.86199400	0.25608100	0.11129900
C	3.81078500	-0.60073400	1.54399100
C	5.33015600	-0.36450300	1.62557000
C	3.46509600	-2.10052700	1.62672200
H	3.35311300	-0.10912800	2.41453800
C	5.90958900	-1.00713900	2.90030400
H	5.82794800	-0.79297700	0.74823500
H	5.55292100	0.70715200	1.63006700
C	4.05941100	-2.73402000	2.89702500
H	3.86609100	-2.62129000	0.74768700
H	2.37750600	-2.23935600	1.60891500
C	5.57397100	-2.50123300	2.99065900
H	6.99439900	-0.85458500	2.92266800
H	5.50402600	-0.48868300	3.78034200
H	3.83335000	-3.80622100	2.91112400
H	3.56825300	-2.29934900	3.77888300
H	5.96463100	-2.92119600	3.92403400
H	6.07601700	-3.03770000	2.17330300
C	3.46204000	2.07869600	0.05493800
C	2.35494000	3.00159500	-0.49550200
C	4.78315500	2.31738000	-0.70213900
H	3.61523200	2.32398400	1.11543100

C	2.77600100	4.48045900	-0.44047800
H	2.13605700	2.72497400	-1.53713000
H	1.42698000	2.85285000	0.06791900
C	5.20309700	3.79707400	-0.62915900
H	4.65187500	2.04007600	-1.75606300
H	5.58440400	1.68789200	-0.30598000
C	4.10540700	4.72360700	-1.16689400
H	1.98322900	5.10255800	-0.87151900
H	2.87467900	4.78484900	0.61099800
H	6.13400700	3.93831100	-1.18956800
H	5.42504700	4.05830400	0.41488400
H	4.40794300	5.77145200	-1.06399000
H	3.97128400	4.54124800	-2.24236900
C	3.22701500	-0.52115300	-1.60631800
C	2.21155600	-1.63119200	-1.94822500
C	4.66892800	-1.01336800	-1.84020700
H	3.03816100	0.32234300	-2.28611000
C	2.39983700	-2.12626500	-3.39252400
H	2.34256300	-2.47287100	-1.25525900
H	1.18843400	-1.26595000	-1.80668500
C	4.84936400	-1.50158200	-3.28997100
H	4.88530800	-1.84392400	-1.15743600
H	5.39680400	-0.22683100	-1.62470200
C	3.83747600	-2.59658000	-3.65220800
H	1.68728100	-2.93331900	-3.59714100
H	2.15349200	-1.30932400	-4.08553000
H	5.87422400	-1.86465800	-3.42624000
H	4.72718400	-0.64997100	-3.97376000
H	3.95746100	-2.89177000	-4.70044200
H	4.04157000	-3.49313300	-3.05015400
Au	0.48619100	0.15598300	0.66884200
TS <sub>25-26</sub>			
C	-2.56522500	0.33689000	0.06935500
C	-1.58143900	0.31042400	1.24142900
C	-1.79374600	1.52589300	1.97286500
H	-1.67402300	2.47695300	1.46296900
H	-1.61145900	1.56989100	3.04518300
O	-3.62396500	1.59053200	1.87124500
H	-3.97746200	1.07952800	2.65773500
C	-2.53906200	-0.86354500	-0.85769100
C	-2.34693800	-2.17002300	-0.38301700
C	-2.65665000	-0.66915700	-2.24142100
C	-2.28376300	-3.24911300	-1.26485300
H	-2.23720900	-2.35578600	0.68113900
C	-2.59895300	-1.74800700	-3.12655200
H	-2.79553500	0.33573800	-2.63041600
C	-2.41361700	-3.04253400	-2.64043600

H	-2.12868400	-4.25199600	-0.87744200
H	-2.69484900	-1.57364200	-4.19404900
H	-2.36543200	-3.88311200	-3.32598900
H	-2.35942200	1.22460200	-0.53851700
H	-1.71177400	-0.56958700	1.87834000
C	-3.98063400	0.71237900	0.75695500
C	-4.92149400	1.46081800	-0.18684500
C	-5.14942700	2.83364000	-0.01608200
C	-5.53563800	0.79620200	-1.26005400
C	-5.97362500	3.52789200	-0.90293500
H	-4.69425000	3.35951400	0.81425200
C	-6.35909900	1.49727300	-2.14142000
H	-5.37892600	-0.26438900	-1.40752900
C	-6.58140900	2.86387000	-1.96801000
H	-6.14340500	4.58972300	-0.75276800
H	-6.83001400	0.96818900	-2.96440500
H	-7.22578700	3.40476000	-2.65410800
C	-4.66791600	-0.46146600	1.49426500
O	-4.69164400	-0.45033700	2.72236100
O	-5.20908300	-1.37951500	0.73027100
C	-5.99251600	-2.44024500	1.38400600
H	-6.70355000	-2.73503900	0.61155800
H	-6.52480500	-1.99216600	2.22470800
C	-5.11105200	-3.59572700	1.81828700
H	-4.55304600	-4.00237800	0.97135000
H	-5.74355400	-4.39052000	2.22594100
H	-4.41242200	-3.28661100	2.59974400
P	2.85640500	0.22255300	0.12742900
C	3.66282600	-1.05890700	1.30756400
C	5.20134900	-1.08566200	1.36145000
C	3.07707800	-2.46738500	1.09018900
H	3.30278700	-0.69691400	2.28134500
C	5.68776600	-2.07123400	2.44122400
H	5.60753300	-1.38733100	0.38954900
H	5.59606100	-0.08837900	1.58018600
C	3.58015400	-3.44523200	2.16669600
H	3.37245300	-2.84052900	0.10122300
H	1.98123900	-2.42674200	1.10000400
C	5.11348000	-3.47806500	2.23040300
H	6.78302700	-2.09828700	2.43966800
H	5.38673300	-1.69879400	3.43026100
H	3.18195200	-4.44615000	1.96574400
H	3.18098900	-3.13993000	3.14403700
H	5.44434800	-4.14592900	3.03315700
H	5.50838100	-3.89668100	1.29409900
C	3.73848200	1.89907200	0.44279500
C	2.78532400	3.08311400	0.18260000
C	5.05957500	2.09422500	-0.32608400

H	3.95856500	1.86497300	1.51909700
C	3.44854000	4.42502700	0.54009800
H	2.49766000	3.09152400	-0.87866600
H	1.86063000	2.95528000	0.75665300
C	5.72195200	3.43381900	0.04646300
H	4.85451400	2.08971600	-1.40440100
H	5.75504200	1.27373000	-0.13057600
C	4.77963400	4.61893300	-0.19818100
H	2.75899400	5.24549300	0.31158700
H	3.62530700	4.45783600	1.62424000
H	6.64682100	3.55258800	-0.52874400
H	6.01430900	3.40944500	1.10533900
H	5.25499500	5.55383000	0.11768300
H	4.58794100	4.71440300	-1.27607900
C	3.06735200	-0.21405900	-1.73214300
C	1.87796100	-1.04617200	-2.25383800
C	4.40415500	-0.87316100	-2.12557200
H	3.01799000	0.77580000	-2.20816100
C	1.96904000	-1.24567400	-3.77637300
H	1.87124200	-2.02597300	-1.75832400
H	0.93020400	-0.56004000	-1.99692900
C	4.48906800	-1.06364900	-3.65178800
H	4.48255200	-1.85426100	-1.64093200
H	5.25507700	-0.27962400	-1.78181400
C	3.30507900	-1.87688800	-4.19066100
H	1.12857400	-1.86367100	-4.11155700
H	1.85774400	-0.27097400	-4.27228400
H	5.43739100	-1.55129000	-3.90364200
H	4.50754900	-0.07786500	-4.13706600
H	3.36548700	-1.95659000	-5.28158800
H	3.36046100	-2.90243000	-3.79920400
Au	0.49674500	0.33639200	0.71860500
<b>26</b>			
C	-2.61031300	0.12723000	0.48750600
C	-1.75681800	-1.03903500	0.92991000
C	-1.18824900	-1.14490500	2.17819200
H	-1.31615100	-0.35253000	2.90941500
H	-0.81930700	-2.10168100	2.54041500
O	-3.86892800	0.17350700	2.49111500
H	-4.50776000	-0.40118600	2.95078400
C	-2.49237000	0.43685700	-0.99933600
C	-2.47812900	-0.55159500	-1.99524800
C	-2.37395500	1.77868400	-1.39249200
C	-2.36110800	-0.20478500	-3.34271700
C	-2.59134300	-1.59682300	-1.73074800
C	-2.26084400	2.12796000	-2.73847000
H	-2.39318800	2.55955000	-0.63690300

C	-2.25502400	1.13518000	-3.72002800
H	-2.36257700	-0.98443600	-4.09891300
H	-2.18509600	3.17431700	-3.01859500
H	-2.17555300	1.40307000	-4.76934900
H	-2.27570600	1.01693100	1.02950500
H	-1.77699000	-1.92668400	0.30094600
C	-4.07288800	-0.04940500	1.10824300
C	-5.06573400	0.97272200	0.52553200
C	-5.36117300	2.12135000	1.27142800
C	-5.67784200	0.79602200	-0.72404100
C	-6.24859800	3.07719600	0.77522900
H	-4.90260600	2.25187500	2.24448200
C	-6.56832900	1.75170700	-1.21362300
H	-5.46143500	-0.08323800	-1.31924200
C	-6.85643200	2.89539100	-0.46746900
H	-6.47040900	3.96035200	1.36711600
H	-7.03899700	1.59868200	-2.18023900
H	-7.55250600	3.63606800	-0.84949200
C	-4.67044100	-1.47328200	1.00276900
O	-5.20327000	-1.98806600	1.96690400
O	-4.56700600	-2.04238400	-0.20099800
C	-5.23302900	-3.33558400	-0.37804700
H	-5.43478400	-3.37817700	-1.44962200
H	-6.17517000	-3.31058400	0.17205600
C	-4.34950000	-4.48276900	0.07992700
H	-3.39316500	-4.48347500	-0.45275500
H	-4.85100200	-5.43271000	-0.12991100
H	-4.16568900	-4.42709000	1.15538900
P	2.82493700	0.06850500	0.20682500
C	3.76664300	-1.60039600	0.15535000
C	5.30510900	-1.52523000	0.14408900
C	3.23362300	-2.51756800	-0.96216300
H	3.46499000	-2.03798200	1.11768100
C	5.90675700	-2.94010400	0.25166700
H	5.65550300	-1.05391200	-0.78083400
H	5.66695300	-0.91270300	0.97605100
C	3.85036600	-3.92332600	-0.85272000
H	3.48389800	-2.09074800	-1.94156100
H	2.13968600	-2.58248800	-0.91416300
C	5.38443600	-3.86909400	-0.85227900
H	6.99923600	-2.87128000	0.21182400
H	5.65662900	-3.36294500	1.23441900
H	3.48731600	-4.54576500	-1.67792700
H	3.50061900	-4.39749500	0.07483200
H	5.79744100	-4.87539600	-0.72508100
H	5.73634400	-3.50919500	-1.82897600
C	3.60814000	1.13965700	1.59435500
C	2.55549300	2.06762200	2.23378200

C	4.84979000	1.94468500	1.16031200
H	3.91389200	0.39547000	2.34277600
C	3.14954600	2.86219000	3.41015100
H	2.17672900	2.76768600	1.47527800
H	1.69512100	1.48097100	2.57720500
C	5.44030600	2.72623300	2.34953500
H	4.56554100	2.65879300	0.37652500
H	5.61521700	1.29019800	0.73369800
C	4.39902400	3.64921400	2.99387200
H	2.38628300	3.53547700	3.81542900
H	3.41029200	2.16360300	4.21711900
H	6.30615200	3.30256800	2.00587100
H	5.81609900	2.01553600	3.09824700
H	4.83024200	4.15964700	3.86150700
H	4.11498200	4.43392300	2.27909100
C	2.88693200	1.06142700	-1.43272400
C	1.70925800	0.71858900	-2.36696800
C	4.22722000	0.98445900	-2.19159500
H	2.74648400	2.09245500	-1.07857500
C	1.70105700	1.65031900	-3.59131700
H	1.79743500	-0.32335800	-2.70151100
H	0.75577200	0.80201700	-1.83369400
C	4.21037500	1.92638400	-3.40956600
H	4.38963100	-0.04296400	-2.53978700
H	5.06761800	1.23813500	-1.54054500
C	3.03600000	1.61831300	-4.34775400
H	0.87377700	1.36870600	-4.25080200
H	1.49542900	2.67646100	-3.25591200
H	5.16322200	1.84255000	-3.94353000
H	4.13895600	2.96561700	-3.06012400
H	3.01772500	2.33235900	-5.17812100
H	3.17865300	0.62436500	-4.79427400
Au	0.55075100	-0.48491700	0.84069900
<b>27</b>			
C	3.22609000	-0.46751100	0.99598100
C	2.10371000	-1.52132400	0.88022900
C	1.77261300	-2.11830800	-0.34770500
C	1.45799900	-1.96874600	2.04087600
C	0.81821100	-3.13551500	-0.40898800
H	2.29157300	-1.82826900	-1.25489600
C	0.50273700	-2.98648200	1.97749800
H	1.72531900	-1.52612500	2.99296200
C	0.18030700	-3.57568500	0.75374400
H	0.59525900	-3.60327600	-1.36380400
H	0.02979100	-3.33337000	2.89179200
H	-0.54201100	-4.38562200	0.70832500
C	4.58134100	-1.18834600	0.75443800

O	5.36691400	-1.34252900	1.66943100
O	4.76068300	-1.60515900	-0.49285400
C	6.02721800	-2.28374600	-0.77060400
H	6.83686000	-1.58826700	-0.53503000
H	6.10608500	-3.14102200	-0.09730300
C	3.07563500	0.70587500	-0.02736000
C	1.96684800	1.70847300	0.23812300
C	1.33612600	2.01446500	1.42317000
H	1.56020000	1.46600400	2.33065100
H	0.81555900	2.96444300	1.52204700
O	3.29394100	0.04532900	2.31000700
H	4.12048600	-0.31608500	2.68825100
C	4.35101000	1.54654300	-0.19321300
C	4.97241100	1.61801100	-1.44832700
C	4.89727800	2.27076900	0.87741800
C	6.12282400	2.38604600	-1.62977400
H	4.55824300	1.06264700	-2.28614000
C	6.05142700	3.03345600	0.69549900
H	4.42551400	2.22692200	1.85253100
C	6.66575700	3.09506500	-0.55655600
H	6.59358600	2.43010900	-2.60731100
H	6.46851300	3.58328700	1.53375900
H	7.56064100	3.69379100	-0.69591500
H	2.87680200	0.25470400	-1.00315800
P	-2.49277600	0.02972200	-0.27686800
C	-3.04751700	-1.13420200	1.14335700
C	-4.26220300	-2.03761800	0.86087000
C	-3.20606300	-0.36230300	2.46774300
H	-2.16376800	-1.77962300	1.23600000
C	-4.50162500	-2.99631600	2.04386500
H	-5.16033700	-1.43031600	0.70285800
H	-4.10354500	-2.62210800	-0.05120000
C	-3.45480500	-1.33069100	3.63735900
H	-4.05144500	0.33343800	2.39429700
H	-2.31285300	0.24274400	2.66533800
C	-4.66119400	-2.24114300	3.37006000
H	-5.38760100	-3.60729100	1.83937200
H	-3.65414800	-3.69163700	2.11958800
H	-3.60104500	-0.75828900	4.55993000
H	-2.55784700	-1.94683700	3.78984600
H	-4.79057700	-2.94990400	4.19501500
H	-5.57597100	-1.63327900	3.33568900
C	-2.40224900	-1.00039000	-1.89285300
C	-1.34100300	-0.42576200	-2.85309200
C	-3.75128100	-1.17388000	-2.61849600
H	-2.05456500	-1.98135200	-1.54220900
C	-1.19533800	-1.29616200	-4.11412100
H	-1.62726500	0.59428700	-3.14689700

H	-0.37482100	-0.34870800	-2.34119000
C	-3.59263300	-2.06042800	-3.86814100
H	-4.12505000	-0.19051000	-2.93144100
H	-4.50467300	-1.60353800	-1.95268400
C	-2.53753700	-1.49879000	-4.82894700
H	-0.46434500	-0.83822400	-4.78992600
H	-0.78547400	-2.27449500	-3.82614100
H	-4.56151900	-2.15116400	-4.37117100
H	-3.30623600	-3.07494700	-3.55838500
H	-2.41160900	-2.16724500	-5.68732000
H	-2.88577900	-0.53720000	-5.23065200
C	-3.68384200	1.50631700	-0.57911800
C	-3.28978900	2.74415300	0.25240200
C	-5.18351400	1.18924800	-0.40771200
H	-3.49900800	1.73998900	-1.63706400
C	-4.16003200	3.95766000	-0.11856700
H	-3.40734500	2.52100400	1.32092800
H	-2.23167500	2.98293300	0.09525300
C	-6.04296900	2.40854300	-0.79167600
H	-5.38453400	0.93089800	0.63921100
H	-5.47672200	0.32601900	-1.01082200
C	-5.65723200	3.65126100	0.02051000
H	-3.88154500	4.81045400	0.51038000
H	-3.94237400	4.25015900	-1.15525100
H	-7.10078700	2.16482600	-0.64422100
H	-5.91734200	2.61587800	-1.86338200
H	-6.25094600	4.51364900	-0.30075400
H	-5.89820600	3.48303500	1.07933600
Au	-0.29617100	0.87106500	0.31684400
C	6.01676200	-2.68953600	-2.22909900
H	5.19197900	-3.37517600	-2.44257600
H	6.95437400	-3.19864000	-2.47054600
H	5.92606300	-1.81589700	-2.88062600
H	1.84013300	2.40807500	-0.58846200
<b>28</b>			
C	2.47279400	0.49182900	0.13567900
C	1.45766100	0.37548300	1.34225900
C	2.04133200	-0.69700000	2.25977100
H	1.33531800	-1.37437400	2.73961000
H	2.77126500	-0.34273300	2.98609400
O	2.84163400	-1.56609100	1.33969100
H	2.14916100	-2.15376700	0.82787000
C	3.01830900	1.90049600	-0.06451500
C	3.62594000	2.62168600	0.97616200
C	2.86040500	2.53162300	-1.30523000
C	4.08442800	3.92215500	0.76961200
H	3.74679700	2.16982200	1.95663600

C	3.31392700	3.83616900	-1.51384600
H	2.36550100	2.00369100	-2.11711800
C	3.93241600	4.53387900	-0.47737500
H	4.55392500	4.46184500	1.58680200
H	3.17869500	4.30501000	-2.48392800
H	4.28560800	5.54832900	-0.63482300
H	1.95667700	0.22128400	-0.78590000
H	1.45998200	1.32202500	1.88918600
C	3.53653500	-0.65444600	0.34782600
C	3.88963500	-1.52096000	-0.84988500
C	4.39128400	-2.81500000	-0.63328100
C	3.79466800	-1.03741500	-2.15943900
C	4.75122200	-3.62175400	-1.71097200
H	4.50444600	-3.19318600	0.37876800
C	4.16732100	-1.84474200	-3.23535800
H	3.46158000	-0.02404000	-2.34781000
C	4.63714200	-3.13958300	-3.01634500
H	5.12930500	-4.62308700	-1.52929100
H	4.09308100	-1.45550200	-4.24608800
H	4.92290900	-3.76563000	-3.85590200
C	4.81782300	-0.19945900	1.08937300
O	4.95247300	-0.24206400	2.29420900
O	5.70841200	0.25275600	0.21696500
C	6.95552200	0.79728500	0.75232800
H	6.72931400	1.32492700	1.68083500
H	7.27103600	1.51252300	-0.00845800
C	7.98113300	-0.30260700	0.96256300
H	7.65409000	-0.99939500	1.73823700
H	8.92847500	0.14256200	1.28249400
H	8.15828700	-0.85479200	0.03569400
P	-2.94158700	-0.03560500	0.13608600
C	-3.67394100	1.69290200	0.53919400
C	-5.20794800	1.81551500	0.58604500
C	-3.04396900	2.78611300	-0.34608800
H	-3.30000200	1.84104900	1.56268200
C	-5.62149700	3.22380800	1.05521800
H	-5.63283600	1.62819400	-0.40643800
H	-5.63314700	1.06878100	1.26438900
C	-3.47425800	4.18779300	0.12118700
H	-3.35975700	2.64238700	-1.38744100
H	-1.95039600	2.70437600	-0.33094200
C	-5.00219400	4.32150100	0.17981400
H	-6.71446000	3.30051800	1.05260700
H	-5.30167000	3.36407000	2.09709300
H	-3.04717300	4.94303200	-0.54801600
H	-3.05206200	4.37877700	1.11756600
H	-5.28089800	5.31024200	0.56010900
H	-5.41322900	4.25159900	-0.83703300

C	-3.87917700	-1.29113000	1.24687600
C	-2.96486600	-2.47247000	1.63094500
C	-5.21874700	-1.80697100	0.68535400
H	-4.08102400	-0.71100600	2.15805900
C	-3.65997700	-3.43210700	2.61283600
H	-2.68705500	-3.02392300	0.71924800
H	-2.03647500	-2.09110200	2.07259300
C	-5.91055800	-2.75517900	1.68254600
H	-5.03570300	-2.35218900	-0.24996300
H	-5.88749900	-0.97677100	0.44254300
C	-5.00434900	-3.93090400	2.06753500
H	-2.99737100	-4.27679800	2.83500900
H	-3.82493600	-2.90744300	3.56397500
H	-6.84717300	-3.11957600	1.24635500
H	-6.18541800	-2.19270000	2.58540200
H	-5.50048200	-4.56650000	2.80885700
H	-4.82950800	-4.56046300	1.18368000
C	-3.20128700	-0.55812300	-1.69407200
C	-2.01069200	-0.12944300	-2.57738700
C	-4.53389700	-0.13954600	-2.34646100
H	-3.18468800	-1.65568400	-1.62612800
C	-2.13673400	-0.71618000	-3.99383900
H	-1.97645300	0.96612200	-2.63951100
H	-1.06595200	-0.44507800	-2.12021000
C	-4.65759600	-0.73562300	-3.76119600
H	-4.57682300	0.95436600	-2.41756100
H	-5.38644800	-0.45274800	-1.73894400
C	-3.47200300	-0.33855900	-4.65039700
H	-1.29658300	-0.37321900	-4.60845000
H	-2.05531300	-1.81090700	-3.93710000
H	-5.60156500	-0.40932200	-4.21156200
H	-4.70992500	-1.83083100	-3.68710900
H	-3.55862400	-0.81410300	-5.63342900
H	-3.49685400	0.74605600	-4.82530300
Au	-0.55423500	0.09916900	0.75110900
O	0.94828400	-2.78950000	0.20091000
H	0.24803800	-2.09978400	0.21349700
H	0.57111300	-3.59026700	0.59085000
TS <sub>28-29</sub>			
C	2.61314000	0.16682500	-0.04581500
C	1.50095600	-0.33965800	0.94030600
C	2.20308700	-1.40538200	1.81094700
H	1.58942900	-2.26889700	2.08200500
H	2.64023800	-0.98032100	2.70800400
O	3.26469500	-1.90326100	0.96186800
H	2.29295100	-2.54635600	-0.18087400
C	2.80053900	1.67647400	-0.01432600

C	3.04599400	2.37943900	1.17549500
C	2.67057900	2.41254500	-1.20281500
C	3.17636100	3.76728200	1.17448000
H	3.14602100	1.84317900	2.11886800
C	2.80161000	3.80278300	-1.20900400
H	2.46297900	1.89269800	-2.13568700
C	3.06015000	4.48300700	-0.01976800
H	3.37375900	4.28894700	2.10762500
H	2.69968300	4.34943400	-2.14293200
H	3.16270800	5.56648200	-0.02306900
H	2.34606500	-0.09581500	-1.07185000
H	1.21181600	0.48967300	1.58955600
C	3.86574100	-0.76504300	0.28957600
C	4.60856600	-1.30710700	-0.92722000
C	5.14734300	-2.60657300	-0.88304900
C	4.80981600	-0.52930600	-2.07407400
C	5.83804800	-3.12083200	-1.97915000
H	5.02117700	-3.20804700	0.00912900
C	5.50765600	-1.04484800	-3.16253300
H	4.44003800	0.48812200	-2.10771000
C	6.02058200	-2.34347900	-3.12455700
H	6.24622200	-4.12494300	-1.93193400
H	5.65517600	-0.42751800	-4.04711400
H	6.56343800	-2.74310300	-3.97504900
C	4.85454900	-0.10470200	1.28404100
O	4.78911000	-0.23680300	2.49193400
O	5.75995600	0.63240000	0.64519200
C	6.73045400	1.36269500	1.45730300
H	6.24020900	1.68036400	2.37988500
H	6.97771500	2.23659200	0.85019200
C	7.95085900	0.50112900	1.73690900
H	7.68339400	-0.36297400	2.34837000
H	8.69403700	1.08868100	2.28618100
H	8.40672300	0.15225900	0.80717500
P	-3.04136600	-0.04473400	0.11846500
C	-3.31987800	1.85339100	0.21387400
C	-4.76229900	2.33133900	0.46905300
C	-2.68830900	2.56611000	-1.00062700
H	-2.72352000	2.11178600	1.09723500
C	-4.79962000	3.86258200	0.62713600
H	-5.40956400	2.04566700	-0.36734500
H	-5.16618200	1.86077500	1.36999500
C	-2.74328400	4.09280400	-0.82858100
H	-3.22848400	2.28440900	-1.91374600
H	-1.65025700	2.24026200	-1.13463700
C	-4.17840600	4.58145800	-0.57601400
H	-5.83674500	4.18299000	0.77574600
H	-4.25434000	4.14668600	1.54262100

H	-2.31854900	4.57716000	-1.71155900
H	-2.10803000	4.38188100	0.02074700
H	-4.18690400	5.66510600	-0.42161700
H	-4.78907600	4.38790700	-1.47099400
C	-3.91886000	-0.82447600	1.64190600
C	-3.18911400	-2.10254500	2.09792600
C	-5.42458800	-1.09713000	1.46613700
H	-3.78332300	-0.05696400	2.41985200
C	-3.80745100	-2.67376600	3.38532700
H	-3.24437900	-2.85816400	1.30214700
H	-2.12360200	-1.89029100	2.25635600
C	-6.03958900	-1.66765400	2.75962100
H	-5.56854800	-1.82464100	0.65547000
H	-5.96160700	-0.18855500	1.17823800
C	-5.30893200	-2.93303000	3.22129600
H	-3.28480100	-3.59654200	3.66648700
H	-3.64775000	-1.95828400	4.20478300
H	-7.10022900	-1.87285800	2.58781900
H	-5.99398400	-0.90384300	3.54633400
H	-5.73745900	-3.29307600	4.16806400
H	-5.46745000	-3.73316400	2.48612500
C	-3.76537300	-0.83967000	-1.46725300
C	-2.73829100	-0.89988100	-2.62059000
C	-5.09332900	-0.23847900	-1.96197800
H	-3.95359800	-1.87295400	-1.14143700
C	-3.29786300	-1.69246400	-3.81569000
C	-2.49418500	0.12163900	-2.94784300
H	-1.80144300	-1.35065100	-2.27749700
C	-5.65315000	-1.04725600	-3.14281300
H	-4.91999000	0.79432300	-2.29138400
H	-5.82939700	-0.19420100	-1.15499300
C	-4.64343000	-1.13664900	-4.29586000
H	-2.56689200	-1.69181000	-4.62840300
H	-3.42912300	-2.74348000	-3.51480000
H	-6.58719700	-0.59047800	-3.48394500
H	-5.91116700	-2.06060700	-2.79631200
H	-5.04668600	-1.76126400	-5.09998200
H	-4.49383400	-0.13606100	-4.72362700
Au	-0.64714900	-0.36599500	0.36624700
O	1.39783200	-2.47968300	-0.65351600
H	0.93754000	-1.49604000	-0.05216800
H	0.87388900	-3.28133500	-0.48849500
<b>29</b>			
C	3.66494000	1.12851000	0.50127900
C	3.36835900	1.43314800	1.99020400
C	2.61272400	0.19862000	2.49548100
H	1.53772800	0.37187100	2.61231000

H	3.02310600	-0.19234000	3.42789800
O	2.76218700	-0.81637900	1.46361300
H	1.41720900	-1.54925000	0.96821700
C	4.77667200	1.97770400	-0.09333000
C	6.05552200	2.05089100	0.48111100
C	4.51042800	2.77653200	-1.21447300
C	7.03967100	2.87166900	-0.06924900
H	6.28836900	1.47930700	1.37411000
C	5.49196900	3.60117200	-1.76646300
H	3.51563600	2.76733200	-1.65497700
C	6.76424900	3.64652700	-1.19770000
H	8.02217900	2.91290400	0.39161300
H	5.25880600	4.21091000	-2.63428900
H	7.53129500	4.28728300	-1.62163900
H	2.75089400	1.32771500	-0.06996900
H	4.29659800	1.56452900	2.54775800
C	3.78987500	-0.43571000	0.50753000
C	3.47602300	-1.18326000	-0.78274400
C	3.34847500	-2.58420800	-0.72284700
C	3.29211900	-0.54741400	-2.01295800
C	3.00654900	-3.32065200	-1.85725700
H	3.52686400	-3.09935300	0.21747100
C	2.96135500	-1.28708900	-3.15398600
H	3.42986400	0.52265200	-2.10143900
C	2.80600600	-2.66997500	-3.08005800
H	2.91994800	-4.40150300	-1.79263900
H	2.83308000	-0.77514500	-4.10301300
H	2.55212300	-3.24158600	-3.96745400
C	5.14995100	-0.87564600	1.10625400
O	5.36528300	-0.89515200	2.30070700
O	6.03676800	-1.17267200	0.15449600
C	7.38140800	-1.53766700	0.58481900
H	7.64043000	-0.94026800	1.46147100
H	8.01333500	-1.24824900	-0.25652900
C	7.47363700	-3.02533300	0.87895800
H	6.84364600	-3.29250500	1.73114500
H	8.50783100	-3.28551800	1.12556200
H	7.17082000	-3.61533700	0.00938400
P	-3.29111400	0.10388400	0.14328900
C	-3.26921700	1.53284800	1.42065200
C	-4.62489900	2.19665500	1.72732200
C	-2.18710700	2.57774000	1.08750400
H	-2.94975000	0.99671200	2.32534400
C	-4.47063700	3.22366300	2.86585200
H	-5.00902300	2.70235000	0.83455600
H	-5.36647200	1.44597700	2.01792400
C	-2.05013700	3.60205500	2.22790400
H	-2.45464400	3.10429200	0.16248700

H	-1.22554200	2.08279300	0.90562900
C	-3.39348400	4.27014500	2.55140500
H	-5.43625800	3.70767800	3.04775300
H	-4.20717500	2.69526100	3.79245700
H	-1.30194600	4.35431800	1.95451500
H	-1.67046400	3.09253300	3.12456200
H	-3.27924400	4.95901400	3.39510300
H	-3.71335600	4.87826500	1.69381800
C	-4.69698100	-1.10079500	0.64664400
C	-4.35308700	-2.55356500	0.25965200
C	-6.09246600	-0.71495400	0.11590200
H	-4.70172100	-1.02753500	1.74304000
C	-5.42990400	-3.53230600	0.75963200
H	-4.27079500	-2.63011600	-0.83407100
H	-3.37644900	-2.83306800	0.67062300
C	-7.16270800	-1.69592100	0.63148000
H	-6.08482000	-0.74414500	-0.98144700
H	-6.35883800	0.30524900	0.40621200
C	-6.82868900	-3.14644800	0.26174700
H	-5.17267900	-4.54780100	0.43936900
H	-5.42188600	-3.54015900	1.85833200
H	-8.13879200	-1.40915500	0.22528100
H	-7.23956800	-1.60341000	1.72350000
H	-7.57953200	-3.82575800	0.67904900
H	-6.87364200	-3.26397900	-0.82991000
C	-3.57674200	0.67378900	-1.66669800
C	-2.25146400	0.98864100	-2.38994900
C	-4.58188300	1.83054800	-1.83895900
H	-4.00470900	-0.22750600	-2.12728200
C	-2.49914800	1.28793800	-3.87896800
H	-1.77216800	1.85656300	-1.91799200
H	-1.55527200	0.14868600	-2.28716100
C	-4.82592600	2.11696500	-3.33275200
H	-4.18118500	2.73484500	-1.36492800
H	-5.53210900	1.60657100	-1.34728900
C	-3.51721800	2.41958800	-4.07334700
H	-1.54804800	1.53916800	-4.36152100
H	-2.86720200	0.37685100	-4.37086400
H	-5.52606000	2.95393900	-3.42926400
H	-5.31515100	1.24680300	-3.79167500
H	-3.71246600	2.57370900	-5.13991800
H	-3.09388600	3.36011200	-3.69415900
Au	-1.21205100	-1.01011200	0.34856400
O	0.62281700	-2.06922400	0.62927100
H	2.78592100	2.35247800	2.08966500
H	0.94804300	-2.52342900	-0.16491400

P<sub>4b</sub>



C	0.61739300	-0.40261300	-1.46166100
C	0.95567800	0.50766900	-2.65932600
C	-0.41235400	1.05241300	-3.09016200
H	-0.81657200	0.52250400	-3.96155400
H	-0.37468200	2.12254600	-3.31674300
O	-1.31795000	0.83417800	-1.99684100
C	1.77933900	-0.74294400	-0.54864700
C	2.64496000	0.23597200	-0.03321600
C	2.02792300	-2.08346000	-0.21747900
C	3.71330000	-0.11697700	0.79184500
H	2.48769700	1.28165300	-0.27743900
C	3.09746100	-2.43931100	0.60539600
H	1.37213100	-2.85653000	-0.60934700
C	3.94497700	-1.45532500	1.11518400
H	4.37045900	0.65738300	1.17800700
H	3.26841900	-3.48530200	0.84416600
H	4.78029000	-1.72809700	1.75374400
H	0.21445800	-1.34358500	-1.85178300
H	1.61292900	1.32317300	-2.35412000
C	-0.65171800	0.31806900	-0.85139900
C	-1.59247400	-0.64593300	-0.12908000
C	-2.88044600	-0.87034400	-0.63100300
C	-1.18109100	-1.35532200	1.00994000
C	-3.73863100	-1.77963500	-0.00889500
H	-3.20190800	-0.32765600	-1.51111500
C	-2.03804700	-2.26672800	1.62570600
H	-0.19368000	-1.19108400	1.42332300
C	-3.32173800	-2.48306700	1.12035700
H	-4.73546600	-1.93627100	-0.41213500
H	-1.70033800	-2.80724000	2.50576500
H	-3.98861700	-3.19174400	1.60352700
C	-0.22059600	1.55071400	-0.01106900
O	0.23060100	2.55520700	-0.52663900
O	-0.37380000	1.39516600	1.31190300
C	0.02563800	2.50757800	2.15298000
H	0.92929600	2.95750300	1.73550500
H	0.25828300	2.04520100	3.11477100
C	-1.09321700	3.52991700	2.27769700
H	-1.30208500	3.99019200	1.30917000
H	-0.79720400	4.31857400	2.97755800
H	-2.00752900	3.06145000	2.65287500
H	1.45516300	-0.05312100	-3.45456600
<b>P<sub>5b</sub></b>			
C	-0.45319500	-0.42853300	-0.45204100
C	-1.95851200	-0.34446300	-0.11812500
C	-2.43107600	0.32067200	1.02233000
C	-2.88865800	-0.90808600	-0.99921000

C	-3.79896200	0.40115100	1.28238000
H	-1.73596400	0.79024400	1.70946600
C	-4.25762700	-0.82565400	-0.73945200
H	-2.52537900	-1.42223800	-1.88100600
C	-4.71918200	-0.17305000	0.40341200
H	-4.14522700	0.91547800	2.17463500
H	-4.96278100	-1.27452800	-1.43361100
H	-5.78422900	-0.11014400	0.60773800
C	-0.00783700	0.96306400	-0.96419100
O	0.31472000	1.14020000	-2.12451100
O	-0.03176800	1.92003100	-0.03496800
C	0.36378300	3.24752100	-0.47410200
H	1.40100400	3.19922300	-0.81835300
H	-0.26116300	3.53058600	-1.32565100
C	0.42493500	-0.83773900	0.77992200
C	0.12388900	-2.20682200	1.35949400
C	-0.56335600	-3.21303500	0.81897000
H	-1.01807800	-3.14892000	-0.16189400
H	-0.68521900	-4.14659000	1.36122700
O	-0.23368100	-1.32508900	-1.52218800
H	0.07230900	-0.77443100	-2.26628700
C	1.92146300	-0.70438800	0.48685200
C	2.66880100	0.32706400	1.07162800
C	2.57821000	-1.61158600	-0.35819000
C	4.03529100	0.45887800	0.81495600
H	2.17571500	1.03158900	1.73682900
C	3.94138300	-1.47745700	-0.62053900
H	2.01116500	-2.42120100	-0.80314600
C	4.67533100	-0.44275200	-0.03565100
H	4.59796500	1.26221200	1.28279600
H	4.43405200	-2.18715400	-1.27955800
H	5.73833900	-0.34433600	-0.23708000
H	0.20077300	-0.10821800	1.56573500
C	0.19066100	4.18663500	0.70289500
H	-0.85008000	4.20596400	1.03824400
H	0.47643400	5.20120000	0.40867500
H	0.82082500	3.88404000	1.54418700
H	0.57333500	-2.35244900	2.34236300
<b>30</b>			
C	2.96534000	0.00980200	-0.72463700
C	1.56217600	0.38251500	-0.20094600
C	0.69890300	-0.65654500	-0.25344600
C	1.37496900	-1.88559200	-0.74837300
H	0.93925600	-2.32871300	-1.64714100
H	1.50546900	-2.65323800	0.02168800
C	1.31629500	1.71843600	0.40090000
C	1.77410500	2.91654100	-0.17489300

C	0.61087000	1.79548300	1.61737900	H	-5.96639100	-3.03644700	0.52258100
C	1.50638800	4.14536700	0.42841400	H	-6.62233200	-1.71511500	-0.45872400
H	2.33139000	2.89708800	-1.10289700	C	-3.52503300	-3.28172500	-0.69061100
C	0.34498400	3.02475600	2.21923900	H	-3.54359700	-3.79404500	0.27252600
H	0.28931700	0.87707000	2.09763600	H	-3.85958800	-3.99753500	-1.45065600
C	0.78883100	4.20748300	1.62383100	H	-2.48962100	-3.00976200	-0.91660600
H	1.86403400	5.05774000	-0.03945200	C	-3.75597200	-2.57393900	2.68472300
H	-0.19297000	3.05680600	3.16243600	H	-4.44359100	-3.27651200	2.20811100
H	0.59085800	5.16588200	2.09455200	H	-2.73495500	-2.81386200	2.37206800
C	3.92347700	0.04585400	0.47950800	H	-3.81945800	-2.74069300	3.76643100
O	4.52760600	1.03646600	0.81410900	C	-5.57925300	-0.83703900	2.77465700
O	3.91460100	-1.11399700	1.16948500	H	-5.72457300	-1.09559000	3.83045800
C	4.64249200	-1.08836600	2.42352100	H	-5.82314900	0.22169000	2.66002800
H	4.30025300	-0.25344400	3.03650300	H	-6.28651000	-1.42463500	2.18634400
H	4.42012700	-2.03897700	2.90671800	C	-3.20484700	-0.18863700	3.21896700
H	5.71288000	-0.98881600	2.23489000	H	-3.40904700	0.86893300	3.03122800
C	3.46389400	0.72220800	-1.97314100	H	-3.38419900	-0.37788400	4.28401400
C	4.81993400	1.00337100	-2.18726500	H	-2.14704400	-0.37999300	3.01399600
C	2.53813200	1.00492400	-2.98986500	C	-6.87955600	0.82280500	-0.49315400
C	5.23740600	1.56858500	-3.39438600	C	-7.21534300	0.64389700	-1.84560000
H	5.55329000	0.79935900	-1.41712400	C	-7.81761200	0.44400700	0.47876200
C	2.95853400	1.56855100	-4.19219500	C	-8.41853800	0.03987700	-2.21306500
H	1.48553200	0.79076700	-2.83052600	H	-6.53444300	0.99733900	-2.61452100
C	4.31106500	1.85363400	-4.39725100	C	-9.02351600	-0.15824900	0.11282600
H	6.28969300	1.78954800	-3.54458100	H	-7.61530500	0.63760100	1.52552200
H	2.23054700	1.78864100	-4.96698600	C	-9.32263000	-0.37361500	-1.23321300
H	4.63885800	2.29755900	-5.33229200	C	-8.65409400	-0.09423300	-3.26469800
O	2.74175400	-1.41338300	-1.14631000	H	-9.73478700	-0.44555700	0.88165000
Au	-1.31730200	-0.70415500	0.14574800	H	-10.26112700	-0.84012000	-1.51690100
P	-3.75275300	-0.71664900	0.50325300	H	4.84841200	-3.24830700	-0.09203700
C	-4.35834500	1.07425100	0.22095100	C	7.53539100	-1.32466600	-0.26647200
C	-5.63449000	1.58443000	-0.13602800	C	6.74771700	-1.94248800	-0.95519900
C	-3.32195500	2.00014900	0.46350300	C	5.80859300	-2.70885000	-1.75547900
C	-5.79291300	2.98217100	-0.21839200	H	5.45372600	-2.14814300	-2.62547000
C	-3.50795800	3.37756700	0.38744800	H	6.25455700	-3.64457000	-2.10821000
H	-2.33109500	1.63543200	0.71367300	O	4.59214700	-3.05144100	-1.00597700
C	-4.75978400	3.87614800	0.04267000	H	3.54972400	-2.09000900	-1.02929100
H	-6.77032400	3.36304000	-0.49789000	C	8.47519400	-0.60636100	0.53561100
H	-2.67253600	4.04123800	0.58776500	C	9.77784000	-1.11305100	0.71464700
H	-4.93420300	4.94529400	-0.03111700	C	8.11100900	0.60919000	1.15001900
C	-4.46649300	-2.05973800	-0.74131000	C	10.69677500	-0.41243900	1.49038200
C	-4.12052400	-1.11005000	2.39337300	H	10.05658400	-2.04824800	0.24009400
C	-4.36015200	-1.43690700	-2.14376500	C	9.03854800	1.29694000	1.92893300
H	-4.64425600	-2.19123600	-2.88695100	H	7.10698100	1.00024700	1.01800200
H	-5.02319200	-0.58205400	-2.26942000	C	10.32974200	0.79101300	2.09890300
H	-3.33561500	-1.11854200	-2.36366800	H	11.70015600	-0.80533600	1.62174800
C	-5.89786200	-2.52620900	-0.44242200	H	8.75381500	2.23218800	2.40097900
H	-6.19268500	-3.25149400	-1.21044100	H	11.04955100	1.33349700	2.70422300

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C	-4.60461300	-0.00176100	-0.64023600	H	2.37678900	0.51003300	-4.37151800
C	-3.27902400	0.12847600	0.17245500	H	4.85756900	0.87596800	-4.42022400
C	-2.24682600	-0.22630400	-0.64728000	C	2.45482900	-1.07595900	1.95181500
C	-2.83850400	-0.51198000	-2.01409700	C	2.06685000	-3.40015300	-0.35215200
H	-2.91573500	-1.59633300	-2.18798400	C	2.67866200	0.44350800	2.02485400
H	-2.28580800	-0.07388700	-2.85104200	H	2.80666700	0.72916100	3.07576400
C	-3.25018600	0.56402800	1.58592100	H	3.56991800	0.75975500	1.48500600
C	-4.38101800	0.43975700	2.41692900	H	1.81961700	0.99527400	1.62962000
C	-2.09124000	1.15262500	2.13577500	C	3.65277300	-1.84572800	2.52452000
C	-4.34386000	0.86368500	3.74604400	H	3.81832400	-1.51027900	3.55544600
H	-5.29194200	-0.00687700	2.03618000	H	3.46041700	-2.92131700	2.56612700
C	-2.06048500	1.57944600	3.46099600	H	4.57354300	-1.67737300	1.97027000
H	-1.20868400	1.27314300	1.51425600	C	1.20154200	-1.41531000	2.78522700
C	-3.18695700	1.43412600	4.27567800	H	0.96670900	-2.48056000	2.78691800
H	-5.22701800	0.74537400	4.36641700	H	1.39846900	-1.12241300	3.82327100
H	-1.15588800	2.03069900	3.85874600	H	0.31706400	-0.86893300	2.44583500
H	-3.16269500	1.76716300	5.30870400	C	1.22185900	-4.16219100	0.68145200
C	-5.56262200	1.18830400	-0.43540300	H	1.69438900	-4.19621000	1.66606600
O	-6.62724000	1.17540700	0.11694400	H	0.21810300	-3.73839600	0.78538100
O	-5.06057400	2.36766700	-0.97296400	H	1.10938400	-5.19821800	0.34127800
C	-5.94710500	3.51671400	-0.87279200	C	3.49043400	-3.96527000	-0.40138000
H	-6.11779800	3.76678200	0.17513200	H	3.43665400	-5.03926300	-0.61629400
H	-5.44102900	4.32725700	-1.39650900	H	4.06987400	-3.50123200	-1.20258600
H	-6.89693300	3.28445600	-1.35404300	H	4.03082900	-3.84131800	0.53896700
C	-5.34489900	-1.32936300	-0.43173200	C	1.41872100	-3.55492700	-1.74016600
C	-6.46065800	-1.60414900	-1.23748300	H	1.96873100	-3.01453700	-2.51515500
C	-4.89922000	-2.30720700	0.46363800	H	1.42318700	-4.61732700	-2.01041300
C	-7.12357400	-2.82373800	-1.13753000	H	0.37991400	-3.21097400	-1.74540100
H	-6.80669400	-0.86292900	-1.95103400	C	5.55738900	-0.67791400	-0.16456200
C	-5.56610400	-3.53181800	0.56443000	C	5.95022700	0.38570300	0.66469800
H	-4.03296400	-2.12164700	1.08940600	C	6.25284900	-1.89205600	-0.06359600
C	-6.67879000	-3.79206000	-0.23258900	C	6.95875000	0.21810900	1.61489500
H	-7.98707000	-3.02018000	-1.76574000	H	5.47336300	1.35492500	0.55005100
H	-5.21057700	-4.27921000	1.26740100	C	7.26409400	-2.05990600	0.88498800
H	-7.19755000	-4.74260800	-0.15305900	H	6.01678500	-2.70508700	-0.74016200
O	-4.14581800	0.09175400	-1.99495000	C	7.61205300	-1.00953300	1.73541700
Au	-0.27796000	-0.69845400	-0.29002800	H	7.24252900	1.05100000	2.25159600
P	2.03172600	-1.47847500	0.07565900	H	7.78812700	-3.00897000	0.94840000
C	3.15499400	-0.65389900	-1.23471800	H	8.39950300	-1.14029200	2.47139000
C	4.55646400	-0.43140500	-1.25753800	H	-2.25556700	1.68996400	-0.95028200
C	2.40980700	-0.28426100	-2.37437400	C	0.54406600	3.90541400	-0.37234600
C	5.12391600	0.12628800	-2.42090400	C	-0.66131400	3.80206200	-0.46938700
C	2.99561500	0.25565400	-3.51619500	C	-2.09804200	3.74907600	-0.53704600
H	1.33393300	-0.42834900	-2.36521700	H	-2.55627000	3.64150500	0.45088300
C	4.37179800	0.46076300	-3.54222500	H	-2.52882800	4.60659600	-1.06096900
H	6.19701600	0.29073500	-2.42910400	O	-2.54575000	2.57453200	-1.36335400
				H	-3.57472600	2.50149300	-1.35096400
				C	1.95936800	4.04489800	-0.25564500

C	2.52829800	4.46115200	0.96441000
C	2.79378900	3.78157500	-1.35918800
C	3.90727000	4.61927600	1.07012000
H	1.88343600	4.66770200	1.81235700
C	4.17250700	3.93254300	-1.23813800
H	2.35568900	3.45690200	-2.29676100
C	4.73087700	4.35618600	-0.02859200
H	4.33997800	4.95243200	2.00830700
H	4.81121400	3.72434800	-2.09036000
H	5.80549700	4.48729400	0.05574800

**TS<sub>31-32</sub>**

C	-4.64591600	-0.10455400	-0.61961400
C	-3.31316400	0.17104000	0.12982100
C	-2.26575600	-0.08187000	-0.73352300
C	-2.88630000	-0.64284600	-2.00871600
H	-2.85073900	-1.74284500	-2.01066400
H	-2.42202400	-0.28283500	-2.93116300
C	-3.27894100	0.74074000	1.48345800
C	-4.42720700	0.73462200	2.30435000
C	-2.09899500	1.32464800	1.99742000
C	-4.39059400	1.27999100	3.58696100
H	-5.34897700	0.28615500	1.95433800
C	-2.07365600	1.88260400	3.27016100
H	-1.20195600	1.34561600	1.38713900
C	-3.21870800	1.85805800	4.07419200
H	-5.28361200	1.25254200	4.20328900
H	-1.15874400	2.33533500	3.64048700
H	-3.19441800	2.28688000	5.07135500
C	-5.59698300	1.11606900	-0.54917900
O	-6.69349900	1.13797000	-0.05380500
O	-5.03707700	2.22155100	-1.13061900
C	-5.89606200	3.39122100	-1.15363400
H	-6.13934000	3.69924100	-0.13545000
H	-5.32883200	4.16444400	-1.67087700
H	-6.81589900	3.16519100	-1.69436100
C	-5.34251700	-1.40521300	-0.21079900
C	-6.50219700	-1.78664200	-0.90319600
C	-4.81356700	-2.27043400	0.75374800
C	-7.12608100	-2.99850700	-0.62215700
H	-6.91554200	-1.13414500	-1.66471300
C	-5.44017400	-3.48821400	1.03382900
H	-3.91479300	-2.00212400	1.29960400
C	-6.59748500	-3.85335800	0.34948400
H	-8.02614200	-3.27721300	-1.16156200
H	-5.01948000	-4.14696900	1.78758800
H	-7.08641300	-4.79775500	0.56850400
O	-4.24087200	-0.17628900	-1.99258300

Au	-0.27474100	-0.57479900	-0.35297600
P	1.98749400	-1.44334300	0.03922900
C	3.16495800	-0.64818600	-1.23911700
C	4.57478400	-0.48576700	-1.22718100
C	2.46046500	-0.23141100	-2.38810000
C	5.19048100	0.06458700	-2.36917400
C	3.09385100	0.30022500	-3.50826000
H	1.37952600	-0.32765300	-2.40514500
C	4.47781400	0.44773500	-3.50080400
H	6.26940400	0.18378300	-2.35168800
H	2.50525300	0.59482000	-4.37182700
H	4.99960000	0.85707100	-4.36058100
C	2.38116100	-1.07325600	1.92910000
C	1.94408800	-3.35876200	-0.40934800
C	2.66080200	0.43575400	2.02214800
H	2.79524500	0.70261100	3.07707100
H	3.56411700	0.72843400	1.48931200
H	1.82474200	1.02424400	1.63147000
C	3.53690000	-1.89653700	2.51431700
H	3.69835700	-1.57656900	3.55068300
H	3.30040600	-2.96376900	2.54265600
H	4.47251100	-1.76049900	1.97656700
C	1.10006100	-1.37314900	2.73456100
H	0.82513100	-2.42867500	2.72173900
H	1.28766600	-1.09624900	3.77864400
H	0.24367800	-0.79025000	2.38318800
C	1.04296800	-4.09081800	0.59784000
H	1.49401000	-4.15793600	1.59077600
H	0.05894400	-3.61985300	0.68728600
H	0.88768900	-5.11627700	0.24312500
C	3.34230500	-3.98682500	-0.43262300
H	3.24388200	-5.05618000	-0.65447900
H	3.95838500	-3.54634600	-1.21959700
H	3.86897000	-3.89200300	0.51884500
C	1.32244500	-3.47022800	-1.81333300
H	1.91310600	-2.94577400	-2.56901100
H	1.28758600	-4.52888300	-2.09560200
H	0.29974100	-3.08162000	-1.83869200
C	5.53949000	-0.79192200	-0.11662800
C	5.95534700	0.23959400	0.74153300
C	6.18397400	-2.03460300	-0.02480500
C	6.93462300	0.01367300	1.71006100
H	5.52074200	1.22941000	0.63597400
C	7.16548200	-2.26088400	0.94266700
H	5.93274100	-2.82408700	-0.72355300
C	7.53539400	-1.24143300	1.82105400
H	7.23686800	0.82268300	2.36860900
H	7.65018300	-3.23107900	0.99855200

H	8.30015100	-1.41750100	2.57135700
H	-2.09594900	1.27656900	-1.09305400
C	0.67090800	3.76241300	-0.48554800
C	-0.50913500	3.62994000	-0.73459400
C	-1.93189200	3.58457100	-0.99419700
H	-2.50602700	3.63421500	-0.06250200
H	-2.24219800	4.40565100	-1.65001600
O	-2.30291700	2.34624300	-1.70348800
H	-3.29036500	2.31075200	-1.76657000
C	2.05763900	3.93870900	-0.19156200
C	2.45352400	4.47823000	1.04854100
C	3.03839100	3.59412500	-1.14124900
C	3.80380100	4.67321600	1.32584100
H	1.69733100	4.75044400	1.77785300
C	4.38686400	3.78775800	-0.85103700
H	2.73584800	3.17621100	-2.09523700
C	4.77257300	4.32988100	0.37836500
H	4.10115500	5.09899000	2.27922500
H	5.13661000	3.52131300	-1.58929700
H	5.82431300	4.49202800	0.59457600
<b>32</b>			
C	-3.99177600	-0.56258900	-0.39709600
C	-3.01092900	0.61290800	-0.16930400
C	-2.38864400	0.87344100	-1.38280700
C	-3.01118500	0.01539400	-2.45547500
H	-2.30666600	-0.46229000	-3.14183400
H	-3.71380300	0.62449200	-3.04418800
C	-3.02600500	1.51084300	1.00527800
C	-3.96444200	1.34266600	2.04161400
C	-2.13469900	2.60384600	1.07751000
C	-4.01491500	2.24208000	3.10722300
H	-4.66880200	0.51969500	2.02129000
C	-2.18638300	3.49119700	2.14581700
H	-1.39604100	2.76518700	0.29858000
C	-3.12757500	3.31550300	3.16637700
H	-4.75255500	2.09823900	3.89038000
H	-1.49528600	4.32803400	2.17809300
H	-3.16741800	4.01228200	3.99804000
C	-5.45379400	0.00352500	-0.40364400
O	-6.35028500	-0.38882500	0.30360600
O	-5.58077000	0.97535800	-1.32333800
C	-6.90597600	1.54072800	-1.44891000
H	-7.22040100	1.97828300	-0.49934900
H	-6.82470300	2.30512500	-2.22013400
H	-7.61856100	0.76788500	-1.74342400
C	-3.90585900	-1.78818600	0.50633400
C	-4.60088900	-2.94008900	0.10589800

C	-3.15697900	-1.82817600	1.68652400
C	-4.54357900	-4.10356500	0.86803400
H	-5.18498200	-2.92310800	-0.80754200
C	-3.10733200	-2.99532200	2.45675800
H	-2.62219400	-0.95092700	2.02937400
C	-3.79765600	-4.13498200	2.04998100
H	-5.08950600	-4.98443700	0.54435200
H	-2.53348400	-3.00397000	3.37891900
H	-3.76345900	-5.03902600	2.65045900
O	-3.69673000	-1.00736300	-1.73513800
Au	-0.71999200	-0.33698900	-0.42056800
P	1.41073800	-1.48333700	-0.12095900
C	2.61720500	-0.73427800	-1.39624100
C	4.03702100	-0.73434900	-1.41870200
C	1.93719500	-0.15492300	-2.48710200
C	4.68138400	-0.16557700	-2.53512600
C	2.59889000	0.39208200	-3.58221900
H	0.85263000	-0.12536900	-2.47841700
C	3.98953100	0.38529200	-3.60840800
H	5.76680200	-0.16682700	-2.54362800
H	2.02611900	0.82438600	-4.39659700
H	4.53338500	0.80692400	-4.44810600
C	1.89281300	-1.23957300	1.76963700
C	1.11120900	-3.35233000	-0.66438700
C	2.37350200	0.21271300	1.91251500
H	2.55943700	0.41512300	2.97349400
H	3.29925600	0.40222200	1.37313700
H	1.61897100	0.92629700	1.56705700
C	2.94437200	-2.24027600	2.27009300
H	3.18460300	-1.99324100	3.31077800
H	2.56463600	-3.26560100	2.26254700
H	3.86967300	-2.20628600	1.69942800
C	0.60540900	-1.40217500	2.60074700
H	0.15696500	-2.39284100	2.51520700
H	0.86465000	-1.24456200	3.65411700
H	-0.14792800	-0.65639800	2.33048400
C	0.21812600	-4.04695700	0.37466800
H	0.72891500	-4.19403000	1.32943200
H	-0.71744200	-3.50939400	0.55325000
H	-0.04367500	-5.04007400	-0.00802100
C	2.43367300	-4.10901100	-0.82953300
H	2.20969500	-5.14620800	-1.10476900
H	3.03624000	-3.67954900	-1.63303200
H	3.02910400	-4.12874700	0.08516600
C	0.38169800	-3.30836400	-2.01884900
H	0.96718000	-2.79541600	-2.78697300
H	0.22010400	-4.33767200	-2.35907500
H	-0.59781700	-2.82624400	-1.94102600

C	4.99182500	-1.23628400	-0.37235600
C	5.56893900	-0.32628700	0.52915300
C	5.47280300	-2.55424500	-0.38753300
C	6.54416000	-0.74066300	1.43749500
H	5.26305200	0.71569600	0.50665800
C	6.45015100	-2.96892700	0.51999300
H	5.09873700	-3.25555000	-1.12416800
C	6.97979600	-2.06682800	1.44373800
H	6.97245300	-0.02311200	2.13112300
H	6.80741100	-3.99407600	0.49274500
H	7.74108600	-2.38916000	2.14750500
H	-1.89625000	1.81161800	-1.63198200
C	1.38452800	4.32523800	-0.48073000
C	0.46688400	4.51099800	-1.25269100
C	-0.59966500	4.82469700	-2.19582600
H	-1.33429400	5.48544700	-1.71109500
H	-0.17313400	5.37826600	-3.04534100
O	-1.23117100	3.61905800	-2.65476600
H	-1.87657100	3.87548900	-3.32774500
C	2.49846000	4.13753200	0.39663200
C	2.33886500	4.21551900	1.79394200
C	3.78252600	3.90107900	-0.13291600
C	3.43732600	4.06431200	2.63732500
H	1.35306900	4.40574100	2.20631500
C	4.87666800	3.75465600	0.71730200
H	3.90912800	3.84540300	-1.20912000
C	4.70798900	3.83596000	2.10280000
H	3.30424700	4.13558200	3.71264900
H	5.86508900	3.59137400	0.29771200
H	5.56430400	3.73219400	2.76244100
<b>TS<sub>4a-33</sub></b>			
C	-4.37832900	-0.49863100	-0.77901400
C	-3.15286600	0.34292200	-0.31584500
C	-1.97965900	-0.27877800	-0.74357600
C	-2.40099000	-1.39177600	-1.67348600
H	-2.49025400	-2.36010400	-1.17172600
H	-1.81094200	-1.48413700	-2.58476900
C	-3.28725200	1.52387900	0.56211000
C	-4.35810500	1.61848000	1.46856800
C	-2.35859100	2.57845500	0.49597700
C	-4.47497200	2.72570700	2.30944200
H	-5.09681000	0.82649500	1.53085700
C	-2.48795800	3.68687600	1.32857000
H	-1.55124700	2.53647900	-0.22789500
C	-3.54214600	3.76080100	2.24362200
H	-5.30136800	2.77855000	3.01115400
H	-1.77290700	4.50078300	1.25579500

H	-3.64147700	4.62618900	2.89148300
C	-5.57892600	0.38633600	-1.19191000
O	-6.67852700	0.29781200	-0.70428600
O	-5.20872600	1.27170700	-2.12398700
C	-6.23731900	2.19184500	-2.56443300
H	-6.57561000	2.79905700	-1.72282800
H	-5.76563700	2.80907800	-3.32666300
H	-7.08104200	1.63688400	-2.97794600
C	-4.76665300	-1.69714200	0.05125200
C	-5.72331500	-2.59303300	-0.45335800
C	-4.17958800	-1.94868300	1.29826900
C	-6.07689100	-3.72372400	0.27708600
H	-6.18998300	-2.40460700	-1.41446000
C	-4.54487200	-3.07926000	2.03252200
H	-3.44942300	-1.25846200	1.70928900
C	-5.48999400	-3.96814500	1.52221200
H	-6.81584600	-4.41141900	-0.12168200
H	-4.09106200	-3.26014500	3.00184700
H	-5.77416000	-4.84688900	2.09288800
O	-3.73314200	-0.91485400	-2.07419900
H	-3.17527600	0.29840700	-1.82413700
Au	-0.01458600	0.06996300	-0.29259400
P	2.36417300	0.38259600	0.24367600
C	3.17438100	-1.34677500	0.23156100
C	4.52771000	-1.73327200	0.04609800
C	2.22877400	-2.35771700	0.50398300
C	4.84771300	-3.10144400	0.15251200
C	2.57394200	-3.70140600	0.61638200
H	1.18608100	-2.08372200	0.63030600
C	3.90094800	-4.07900200	0.43871400
H	5.88368600	-3.38954400	0.00419100
H	1.80776000	-4.43944600	0.83294600
H	4.19945300	-5.11999800	0.51458400
C	3.03060500	1.64730600	-1.10624500
C	2.49050300	1.02540800	2.09756700
C	3.12467500	0.85888000	-2.42335200
H	3.40741100	1.54973200	-3.22606300
H	3.87598700	0.07169900	-2.38347700
H	2.16278200	0.41072400	-2.69431900
C	4.36719200	2.31490800	-0.75391500
H	4.65456500	2.97013600	-1.58475600
H	4.28419700	2.94471300	0.13615200
H	5.17341700	1.60109000	-0.60158700
C	1.95874600	2.74345300	-1.28061400
H	1.82231300	3.35270300	-0.38578000
H	2.28612000	3.41090200	-2.08609000
H	0.98871600	2.32627500	-1.56908200
C	1.93590400	2.45618400	2.17874400

H	2.57953500	3.18405900	1.67877900
H	0.92597000	2.53126900	1.76350200
H	1.87939100	2.74599800	3.23441000
C	3.92578500	0.97493200	2.63131100
H	3.93482400	1.36290000	3.65671300
H	4.29501300	-0.05249500	2.66733500
H	4.62004700	1.57621300	2.04161800
C	1.60641000	0.09297900	2.94589800
H	1.94519400	-0.94568800	2.90541700
H	1.65928000	0.41761100	3.99162500
H	0.55733300	0.13047800	2.63564500
C	5.70806200	-0.86916400	-0.29635000
C	6.15107600	-0.80119500	-1.62782500
C	6.50014600	-0.27683600	0.69860400
C	7.31052000	-0.10041100	-1.96300200
H	5.59248900	-1.31729900	-2.40331800
C	7.66261900	0.42190200	0.36510600
H	6.22119100	-0.37974000	1.74053800
C	8.06464100	0.52326600	-0.96754100
H	7.63103000	-0.05530100	-2.99956500
H	8.26113500	0.87362500	1.15065300
H	8.96943300	1.06486800	-1.22584400
<b>33</b>			
C	-4.30553000	-0.72681800	-0.84239100
C	-5.07184800	-0.98424100	0.44377400
C	-5.78436500	0.05048300	1.06811200
C	-5.08654200	-2.26257100	1.01408800
C	-6.48059100	-0.18806600	2.25140500
H	-5.80125100	1.04462300	0.63188600
C	-5.78152300	-2.49766200	2.20216700
H	-4.58624500	-3.08031600	0.50748300
C	-6.47606500	-1.46145900	2.82582900
H	-7.03075000	0.62070600	2.72256600
H	-5.78986000	-3.49542500	2.63046600
H	-7.02130900	-1.64586900	3.74638900
Au	0.03787700	-0.24422300	-0.23579300
C	-5.16948600	-0.15907400	-2.00067700
O	-4.72180900	0.62570900	-2.81719700
O	-6.38805200	-0.67247800	-2.02133500
C	-7.23094400	-0.27611000	-3.13053400
H	-6.77233500	-0.57863300	-4.07377900
H	-8.17478100	-0.79413200	-2.97231300
H	-7.37334400	0.80615000	-3.12388200
P	2.39056900	0.32995200	0.21282900
C	3.34471300	-1.30676500	0.43011500
C	4.72287300	-1.60035100	0.25970600
C	2.49476000	-2.34357700	0.86940000

C	5.16024600	-2.91069500	0.53797600
C	2.95585400	-3.62577000	1.15227500
H	1.43527700	-2.14194200	0.99278900
C	4.30620600	-3.91426300	0.98221900
H	6.21408600	-3.12990200	0.39850600
H	2.26097000	-4.38717700	1.49270000
H	4.69370500	-4.90738100	1.18710200
C	2.92092800	1.44421500	-1.32118100
C	2.45210700	1.24579500	1.95173200
C	3.09214000	0.48416300	-2.50965700
H	3.28443500	1.07555700	-3.41221200
H	3.93113500	-0.19611100	-2.37362600
H	2.18698400	-0.10657200	-2.68713700
C	4.18661700	2.28034900	-1.08774900
H	4.40093200	2.84153800	-2.00494800
H	4.04932400	3.01401400	-0.28854200
H	5.06082000	1.67438400	-0.85971100
C	1.74405900	2.39198500	-1.63264200
H	1.53616800	3.09888200	-0.82832600
H	2.00829600	2.97439000	-2.52266800
H	0.82207200	1.84643500	-1.85797400
C	1.75815300	2.61153100	1.83017500
H	2.32630900	3.31564600	1.21755600
H	0.74433400	2.52897000	1.42611500
H	1.67746600	3.04761700	2.83250600
C	3.88791900	1.41614400	2.45963800
H	3.86254500	1.95971600	3.41148900
H	4.35656900	0.44774400	2.64902700
H	4.51718200	1.98098000	1.76979900
C	1.67033600	0.36418600	2.94230200
H	2.10879200	-0.63203100	3.04415000
H	1.69739800	0.83989500	3.92946300
H	0.62021400	0.25597900	2.65246500
C	5.81803100	-0.69238300	-0.22264000
C	6.25322000	-0.78242600	-1.55558000
C	6.55131700	0.11104500	0.66343400
C	7.34259800	-0.03545700	-2.00604700
H	5.74472700	-1.45660700	-2.23889800
C	7.64395300	0.85636300	0.21466200
H	6.28372700	0.13769500	1.71313200
C	8.03519900	0.79536700	-1.12362900
H	7.65777500	-0.11516500	-3.04212000
H	8.19817400	1.47218900	0.91673700
H	8.88613000	1.37316800	-1.47107400
C	-3.02827800	0.20381300	-0.71018400
C	-1.88385100	-0.69163000	-0.65781900
C	-2.38291300	-2.02585100	-1.03568100
H	-1.80736500	-2.50826500	-1.83524900

H	-2.24597300	-2.65165800	-0.12792300
O	-3.75189900	-1.93467800	-1.39414500
H	-2.89965700	0.50578800	-1.79035300
C	-3.05422600	1.46754000	0.11298600
C	-3.42643500	2.68312300	-0.47829200
C	-2.72710600	1.43955500	1.47743700
C	-3.46212900	3.85308400	0.28222600
H	-3.69423200	2.70769700	-1.53041100
C	-2.76392000	2.61035100	2.23457400
H	-2.46622000	0.49791800	1.95247200
C	-3.12995200	3.81948000	1.63804200
H	-3.75046400	4.78944300	-0.18547100
H	-2.51888300	2.57602700	3.29186600
H	-3.16274100	4.72957100	2.22919400
<b>TS<sub>33-34</sub></b>			
C	4.32927900	-0.59934700	-0.85830500
C	3.07756000	-0.23750100	-0.02099600
C	1.92117900	-0.67535500	-0.68661900
C	2.37333800	-1.27187300	-1.99708500
H	1.90048500	-0.72648700	-2.82359900
H	2.09810400	-2.32971900	-2.08952700
C	3.10944100	0.53181100	1.24533400
C	3.82106800	0.08561700	2.37155800
C	2.42551000	1.75758700	1.29613400
C	3.83629600	0.85634000	3.53261100
H	4.32526800	-0.87419200	2.34952900
C	2.46783900	2.53463900	2.45309100
H	1.88809200	2.10761900	0.42087000
C	3.16882400	2.08336500	3.57297300
H	4.37142200	0.49861200	4.40655300
H	1.95396700	3.49043000	2.47905200
H	3.19547500	2.68565400	4.47580200
C	4.99738800	-1.83402100	-0.19287200
O	4.34724900	-2.59816500	0.50314800
O	6.25755500	-2.00488600	-0.54794200
C	6.89239400	-3.22794000	-0.09742200
H	6.36299800	-4.09192800	-0.50297000
H	7.90974600	-3.17909500	-0.48024500
H	6.88608000	-3.27379500	0.99312600
C	5.22435400	0.60350700	-1.11740600
C	6.13535800	1.04741400	-0.14965300
C	5.10962600	1.30112800	-2.32487300
C	6.91784800	2.17555000	-0.38770900
H	6.24572500	0.51251200	0.78814600
C	5.89607800	2.42988800	-2.56041600
H	4.42603700	0.94270500	-3.08559800
C	6.79929800	2.87094700	-1.59326600

H	7.62527000	2.50711600	0.36609800
H	5.80607400	2.95847800	-3.50448900
H	7.41353400	3.74670600	-1.77888700
O	3.79459800	-1.11316000	-2.08132200
H	2.47939000	-1.41326800	0.22187300
Au	-0.07452500	-0.50490000	-0.16351700
P	-2.46088100	-0.37922300	0.38019400
C	-3.12748600	1.24921300	-0.36087000
C	-4.44568200	1.62572500	-0.72845200
C	-2.10143300	2.20686800	-0.50281100
C	-4.65220400	2.93416400	-1.20933700
C	-2.33479700	3.49722400	-0.96910900
H	-1.08470700	1.93067700	-0.24179700
C	-3.62725400	3.86643500	-1.32764000
H	-5.66198700	3.21219800	-1.49426900
H	-1.50991800	4.19753200	-1.05766200
H	-3.83881000	4.86361700	-1.70093900
C	-3.23001300	-2.03610900	-0.35313000
C	-2.62186100	-0.20404100	2.33150600
C	-3.26948100	-1.84898400	-1.87899300
H	-3.59737800	-2.78823900	-2.33913100
H	-3.96523900	-1.06913400	-2.18485000
H	-2.27895000	-1.61010800	-2.28071500
C	-4.61301100	-2.39628300	0.20657700
H	-4.95421300	-3.31478400	-0.28543200
H	-4.57539000	-2.60323700	1.27972700
H	-5.36032500	-1.62716000	0.02451300
C	-2.24898000	-3.18389100	-0.03608200
H	-2.15450800	-3.38449800	1.03204900
H	-2.63452700	-4.09482100	-0.50811600
H	-1.24985900	-2.99743600	-0.44220000
C	-2.16607900	-1.51337600	2.99454100
H	-2.86676200	-2.33422600	2.82366100
H	-1.17181600	-1.82326500	2.65728900
H	-2.11170800	-1.35402400	4.07760200
C	-4.04926500	0.14794200	2.76405000
H	-4.08311800	0.20023700	3.85866400
H	-4.34502600	1.12678200	2.38022600
H	-4.78530700	-0.59113900	2.44302400
C	-1.67560600	0.93473700	2.75274900
H	-1.94015200	1.88498500	2.28086700
H	-1.75636800	1.07083900	3.83747800
H	-0.63026200	0.70895300	2.52073500
C	-5.69415200	0.79046400	-0.71525400
C	-6.15427700	0.21933500	-1.91357900
C	-6.52016700	0.71740500	0.41626900
C	-7.36866100	-0.46661400	-1.96132500
H	-5.56384700	0.33026400	-2.81854800



C	-7.73742200	0.03413100	0.36912100
H	-6.22376500	1.21456400	1.33227000
C	-8.15941500	-0.57075300	-0.81568500
H	-7.70197300	-0.90596300	-2.89674500
H	-8.36200100	-0.01127700	1.25636600
H	-9.10685700	-1.09967200	-0.85170200
<b>34</b>			
C	3.33437000	0.90941700	-0.47107500
C	2.88854300	-0.57622900	-0.44626800
C	2.58389700	-0.92693100	-1.75334400
C	2.92262900	0.21586700	-2.67799800
H	2.17832800	0.43116100	-3.44929100
H	3.88966000	0.01372200	-3.15952800
C	3.13948300	-1.51140800	0.67148500
C	3.83456700	-1.09641500	1.82252100
C	2.74298200	-2.86243300	0.58149700
C	4.13054100	-2.00303300	2.84057400
H	4.15476700	-0.06668200	1.92901200
C	3.03129800	-3.76045000	1.60226800
H	2.20044800	-3.21391200	-0.29064100
C	3.72982600	-3.33425300	2.73727500
H	4.67612100	-1.66327700	3.71520200
H	2.71794900	-4.79585200	1.51177600
H	3.95935000	-4.03747900	3.53170200
C	4.89951300	0.87952200	-0.42489300
O	5.53846500	0.18859700	-1.18882200
O	5.42696500	1.68907600	0.49527200
C	6.87445900	1.73105900	0.53324000
H	7.26331700	2.08301300	-0.42396800
H	7.12107500	2.42698300	1.33305100
H	7.27339300	0.73634000	0.74132800
C	2.67280800	1.89523900	0.48402800
C	1.83564300	1.50596800	1.53649800
C	2.87637000	3.26553900	0.25433700
C	1.22480100	2.46552900	2.35126800
H	1.65995700	0.45746900	1.74642000
C	2.26316400	4.21917700	1.06214800
H	3.51331500	3.58258500	-0.56403800
C	1.43663500	3.82249000	2.11781800
H	0.58742300	2.14307600	3.16925500
H	2.43405400	5.27418500	0.87069100
H	0.96655300	4.56732700	2.75279000
O	3.00042000	1.34355700	-1.80613600
H	2.54636600	-1.95070600	-2.11041400
Au	0.48826100	-0.54595800	-0.91475000
P	-1.93830100	-0.38191900	-0.78584800
C	-2.43128000	-0.80062500	1.00877900

C	-3.59974400	-0.45303000	1.73538400
C	-1.46906000	-1.61390900	1.64284300
C	-3.72932700	-0.94145000	3.05083200
C	-1.63004000	-2.09480500	2.93875600
H	-0.56363300	-1.88004600	1.10707000
C	-2.77394200	-1.75273000	3.65331300
H	-4.62195100	-0.66668900	3.60379500
H	-0.86138200	-2.72160700	3.37989600
H	-2.92319700	-2.10703400	4.66852000
C	-2.34137000	1.44244600	-1.41002600
C	-2.65268600	-1.82354100	-1.91940200
C	-1.95574800	2.38636600	-0.26050000
H	-2.09123500	3.41933400	-0.60098900
H	-2.58066100	2.24392800	0.61976000
H	-0.90713000	2.26866700	0.02877800
C	-3.80198700	1.63770700	-1.84151400
H	-3.92849300	2.68091800	-2.15351100
H	-4.05946900	1.01312100	-2.70125900
H	-4.51399700	1.44422300	-1.04179700
C	-1.41805000	1.74280300	-2.60884000
H	-1.61023500	1.10317400	-3.47158300
H	-1.60552100	2.77667800	-2.92011000
H	-0.35881500	1.66887900	-2.34398700
C	-2.33152200	-1.51609700	-3.38967800
H	-2.89895100	-0.66491400	-3.77296700
H	-1.26479800	-1.32827100	-3.54879400
H	-2.60591900	-2.38802100	-3.99419000
C	-4.16270200	-2.00162500	-1.72313200
H	-4.51276300	-2.78957100	-2.40008000
H	-4.39115100	-2.32060800	-0.70382900
H	-4.73032500	-1.09613500	-1.94392500
C	-1.93708600	-3.12017800	-1.50052100
H	-2.10910600	-3.36628900	-0.44937400
H	-2.33269100	-3.94574700	-2.10309900
H	-0.85752200	-3.06641700	-1.67424100
C	-4.74569800	0.41527500	1.30089800
C	-4.80480600	1.75051200	1.73381400
C	-5.85859900	-0.11748800	0.63317500
C	-5.91165000	2.54951500	1.44404400
H	-3.98492800	2.15966800	2.31704700
C	-6.96835000	0.68024400	0.34531000
H	-5.87096500	-1.16562400	0.35867900
C	-6.99310000	2.01909300	0.73847000
H	-5.93380200	3.58104000	1.78248200
H	-7.81979700	0.24851800	-0.17227000
H	-7.85725900	2.63768900	0.51677100

C	-3.22377400	1.96375600	0.65900400
C	-2.96180200	3.37433400	0.15080200
C	-1.69558900	3.95301200	0.28986200
C	-3.99278500	4.09988000	-0.46152200
C	-1.45635200	5.24397400	-0.18491000
H	-0.89950100	3.40282300	0.78436500
C	-3.75256500	5.39145700	-0.92687300
H	-4.97825400	3.65680100	-0.55505900
C	-2.48433800	5.96367500	-0.79480000
H	-0.47343100	5.69000600	-0.06704100
H	-4.55652600	5.95360700	-1.39201200
H	-2.30147600	6.96990900	-1.15918700
Au	-0.29659400	0.08000100	-0.26321100
C	-3.26510400	1.02268100	-0.55439600
O	-2.28369200	0.40004400	-1.00272000
O	-4.42088200	0.99176200	-1.16307800
C	-4.54729600	0.17119600	-2.35366200
H	-4.38916200	-0.87657300	-2.09351900
H	-5.56523400	0.33682600	-2.70015100
H	-3.82217400	0.48870600	-3.10451600
P	1.94055900	-0.41972900	0.39722100
C	2.93084600	-0.65647400	-1.21776400
C	4.32542900	-0.54031700	-1.45500600
C	2.10372100	-1.05315900	-2.28934500
C	4.80195400	-0.83123800	-2.74875700
C	2.60365300	-1.34530800	-3.55460000
H	1.03301600	-1.13357800	-2.13264600
C	3.97032100	-1.23238900	-3.78837100
H	5.86840600	-0.73388000	-2.92525100
H	1.92422400	-1.64794100	-4.34509800
H	4.38762800	-1.44683600	-4.76725500
C	2.48461000	1.08249500	1.54592900
C	1.89707800	-2.17151100	1.28917900
C	2.70841900	2.27771400	0.60567000
H	2.91233200	3.16687400	1.21313600
H	3.55875000	2.12701700	-0.05744700
H	1.82234900	2.48394900	-0.00388100
C	3.72628300	0.79401500	2.40173000
H	3.95865300	1.69653600	2.97877400
H	3.54629400	-0.00895000	3.12154300
H	4.60436700	0.54475200	1.81100100
C	1.30394100	1.41079500	2.48144600
H	1.08238400	0.61075700	3.18897200
H	1.57502000	2.29888000	3.06336400
H	0.39063300	1.64079700	1.92520300
C	1.17262600	-2.04071900	2.63749000
H	1.74922000	-1.46943300	3.36885400
H	0.18302400	-1.58481200	2.53331200

H	1.03096900	-3.04534700	3.05174500
C	3.31123000	-2.72904300	1.48937100
H	3.23773700	-3.68701700	2.01698800
H	3.79849700	-2.92063000	0.53079000
H	3.94830600	-2.07048300	2.08251100
C	1.10511800	-3.12070600	0.37270400
H	1.57070700	-3.23088400	-0.61015700
H	1.08167300	-4.11204200	0.83975200
H	0.07131200	-2.78935200	0.23347100
C	5.40404700	-0.10371800	-0.50543900
C	5.88032800	1.21694800	-0.56192800
C	6.08624000	-1.02308300	0.30571400
C	6.95848700	1.62416300	0.22520100
H	5.41409900	1.92402100	-1.24212700
C	7.16702600	-0.61734100	1.09189000
H	5.78855600	-2.06512500	0.30677000
C	7.59827800	0.70975900	1.06382500
H	7.30673300	2.65121300	0.17060200
H	7.68130800	-1.34424200	1.71348200
H	8.44038200	1.02344200	1.67298500
C	-4.50417000	-1.57767100	1.23686700
C	-4.53077600	-0.46567500	1.72462600
C	-4.56655300	0.87221500	2.31867700
H	-5.53005600	1.04967200	2.80560500
H	-3.78382100	0.95823300	3.08825900
O	-4.43299200	1.94799400	1.37884600
C	-2.37861200	1.63224100	1.28010800
C	-4.50687400	-2.88020600	0.64705500
C	-3.45032100	-3.78121200	0.88479200
C	-5.57578700	-3.27973100	-0.18016400
C	-3.46331000	-5.04643600	0.30254000
H	-2.63571200	-3.48311800	1.53737900
C	-5.57860200	-4.54588400	-0.76024500
H	-6.39950600	-2.59380900	-0.35065900
C	-4.52382200	-5.43072600	-0.52227900
H	-2.64891100	-5.73778200	0.49715900
H	-6.40834200	-4.84613700	-1.39281000
H	-4.53165800	-6.41874000	-0.97223700
<b>35</b>			
C	4.76223600	-1.01754000	0.15508900
C	6.22841300	-0.92451700	-0.22267100
C	6.76673900	-1.84321400	-1.13304600
C	7.05100600	0.05349200	0.34281600
C	8.11589500	-1.77474300	-1.47701800
H	6.12468500	-2.60065800	-1.57161900
C	8.40286400	0.11674900	0.00115900
H	6.63664400	0.76613800	1.05127000

C	8.93639500	-0.79643700	-0.90957300
H	8.52810300	-2.48646200	-2.18600600
H	9.03636500	0.88002100	0.44298600
H	9.98750800	-0.74604800	-1.17742000
Au	-0.16463800	0.44006900	-0.40940500
C	4.51875600	-2.28801500	0.98991300
O	3.98262400	-3.29576400	0.58163200
O	4.99753100	-2.12347600	2.23113800
C	4.92254500	-3.28015200	3.09120700
H	5.48577600	-4.10983600	2.65899400
H	5.36252000	-2.96893800	4.03746900
H	3.88299300	-3.58587300	3.22944000
P	-2.59022600	0.31305900	-0.52192000
C	-3.04368500	-1.52211200	-0.27222800
C	-4.25090700	-2.11018900	0.18721400
C	-1.99104100	-2.37840300	-0.65741600
C	-4.32483200	-3.51658700	0.23417500
C	-2.09565900	-3.76518800	-0.61381800
H	-1.05684200	-1.94612300	-1.00205600
C	-3.27757800	-4.34220200	-0.15990200
H	-5.24804100	-3.95995600	0.59352100
H	-1.25642300	-4.37998300	-0.92348700
H	-3.38569000	-5.42103100	-0.10747200
C	-3.21401700	1.55945600	0.86681900
C	-3.10986600	0.78319100	-2.35976900
C	-2.94487900	0.86853100	2.21327400
H	-3.18863400	1.56931400	3.01991500
H	-3.55635400	-0.02173300	2.35098600
H	-1.89120300	0.59001800	2.32084300
C	-4.68859000	1.96285500	0.72261400
H	-4.94559500	2.62237200	1.55974300
H	-4.86740200	2.52757700	-0.19649400
H	-5.36737100	1.11367900	0.74950800
C	-2.34061100	2.82823300	0.78855100
H	-2.45639800	3.37145900	-0.15041300
H	-2.65413000	3.49891500	1.59668900
H	-1.27813300	2.61047600	0.93496400
C	-2.82287500	2.27283000	-2.60083200
H	-3.49331200	2.92572500	-2.03703600
H	-1.78806800	2.53802200	-2.36164100
H	-2.97974900	2.48777700	-3.66394100
C	-4.58534400	0.46589200	-2.62715800
H	-4.82926400	0.77017300	-3.65158800
H	-4.77598000	-0.60680000	-2.55056600
H	-5.26334000	0.99248600	-1.95301200
C	-2.23328800	-0.06386600	-3.29906600
H	-2.38179200	-1.13643600	-3.14838400
H	-2.51009600	0.16582700	-4.33424800

H	-1.16897500	0.16278000	-3.18017300
C	-5.49517600	-1.42682000	0.67761500
C	-5.72738800	-1.32210400	2.05938100
C	-6.52524900	-1.05659000	-0.20001200
C	-6.92385000	-0.79450000	2.54706900
H	-4.97198100	-1.67411200	2.75607500
C	-7.72432300	-0.53130900	0.28690200
H	-6.40164300	-1.20137200	-1.26674300
C	-7.92242400	-0.38670600	1.66085400
H	-7.08024200	-0.71694900	3.61882200
H	-8.50914800	-0.25089000	-0.40927700
H	-8.85589000	0.01904800	2.03852300
C	2.11759700	1.36345000	-0.03738300
C	2.01034400	0.19748600	-0.46271400
C	2.60459300	-1.10176300	-0.92721700
H	2.28665400	-1.91133200	-0.26050600
H	2.22346600	-1.32533200	-1.92734200
O	4.00574700	-1.04001600	-1.05114300
H	4.48978700	-0.15147600	0.77430400
C	2.29033500	2.69570000	0.43068000
C	2.34888400	2.96006300	1.81677600
C	2.44428600	3.75253200	-0.49328700
C	2.55749500	4.25992600	2.26368600
H	2.23751200	2.14253500	2.52186000
C	2.65295100	5.04763900	-0.03224800
H	2.40705700	3.54065800	-1.55680900
C	2.70841800	5.30175600	1.34216000
H	2.60665100	4.46376500	3.32842800
H	2.77660100	5.85966000	-0.74139900
H	2.87293200	6.31471300	1.69651300
<b>TS<sub>35-36</sub></b>			
C	4.72558300	-1.04610000	-0.14751000
C	5.80264500	-0.79647800	-1.15214400
C	5.74542700	-1.45448400	-2.39482700
C	6.85696200	0.09820800	-0.89210400
C	6.73540300	-1.23444800	-3.34714200
H	4.93681800	-2.14617700	-2.59634700
C	7.84022500	0.31475400	-1.85452200
H	6.90336000	0.62450500	0.05297200
C	7.78496400	-0.35029800	-3.08107100
H	6.69093300	-1.75707200	-4.29745000
H	8.65231500	1.00357600	-1.64437600
H	8.55625400	-0.18189700	-3.82634300
Au	-0.12228100	-0.59268100	0.26559300
C	5.09023000	-1.05782400	1.35140900
O	5.00109700	-2.05561500	2.02594300
O	5.47165400	0.14691300	1.79016500

C	5.85820800	0.20930100	3.18646600
H	6.70859900	-0.44993700	3.36929900
H	6.12594400	1.24906200	3.36454600
H	5.02227600	-0.09297300	3.81983000
P	-2.56495200	-0.56506900	0.41693200
C	-3.15173400	1.17060800	-0.12044600
C	-4.40594900	1.60825700	-0.62168800
C	-2.14253700	2.13666900	0.07436500
C	-4.57092200	2.98206300	-0.88802900
C	-2.33619800	3.49004800	-0.18592800
H	-1.17030800	1.81877200	0.43706000
C	-3.56623900	3.91935800	-0.67343500
H	-5.53061800	3.30788000	-1.27666800
H	-1.52535100	4.19176000	-0.01676900
H	-3.74459600	4.96764900	-0.89233800
C	-3.16181100	-2.06214300	-0.71321700
C	-3.03870000	-0.74419700	2.31671700
C	-2.97152900	-1.60117500	-2.16750000
H	-3.20500200	-2.43920700	-2.83433700
H	-3.62966800	-0.77451400	-2.43000800
H	-1.93673700	-1.29959500	-2.36115100
C	-4.60325100	-2.51795300	-0.44743700
H	-4.83999900	-3.33296300	-1.14156100
H	-4.72208700	-2.91412600	0.56474700
H	-5.33596300	-1.72891400	-0.60201200
C	-2.20807100	-3.24661000	-0.45690900
H	-2.27160000	-3.63613700	0.56018900
H	-2.48913000	-4.05801200	-1.13808800
H	-1.16588600	-2.98437900	-0.66334900
C	-2.66267600	-2.15308600	2.80128700
H	-3.30774000	-2.92697500	2.37834400
H	-1.62042400	-2.40151000	2.57734300
H	-2.78366000	-2.19018200	3.89002400
C	-4.52532100	-0.46870300	2.56780400
H	-4.73470300	-0.60955600	3.63484400
H	-4.78115400	0.56333700	2.31773400
H	-5.18169200	-1.13803700	2.00871200
C	-2.19916400	0.29525500	3.08101400
H	-2.40170500	1.31599100	2.74553400
H	-2.45681200	0.23833700	4.14494900
H	-1.12616300	0.10210700	2.98396500
C	-5.61710500	0.78540200	-0.95831200
C	-5.86507000	0.43748300	-2.29675900
C	-6.61024700	0.51192900	-0.00590400
C	-7.03607300	-0.22941300	-2.65950400
H	-5.14187500	0.70744000	-3.06092200
C	-7.78415100	-0.15263800	-0.36791800
H	-6.47737900	0.83777500	1.01892200

C	-7.99513900	-0.53681300	-1.69290600
H	-7.20374400	-0.49522500	-3.69894200
H	-8.53975700	-0.35588600	0.38516600
H	-8.90875000	-1.05177200	-1.97370400
C	2.67335500	0.38316900	0.00773300
C	1.95938300	-0.70084800	0.12505000
C	2.59262700	-2.07702000	0.13276600
H	2.69013300	-2.44526700	1.15970400
H	2.02190600	-2.79667200	-0.45323500
O	3.88876600	-2.04206300	-0.50169400
H	3.94153100	-0.00991400	-0.21435100
C	2.72385400	1.82605100	0.10896500
C	2.32651500	2.46716600	1.30092900
C	3.19177200	2.60042200	-0.97150100
C	2.36416700	3.85575400	1.39024000
H	1.98465300	1.86697700	2.13790600
C	3.23447900	3.98754100	-0.86961400
H	3.51009000	2.10678500	-1.88449500
C	2.81917300	4.61642500	0.30826600
H	2.04787000	4.34637800	2.30563500
H	3.58911000	4.57980900	-1.70712300
H	2.85454000	5.69890100	0.38488200
<b>36</b>			
C	5.02260400	-1.16353200	-0.19681900
C	6.33707600	-1.05058200	-0.77319600
C	6.51024200	-1.30872000	-2.15804300
C	7.46467300	-0.72839500	0.02187800
C	7.77202200	-1.23816600	-2.72309100
H	5.64768600	-1.55937100	-2.76413500
C	8.72504700	-0.66976000	-0.55662900
H	7.34703500	-0.52005800	1.07736300
C	8.88035400	-0.92143900	-1.92388800
H	7.90314900	-1.43119700	-3.78250800
H	9.58814100	-0.42633900	0.05354900
H	9.86854000	-0.87135600	-2.37108100
Au	-0.00887800	-0.36508800	0.08658800
C	4.74878500	-0.97273500	1.29660700
O	4.21199400	-1.84783700	1.93663200
O	5.18792900	0.19554700	1.74578000
C	4.91107100	0.47995700	3.14556300
H	5.35742600	-0.28883700	3.77810700
H	5.35902200	1.45388500	3.32963300
H	3.83172500	0.51118400	3.30290000
P	-2.44190000	-0.57438600	0.43937500
C	-3.25549000	0.99803300	-0.28210100
C	-4.57724100	1.24122300	-0.74099500
C	-2.34275700	2.07302700	-0.30087900

C	-4.90174300	2.54209400	-1.17437600
C	-2.69152400	3.35215300	-0.72455500
H	-1.31977000	1.90518300	0.01785100
C	-3.98863700	3.59138700	-1.16558400
H	-5.91266800	2.71751600	-1.52896600
H	-1.94479600	4.14011000	-0.71600600
H	-4.28927900	4.57678400	-1.50836800
C	-2.94597800	-2.25913000	-0.43680100
C	-2.81228800	-0.53749100	2.36813400
C	-2.87470100	-1.98629700	-1.94880200
H	-3.04449500	-2.92692100	-2.48571400
H	-3.63145400	-1.27511500	-2.27674000
H	-1.89025800	-1.60604500	-2.24114500
C	-4.31822500	-2.81540400	-0.03168800
H	-4.50397300	-3.73065400	-0.60679000
H	-4.34836400	-3.09186500	1.02601200
H	-5.13515900	-2.12683300	-0.23533100
C	-1.86668600	-3.30538400	-0.08797800
H	-1.85144200	-3.56515500	0.97171900
H	-2.09015900	-4.22099500	-0.64804700
H	-0.86509100	-2.97112200	-0.37436100
C	-2.26485600	-1.82057600	3.01270300
H	-2.84237500	-2.70584800	2.73559900
H	-1.21393700	-1.99202700	2.75898900
H	-2.33015600	-1.71918000	4.10236200
C	-4.30477100	-0.37827500	2.67597600
H	-4.44524600	-0.38791300	3.76361000
H	-4.68070900	0.57806900	2.30573300
H	-4.91313900	-1.18045500	2.25374200
C	-2.05090700	0.67412500	2.93533600
H	-2.37750300	1.61418100	2.48234000
H	-2.24516100	0.73869100	4.01252300
H	-0.97049300	0.57481400	2.79201600
C	-5.71333500	0.26760900	-0.88013800
C	-5.99064600	-0.29381200	-2.13784400
C	-6.62447100	0.04143200	0.16238400
C	-7.10290900	-1.11473500	-2.32835500
H	-5.33805200	-0.07002200	-2.97671300
C	-7.73931500	-0.77827100	-0.02685700
H	-6.47458900	0.52353600	1.12117200
C	-7.97550500	-1.36921400	-1.26892500
H	-7.29375200	-1.54331300	-3.30778400
H	-8.43072800	-0.94172300	0.79458800
H	-8.84330500	-2.00501400	-1.41567100
C	2.74111600	0.90834700	-0.49775100
C	2.02060200	-0.21916700	-0.32366500
C	2.59935500	-1.57819900	-0.53638900
H	2.55413500	-2.20898000	0.35128600

H	2.16434000	-2.09950700	-1.39006700
O	4.07250700	-1.57023200	-0.95177700
H	3.75449600	0.84020800	-0.90565200
C	2.33507200	2.30383200	-0.24757200
C	1.43311800	2.67149400	0.76740400
C	2.90350100	3.32560200	-1.02978500
C	1.08491900	4.00748700	0.96490000
H	1.02375200	1.90291500	1.41587800
C	2.55051900	4.66010900	-0.83880800
H	3.61712200	3.06433600	-1.80751100
C	1.63604700	5.00692800	0.15832200
H	0.39476300	4.27181100	1.76130900
H	2.99213500	5.42995100	-1.46465600
H	1.36820900	6.04724600	0.31661300
<b>TS<sub>36-33</sub></b>			
C	4.48535200	1.30405100	-0.17980300
C	5.02658800	0.76090500	1.05891000
C	6.03877200	-0.22974900	1.07790000
C	4.49885700	1.22128800	2.29097300
C	6.50573400	-0.72500200	2.29061300
H	6.44705000	-0.59422800	0.14615800
C	4.98566600	0.73070700	3.49264600
H	3.72925000	1.98348000	2.28359400
C	5.98962700	-0.24738200	3.49748300
H	7.28078600	-1.48460100	2.29356000
H	4.58927300	1.10803800	4.43001600
H	6.36542700	-0.63350900	4.44023000
Au	0.02229300	0.24288500	-0.21299800
C	5.33659800	1.32525100	-1.44438000
O	6.24696600	0.56329200	-1.69009700
O	4.92094600	2.29658100	-2.27263800
C	5.67513700	2.42868300	-3.50066500
H	5.60753900	1.51076000	-4.08873100
H	5.21974200	3.26436200	-4.02901300
H	6.72290400	2.63577200	-3.27633000
P	-2.32379700	-0.38746800	0.21836900
C	-3.28168700	1.22186100	0.58903700
C	-4.66086700	1.52925900	0.45621500
C	-2.42938700	2.21578000	1.11417000
C	-5.09783300	2.80729900	0.85823100
C	-2.88958800	3.46552700	1.51849200
H	-1.36880900	2.00443300	1.20580100
C	-4.24144800	3.76666300	1.38739900
H	-6.15292800	3.03676600	0.74732200
H	-2.19241900	4.19351000	1.92183100
H	-4.62822200	4.73579400	1.68688900
C	-2.87471600	-1.37541500	-1.39383200

C	-2.38071300	-1.44656000	1.87561900
C	-3.03614700	-0.32292900	-2.50317300
H	-3.25407100	-0.83814600	-3.44575100
H	-3.85537500	0.36658100	-2.30519500
H	-2.11724300	0.25576500	-2.64541500
C	-4.14897700	-2.21327300	-1.22290500
H	-4.37607100	-2.69346600	-2.18219900
H	-4.01440000	-3.01336000	-0.48934100
H	-5.01429600	-1.61950200	-0.93724800
C	-1.71063800	-2.30974600	-1.78333300
H	-1.52611000	-3.09362000	-1.04764900
H	-1.97663800	-2.80097300	-2.72647300
H	-0.77677100	-1.76328400	-1.94583900
C	-1.71088700	-2.80712200	1.63023000
H	-2.30272100	-3.45037600	0.97512000
H	-0.70648800	-2.70534100	1.20761600
H	-1.61499100	-3.32517600	2.59156500
C	-3.81292700	-1.63802100	2.38593600
H	-3.78496200	-2.24494300	3.29875400
H	-4.27028000	-0.67989200	2.64378900
H	-4.45375400	-2.14932900	1.66526700
C	-1.57298300	-0.66531800	2.92780300
H	-1.99867000	0.32194600	3.12598400
H	-1.58935800	-1.22711600	3.86905900
H	-0.52697500	-0.53946300	2.62979200
C	-5.75958300	0.66986900	-0.10135500
C	-6.19430600	0.87364200	-1.42163000
C	-6.49567200	-0.20279800	0.71403800
C	-7.28743800	0.17261900	-1.93272900
H	-5.68222000	1.60018500	-2.04600000
C	-7.59187300	-0.90252500	0.20480400
H	-6.22621700	-0.32062100	1.75706300
C	-7.98372400	-0.72650400	-1.12313900
H	-7.60249100	0.34087100	-2.95822400
H	-8.14803100	-1.57370000	0.85255400
H	-8.83735800	-1.26913000	-1.51754300
C	2.97928500	-0.05778300	-1.03546000
C	1.93087400	0.77935400	-0.65620300
C	2.34473800	2.23953500	-0.62752800
H	2.32138300	2.63850200	-1.65626100
H	1.68819500	2.85675900	-0.01378400
O	3.64116700	2.36382500	-0.03111800
H	3.45574300	0.28689200	-1.95477300
C	3.12868700	-1.49417300	-0.77920600
C	3.82110600	-2.29521100	-1.70555500
C	2.64810800	-2.08724000	0.40377900
C	3.99170900	-3.65865600	-1.47667300
H	4.22254000	-1.84525300	-2.60971400

C	2.82250100	-3.45052500	0.63080900
H	2.15069200	-1.47172800	1.14774300
C	3.48923600	-4.24041100	-0.31018600
H	4.51948000	-4.26605300	-2.20529700
H	2.45088200	-3.89678200	1.54847400
H	3.62703200	-5.30200800	-0.12923700
TS <sub>8-37</sub>			
C	3.46071500	0.77573400	0.20939600
C	4.73511400	1.52612400	-0.09229200
C	4.97326400	1.81674300	-1.44364500
C	5.61444500	1.99165300	0.89028600
C	6.09459900	2.55938400	-1.80851000
H	4.28347600	1.45562400	-2.19506500
C	6.73708200	2.73399300	0.51577100
H	5.42973100	1.75834800	1.93188800
C	6.97922900	3.01873700	-0.82918400
H	6.27686100	2.77707100	-2.85630000
H	7.42149500	3.08862100	1.28009100
H	7.85362400	3.59543400	-1.11434700
Au	0.12675800	-0.69058400	0.52256300
C	2.28342400	1.76768300	0.18322400
O	1.81357500	2.29537400	1.17414700
O	1.97720300	2.06051000	-1.07336900
C	1.02761400	3.13440600	-1.28160300
H	1.32404500	4.01117900	-0.70361900
H	1.06387000	3.34161700	-2.34975500
H	0.03042900	2.81042200	-0.98184200
P	-2.34690000	-0.65618000	0.41966800
C	-2.89515600	1.17499300	0.36518500
C	-4.08433500	1.78193700	-0.11763500
C	-1.93241900	2.00026600	0.98558100
C	-4.23944100	3.17247600	0.05952100
C	-2.10581300	3.37352400	1.13728300
H	-1.01077400	1.56190600	1.35264100
C	-3.27431000	3.96666800	0.66864500
H	-5.15293800	3.62963300	-0.30772700
H	-1.33022300	3.96198400	1.61762000
H	-3.43963900	5.03409900	0.77916400
C	-2.79879300	-1.73563900	-1.15552400
C	-3.05367000	-1.37555900	2.10341400
C	-2.38711300	-0.88342400	-2.36708400
H	-2.60259300	-1.44361100	-3.28417700
H	-2.93248400	0.05825900	-2.41874200
H	-1.31371600	-0.66634300	-2.35093500
C	-4.27291400	-2.17351300	-1.23691200
H	-4.42262100	-2.71379300	-2.17849200
H	-4.53805900	-2.85975400	-0.42811500

H	-4.94995400	-1.32388000	-1.22061100
C	-1.92192300	-3.01400900	-1.12784400
H	-2.22125500	-3.72250500	-0.35292100
H	-2.03682000	-3.50922700	-2.09855700
H	-0.85911600	-2.78987800	-0.99260900
C	-2.74717900	-2.88018200	2.17419000
H	-3.36625400	-3.46764500	1.49120700
H	-1.69430300	-3.09569800	1.96316800
H	-2.95639100	-3.23584400	3.18954000
C	-4.56059100	-1.13087000	2.24984500
H	-4.90602200	-1.59179000	3.18268200
H	-4.77774900	-0.06136800	2.30965500
H	-5.14518800	-1.55758800	1.43302500
C	-2.32228600	-0.64941000	3.24891900
H	-2.48394400	0.43281000	3.21865700
H	-2.71680900	-1.01613900	4.20359200
H	-1.24509300	-0.84225400	3.23448900
C	-5.23034800	1.13646900	-0.84402500
C	-5.27753300	1.18645900	-2.24643500
C	-6.34817600	0.63734600	-0.15869500
C	-6.37591100	0.68340900	-2.94561200
H	-4.45536700	1.63889500	-2.79332100
C	-7.44748400	0.13312300	-0.85579500
H	-6.36947000	0.66389200	0.92487200
C	-7.45906400	0.14198900	-2.25188200
H	-6.38909000	0.72655200	-4.03060600
H	-8.30110400	-0.25226400	-0.30614100
H	-8.31537200	-0.24811700	-2.79348200
C	3.22801700	-0.59832800	-0.22549100
C	2.13397200	-1.02824700	0.61628900
C	2.81196200	-1.22840600	1.89124700
H	2.22509400	-1.28395000	2.80334400
H	3.75815900	-1.76100500	1.93777100
O	3.48505500	0.39238600	1.95014800
H	2.80146800	1.02573000	2.27665700
C	4.20525000	-1.56755000	-0.65974400
C	5.61391400	-1.39517800	-0.73567300
C	3.66633500	-2.82933700	-1.03550200
C	6.42404900	-2.44112500	-1.14703600
H	6.06562400	-0.46024900	-0.43322100
C	4.49256200	-3.87791300	-1.43014400
H	2.58806500	-2.94651700	-1.05983600
C	5.87189900	-3.68540200	-1.49315000
H	7.49972400	-2.30013400	-1.18625500
H	4.05929100	-4.83156800	-1.71457300
H	6.52044600	-4.49243200	-1.81998100

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C	3.19117200	1.01222100	-0.01799000
C	4.24722100	2.00081100	-0.23647300
C	5.27129900	1.80570300	-1.19323400
C	4.21694200	3.22425600	0.47821000
C	6.21478700	2.79813300	-1.42638800
H	5.30202300	0.89454900	-1.77489400
C	5.18875800	4.19320000	0.26706400
H	3.45413300	3.38895600	1.23171000
C	6.18659100	3.98690100	-0.69066900
H	6.97808400	2.64370200	-2.18215700
H	5.16782000	5.11168300	0.84455200
H	6.93768200	4.75113600	-0.86545900
Au	0.22445300	-0.91032900	0.11986900
C	1.87866300	1.66562300	0.36684400
O	1.52009200	1.77411100	1.52093400
O	1.29612100	2.23316600	-0.69121200
C	0.17304800	3.10658300	-0.41172800
H	0.49528000	3.92338000	0.23765000
H	-0.13766100	3.48772400	-1.38273500
H	-0.63334300	2.55287700	0.06937400
P	-2.23893200	-0.80536800	-0.03182700
C	-2.84001400	0.67090700	1.01945200
C	-4.04162500	1.42574800	0.96211300
C	-1.91440300	0.97416400	2.04043300
C	-4.24197400	2.42858000	1.93125000
C	-2.14352200	1.96256000	2.99404500
H	-0.97874700	0.42759500	2.09068800
C	-3.32264300	2.69857800	2.93999700
H	-5.16064600	3.00446000	1.87805200
H	-1.39718400	2.15321500	3.75863100
H	-3.52708800	3.47813900	3.66748200
C	-2.64840800	-0.72412200	-1.95313000
C	-2.93240800	-2.41233400	0.87421300
C	-2.28915700	0.70044500	-2.40741400
H	-2.42720600	0.76940600	-3.49268100
H	-2.92324800	1.45584900	-1.94483400
H	-1.24171400	0.93404200	-2.19023600
C	-4.09627000	-1.08229700	-2.31413100
H	-4.21821700	-0.97600200	-3.39859200
H	-4.33123700	-2.12080800	-2.06572600
H	-4.82731100	-0.43627500	-1.83357900
C	-1.69729800	-1.70365300	-2.67257800
H	-1.88549900	-2.74736000	-2.41629500
H	-1.85824500	-1.59789400	-3.75177200
H	-0.64550300	-1.47879600	-2.46954800
C	-2.60155600	-3.65651800	0.03571500
H	-3.16851300	-3.69824600	-0.89711000
H	-1.53430600	-3.72461000	-0.19649900

H	-2.86636900	-4.54681300	0.61744400
C	-4.44232500	-2.32449800	1.12094800
H	-4.77145800	-3.24531500	1.61690000
H	-4.68484200	-1.49137600	1.78461200
H	-5.01829100	-2.21916700	0.19939300
C	-2.20120500	-2.50548800	2.22584300
H	-2.38464100	-1.62978600	2.85395700
H	-2.57940800	-3.38175900	2.76526800
H	-1.12116100	-2.62987700	2.10182600
C	-5.15861200	1.32709100	-0.03769900
C	-5.21112100	2.22897200	-1.11330500
C	-6.25652300	0.47916100	0.17283000
C	-6.29429900	2.23393300	-1.99339600
H	-4.40541300	2.94467400	-1.24969100
C	-7.34226200	0.48448300	-0.70555600
H	-6.27318500	-0.17456300	1.03701000
C	-7.35916800	1.35284300	-1.79808800
H	-6.31163700	2.93580700	-2.82185900
H	-8.18125300	-0.18114200	-0.52568100
H	-8.20458300	1.35789000	-2.47920600
C	3.35185200	-0.37748700	-0.01957700
C	2.24612300	-1.24884100	0.20702600
C	2.59023300	-2.67421200	0.53737800
H	3.20920900	-3.10560800	-0.26407000
H	3.24672900	-2.66220900	1.42096800
O	1.49781800	-3.51186800	0.85735500
H	1.06133400	-3.77468200	0.03667500
C	4.73506200	-0.96869100	-0.11459300
C	5.62404000	-0.85813500	0.96438200
C	5.13799200	-1.67373600	-1.26055800
C	6.89226300	-1.43803500	0.89645800
H	5.32350600	-0.31518900	1.85617900
C	6.40866600	-2.24558100	-1.32896400
H	4.45996400	-1.76080200	-2.10652500
C	7.28760300	-2.13026900	-0.24912000
H	7.57020500	-1.34727900	1.73959600
H	6.71175500	-2.78010600	-2.22411200
H	8.27503300	-2.57817400	-0.30122800
<b>38</b>			
C	3.85847100	0.47204400	0.23381700
C	5.01959500	-0.37131300	0.41982400
C	5.77221100	-0.77251200	-0.71202600
C	5.47290700	-0.75878900	1.70462000
C	6.93003800	-1.52698700	-0.56318900
H	5.45304400	-0.45081900	-1.69879200
C	6.62014300	-1.52762900	1.84378700
H	4.91068400	-0.46637900	2.58490400

C	7.35357900	-1.90898400	0.71320600
H	7.50731700	-1.81042100	-1.43730800
H	6.95037000	-1.83028000	2.83215900
H	8.25762700	-2.49865200	0.82954200
Au	0.25299600	-0.88097400	-0.57462100
C	3.49584300	1.47081700	1.31189800
O	2.35889800	1.65040700	1.70010100
O	4.57431500	2.10278300	1.79504000
C	4.31864000	3.06892100	2.84067900
H	3.85762500	2.58106300	3.70197600
H	5.29395000	3.47632700	3.10092900
H	3.65503700	3.85399500	2.47225500
P	-2.10912800	-0.89624000	0.09430900
C	-2.43727200	0.80320100	0.89951300
C	-3.65126900	1.51400500	1.09095000
C	-1.24786300	1.37347500	1.39954700
C	-3.59737000	2.74609000	1.77212700
C	-1.22471000	2.58749800	2.08000000
H	-0.30033400	0.86540700	1.25376800
C	-2.41418700	3.28324800	2.26905500
H	-4.52848900	3.28704100	1.90923600
H	-0.27695500	2.97367000	2.44079900
H	-2.42735200	4.23552700	2.79053200
C	-3.13479600	-1.29472100	-1.53403900
C	-2.29663900	-2.23423100	1.52497900
C	-3.10285800	-0.01661300	-2.38815000
H	-3.57726300	-0.22749500	-3.35345000
H	-3.64475300	0.80572200	-1.92364000
H	-2.07605400	0.30861400	-2.58564400
C	-4.57528600	-1.76091300	-1.27928500
H	-5.06044000	-1.92687200	-2.24849400
H	-4.60673700	-2.71156000	-0.73960500
H	-5.16832600	-1.03037800	-0.73330000
C	-2.37810600	-2.40142100	-2.29734900
H	-2.34421300	-3.34752000	-1.75488100
H	-2.90533700	-2.58292700	-3.24101300
H	-1.35319000	-2.10378000	-2.54095000
C	-2.12180500	-3.63963700	0.93024300
H	-2.95227400	-3.92628800	0.28073200
H	-1.18521300	-3.73681400	0.37271200
H	-2.08847400	-4.36291900	1.75299100
C	-3.64400200	-2.11873000	2.24551400
H	-3.70013300	-2.89942100	3.01338300
H	-3.73559000	-1.15492200	2.75119100
H	-4.49745600	-2.24686200	1.57682100
C	-1.16222900	-1.96386200	2.53002900
H	-1.22508900	-0.96140500	2.96176800
H	-1.24637200	-2.68511700	3.35124500



H	-0.17510300	-2.08752300	2.07417300
C	-5.03071600	1.14790500	0.62217900
C	-5.54962000	1.75245200	-0.53512400
C	-5.89199600	0.36255400	1.40305400
C	-6.86541300	1.52089500	-0.93841100
H	-4.92098000	2.42419800	-1.11266600
C	-7.21022400	0.13226400	1.00275600
H	-5.54029200	-0.05361500	2.33975900
C	-7.69758000	0.70003500	-0.17532400
H	-7.24299400	1.99387500	-1.84009100
H	-7.85970400	-0.47945300	1.62197100
H	-8.72299100	0.52211300	-0.48452000
C	2.93658500	0.40161100	-0.85833000
C	2.31091100	-0.86051300	-0.88834400
C	2.96260100	-2.20940300	-0.85183100
H	3.34456300	-2.36797400	-1.87819400
H	3.84441700	-2.24744800	-0.20429700
O	2.13542800	-3.27444300	-0.43577800
H	1.37700500	-3.32979600	-1.03368900
C	2.47135200	1.62987100	-1.52683800
C	3.29451400	2.77324700	-1.45562800
C	1.32480600	1.69058300	-2.34399000
C	2.95173200	3.94852300	-2.11849000
H	4.22601200	2.73278200	-0.89889100
C	0.98986400	2.86158700	-3.01482700
H	0.69089000	0.81666400	-2.45078800
C	1.79411100	3.99961100	-2.89657900
H	3.60003500	4.81610900	-2.04610900
H	0.10017300	2.88822500	-3.63642400
H	1.53073300	4.91078900	-3.42472600
<b>TS<sub>38-39</sub></b>			
C	3.69375800	0.21712500	0.34839400
C	5.02745200	-0.35708400	0.10079000
C	5.83743800	0.19532300	-0.91257000
C	5.51819500	-1.45346000	0.83922000
C	7.10438500	-0.32462500	-1.17217800
H	5.47973800	1.05180800	-1.47683200
C	6.78452200	-1.96458900	0.57893600
H	4.90142000	-1.90058900	1.60991400
C	7.58097900	-1.40313000	-0.42551100
H	7.72107300	0.11856400	-1.94779800
H	7.15193400	-2.80820900	1.15467000
H	8.56961000	-1.80601400	-0.62267800
Au	0.33999600	-0.59121400	-0.50471000
C	3.15886100	0.45223300	1.72748800
O	1.99003900	0.71863500	1.95877900
O	4.10136000	0.34903800	2.67278900

C	3.65841800	0.55203400	4.03183100
H	2.91234500	-0.19777800	4.30391600
H	4.55242600	0.44697600	4.64423600
H	3.22615400	1.54840900	4.14480000
P	-2.03717600	-0.87040600	0.00281100
C	-2.58074200	0.73209100	0.88562100
C	-3.86527300	1.32383400	1.00879900
C	-1.49329700	1.35406500	1.53491200
C	-3.98148400	2.50085500	1.77420100
C	-1.64186500	2.50927800	2.29768000
H	-0.49710300	0.93247300	1.44857500
C	-2.89936400	3.09165700	2.41807800
H	-4.96538900	2.95140000	1.85922800
H	-0.77336500	2.94383100	2.78245200
H	-3.04195700	3.99603000	3.00170700
C	-2.89282200	-1.24814200	-1.72758700
C	-2.20571200	-2.31303400	1.32864700
C	-2.90215000	0.08076100	-2.50060500
H	-3.28596600	-0.10384200	-3.51060000
H	-3.54175900	0.82808500	-2.03355500
H	-1.89258300	0.49409500	-2.59744400
C	-4.30334500	-1.84399000	-1.61729200
H	-4.69430500	-1.99325200	-2.63061200
H	-4.29367300	-2.82308600	-1.13040200
H	-4.99806100	-1.19716300	-1.08598400
C	-1.98815700	-2.23897700	-2.48901400
H	-1.92049900	-3.21541400	-2.00652700
H	-2.42105000	-2.39466600	-3.48385400
H	-0.97531500	-1.84649400	-2.62314100
C	-1.85853900	-3.65554000	0.66827000
H	-2.60536400	-3.96839000	-0.06513400
H	-0.87702200	-3.63495500	0.18421100
H	-1.82358200	-4.42684100	1.44603500
C	-3.61109200	-2.36432400	1.93875900
H	-3.65549200	-3.19861600	2.64877200
H	-3.83141900	-1.45003100	2.49427000
H	-4.39294100	-2.51927100	1.19303200
C	-1.18400900	-2.01465200	2.44079100
H	-1.37742500	-1.05761800	2.93202800
H	-1.26005300	-2.80076800	3.20103200
H	-0.15636400	-2.00699400	2.06450100
C	-5.16177000	0.87846900	0.39463100
C	-5.63492200	1.51836900	-0.76306500
C	-6.01064600	-0.02935300	1.04565700
C	-6.88728700	1.20704500	-1.29449900
H	-5.02308800	2.27938400	-1.23892700
C	-7.26558100	-0.33975600	0.51692100
H	-5.70037200	-0.48055900	1.98083900

C	-7.70278800	0.26759000	-0.66119000
H	-7.23025000	1.70944300	-2.19406800
H	-7.90671700	-1.04609800	1.03595700
H	-8.67923900	0.02702600	-1.07027900
C	2.91661900	0.79830100	-0.72375100
C	2.41525000	-0.46693500	-0.93635100
C	2.97547100	-1.74502000	-1.53796100
H	2.63542800	-1.74081600	-2.58687000
H	4.06702300	-1.74027000	-1.54452500
O	2.58498800	-2.91600200	-0.86015500
H	1.61854900	-2.97000300	-0.88253400
C	2.51476200	2.14965900	-1.00108300
C	3.17251300	3.21011700	-0.34164000
C	1.54404000	2.43811700	-1.98637900
C	2.85281900	4.52771100	-0.64724400
H	3.93884100	2.98665700	0.39444500
C	1.23280200	3.75578600	-2.28934400
H	1.04298000	1.62015400	-2.49519200
C	1.88340300	4.80063200	-1.61799900
H	3.35913600	5.34213800	-0.13957000
H	0.48811200	3.97892200	-3.04652600
H	1.63742000	5.83035600	-1.85915300
<b>39</b>			
C	3.45557500	-0.24909100	0.27234800
C	4.95328400	-0.17573100	0.07260200
C	5.69179500	0.96701100	0.40533400
C	5.62193900	-1.28909500	-0.46052400
C	7.07283800	0.99825000	0.20621800
H	5.19265200	1.83538000	0.82311200
C	7.00247200	-1.25625100	-0.65677900
H	5.05821600	-2.18223500	-0.71682800
C	7.73074100	-0.11207700	-0.32476700
H	7.63402000	1.89000700	0.46877500
H	7.50809900	-2.12430200	-1.06886300
H	8.80521900	-0.08642600	-0.47841900
Au	0.38759600	-0.40888800	-0.34829300
C	2.96374500	-0.91314400	1.54248200
O	1.78618500	-1.11942900	1.80728300
O	3.96184800	-1.24355300	2.35429400
C	3.60255900	-1.89678100	3.59210600
H	3.07989300	-2.83294100	3.38609100
H	4.54643900	-2.08509900	4.10043200
H	2.96255200	-1.24600800	4.19147800
P	-2.01819200	-0.74535600	-0.30563100
C	-2.63379400	0.14045900	1.27071800
C	-3.90917200	0.68287400	1.57598800
C	-1.62842000	0.19936100	2.25899100

C	-4.09611700	1.25759500	2.84893500
C	-1.84821400	0.75872300	3.51457800
H	-0.64356700	-0.20428700	2.04982500
C	-3.09515000	1.29828100	3.81323200
H	-5.07199200	1.67638500	3.07347800
H	-1.04368000	0.77398600	4.24313900
H	-3.29107900	1.74739000	4.78197600
C	-2.67609400	-0.04497100	-2.02580700
C	-2.34762600	-2.66503400	-0.02273600
C	-2.58164300	1.48616700	-1.93196800
H	-2.85359000	1.91231900	-2.90457400
H	-3.26120000	1.89902300	-1.18830100
H	-1.56317200	1.81274500	-1.69693600
C	-4.09694600	-0.50427700	-2.38345900
H	-4.37894000	-0.03613200	-3.33365800
H	-4.14842800	-1.58642300	-2.53139700
H	-4.83778600	-0.21797800	-1.64050900
C	-1.70532200	-0.51981100	-3.12531800
H	-1.70980900	-1.60197700	-3.26365600
H	-2.02184600	-0.06692500	-4.07181900
H	-0.67879200	-0.19824200	-2.92574900
C	-1.95051500	-3.44328500	-1.28597500
H	-2.61765200	-3.24592900	-2.12817400
H	-0.92258700	-3.23038200	-1.59706600
H	-2.01064700	-4.51531100	-1.06728500
C	-3.81465300	-2.93547000	0.33219200
H	-3.95127400	-4.01588800	0.45801000
H	-4.08449100	-2.45943800	1.27766400
H	-4.50825600	-2.60029800	-0.44102600
C	-1.45547800	-3.10371800	1.15187600
H	-1.69940000	-2.57111400	2.07461800
H	-1.62284600	-4.17179600	1.33266400
H	-0.39131200	-2.95823100	0.94379100
C	-5.12866800	0.75572800	0.70260400
C	-5.45343100	1.96329600	0.06234600
C	-6.05975400	-0.29295100	0.65623000
C	-6.63925700	2.09427900	-0.66192600
H	-4.77963100	2.81103500	0.14843600
C	-7.24866100	-0.16175900	-0.06495600
H	-5.86731000	-1.20814400	1.20377300
C	-7.53645000	1.02747100	-0.73644400
H	-6.86754900	3.03469800	-1.15457200
H	-7.95615000	-0.98531000	-0.08791700
H	-8.46181800	1.12962900	-1.29491600
C	2.60675400	0.82335400	-0.38510600
C	2.59607100	-0.37249900	-0.99805100
C	2.77597200	-1.08525200	-2.31018400
H	2.11635200	-0.64091700	-3.06820900

H	3.81210500	-0.92213500	-2.62745900
O	2.61446400	-2.48422400	-2.20270000
H	1.70142700	-2.66519500	-1.94071100
C	2.40391700	2.25293300	-0.41749800
C	2.61836900	3.02060300	0.74335100
C	1.99562000	2.89008800	-1.60777600
C	2.43244900	4.39968300	0.71253700
H	2.92510800	2.52776400	1.66078500
C	1.81659500	4.26843100	-1.63182400
H	1.83693400	2.29983700	-2.50515800
C	2.03316900	5.02347000	-0.47299000
H	2.59953400	4.98891000	1.60839300
H	1.51500700	4.75915700	-2.55169600
H	1.89310100	6.09978200	-0.49645300
<b>TS</b> <sub>38-40</sub>			
C	4.20009500	-0.14786400	0.64487800
C	5.34731600	-0.71843700	0.03340000
C	5.62726200	-0.42064000	-1.33282500
C	6.27113900	-1.52510600	0.75678500
C	6.77038300	-0.91400100	-1.93947100
H	4.95289900	0.23021700	-1.87676800
C	7.40547700	-2.01575700	0.13916700
H	6.07640400	-1.76724800	1.79475400
C	7.65727700	-1.71268300	-1.20848400
H	6.98661200	-0.66824600	-2.97377600
H	8.10261600	-2.63496800	0.69384700
H	8.55718500	-2.09190500	-1.68367200
Au	0.13302900	-0.09536900	-0.64788100
C	4.04808900	-0.18214200	2.15118200
O	3.07421800	-0.67826500	2.67246900
O	5.08952000	0.35278400	2.80029200
C	4.99576300	0.34114900	4.24808800
H	4.90302700	-0.68405300	4.61099600
H	5.91929400	0.79820500	4.59815600
H	4.12735700	0.91912100	4.57041600
P	-2.32779900	0.10736600	-0.63526100
C	-3.01002400	-1.43532800	0.26865800
C	-4.26785700	-1.67251400	0.88426000
C	-2.08501900	-2.49926200	0.23095000
C	-4.52308600	-2.95796300	1.40194400
C	-2.36455600	-3.76250700	0.74400700
H	-1.10949700	-2.32648300	-0.21168500
C	-3.60164200	-3.99732200	1.33444200
H	-5.48541600	-3.12828600	1.87440500
H	-1.61523900	-4.54607600	0.68716700
H	-3.84785700	-4.97099800	1.74674500
C	-2.76719900	1.83438400	0.19091100

C	-2.93834100	-0.06285800	-2.49826800
C	-2.49673600	1.66760700	1.69573500
H	-2.64203200	2.63643200	2.18791200
H	-3.17437000	0.95378400	2.16181900
H	-1.46667500	1.34839600	1.88599000
C	-4.19666800	2.32680200	-0.07434300
H	-4.32875900	3.28823600	0.43609100
H	-4.37326600	2.50179600	-1.13904500
H	-4.95945600	1.64756700	0.29885400
C	-1.77284400	2.87455000	-0.36004500
H	-1.89052900	3.05266300	-1.43025300
H	-1.96259400	3.82475400	0.15293800
H	-0.73537900	2.59460200	-0.16507700
C	-2.51490700	1.18580200	-3.28763300
H	-3.07988800	2.07511800	-2.99788000
H	-1.44617700	1.39737400	-3.18216900
H	-2.71232200	1.00869000	-4.35129000
C	-4.45356300	-0.27166400	-2.59785600
H	-4.73170100	-0.33966800	-3.65641200
H	-4.75261700	-1.20721600	-2.12003800
H	-5.02567400	0.54531800	-2.15462300
C	-2.22603500	-1.29556600	-3.08464500
H	-2.45235900	-2.20753800	-2.52553500
H	-2.57247700	-1.44397600	-4.11417500
H	-1.14005900	-1.16257800	-3.10937300
C	-5.39428200	-0.70607000	1.11935700
C	-5.50964700	-0.07314700	2.36833500
C	-6.44452000	-0.55941200	0.20094700
C	-6.60461100	0.74075300	2.66165100
H	-4.74423000	-0.23608300	3.12136300
C	-7.54188800	0.25343900	0.49357800
H	-6.41503500	-1.09654300	-0.73975900
C	-7.61956200	0.91603100	1.71946900
H	-6.67025900	1.22544500	3.63122800
H	-8.34263100	0.35587800	-0.23288700
H	-8.47397000	1.54613800	1.94698700
C	3.07511800	0.40926500	-0.09495300
C	2.18821000	-0.51752200	-0.60846200
C	2.34805100	-1.99767800	-0.84660700
H	1.75627300	-2.49810900	-0.06105000
H	1.82443400	-2.20152300	-1.79515000
O	3.66114600	-2.53272400	-0.89119100
H	3.57722400	-3.47446700	-1.09012000
C	2.81683600	1.87259100	-0.03369200
C	3.35517700	2.69800300	0.96987700
C	2.11502200	2.48612900	-1.08854400
C	3.14111300	4.07540200	0.95353500
H	3.96102400	2.28072400	1.76574500

C	1.92303200	3.86630200	-1.11547900
H	1.74494500	1.87602200	-1.90635100
C	2.42216700	4.66712800	-0.08653400
H	3.55465300	4.68962200	1.74765300
H	1.39372800	4.31740800	-1.94954700
H	2.27417200	5.74236300	-0.10738000
<b>40</b>			
C	-2.23312800	-0.73766400	-0.78327600
C	-2.79664200	-1.94794700	-1.45479100
H	-2.45641500	-2.84143200	-0.90247600
H	-2.23751900	-1.97820400	-2.40966500
C	-3.00016600	0.42447800	-0.49246500
C	-2.31190100	1.75301500	-0.63540400
C	-1.72933800	2.11951900	-1.85996000
C	-2.24464500	2.64789100	0.44473100
C	-1.09730100	3.35473100	-2.00152500
H	-1.79880500	1.44633300	-2.70917400
C	-1.60068900	3.87844300	0.30360600
H	-2.69245800	2.37851300	1.39626800
C	-1.02786200	4.23478000	-0.91861400
H	-0.66809500	3.63367700	-2.95909900
H	-1.54982700	4.55883500	1.14835300
H	-0.53646400	5.19657000	-1.02958100
C	-4.32753400	0.41627200	-0.05293300
C	-5.15025300	1.67810500	-0.21380400
O	-5.52887400	2.05667800	-1.29880300
O	-5.43981400	2.25098100	0.95908000
C	-6.23335900	3.46063300	0.88356400
H	-6.36222800	3.78553200	1.91440400
H	-5.70731500	4.21752000	0.29830700
H	-7.19828000	3.24941600	0.41887000
C	-4.97015400	-0.69299700	0.61595000
C	-4.21674500	-1.60780100	1.38730300
C	-6.37355600	-0.86401100	0.53451500
C	-4.83722000	-2.68668400	2.00729400
H	-3.15916000	-1.42354400	1.54673700
C	-6.98236900	-1.95032800	1.14298000
H	-6.96552200	-0.17077200	-0.05466300
C	-6.21674300	-2.86571400	1.87897600
H	-4.25337200	-3.37269900	2.61292300
H	-8.05468100	-2.09009800	1.05149100
H	-6.70258200	-3.70263100	2.37131500
O	-4.18319400	-1.95206000	-1.68770800
P	2.25165000	-0.83204300	-0.19938800
C	3.01784000	-0.23304200	-1.90789300
C	2.71918000	-2.67785500	0.29075800
C	2.47015300	-3.59787700	-0.91470200

H	3.19170400	-3.43645500	-1.71907300
H	2.57776000	-4.63840900	-0.58718000
H	1.45967400	-3.48218000	-1.31950200
C	4.16869900	-2.80736900	0.77110900
H	4.32949700	-2.23993000	1.69029800
H	4.37313300	-3.86094800	0.99600100
H	4.89475700	-2.47859000	0.02519500
C	1.77263000	-3.07823900	1.43687100
H	0.72389200	-3.05241600	1.12419500
H	2.00871200	-4.10316800	1.74591300
H	1.88968100	-2.43316100	2.31188700
C	4.49432500	-0.59965200	-2.11018100
H	4.63892700	-1.68219400	-2.16658100
H	4.82537600	-0.18185100	-3.06842100
H	5.14347000	-0.20091100	-1.33365500
C	2.18704800	-0.87445500	-3.03866100
H	1.12633600	-0.61460500	-2.96788900
H	2.56207400	-0.48764000	-3.99331800
H	2.27484000	-1.96160400	-3.06952600
C	2.80119800	1.28869900	-1.96026900
H	1.74650300	1.55151500	-1.82891800
H	3.38604400	1.81661000	-1.20854900
H	3.11685400	1.65392800	-2.94461900
C	2.68161800	0.23928000	1.32006000
C	3.90005600	0.85852700	1.70505900
C	1.57850100	0.35101200	2.19198600
C	3.93951000	1.53522000	2.94028500
C	1.64781900	1.01564700	3.41298200
H	0.63232100	-0.09490900	1.90244200
C	2.84429500	1.61416200	3.79382800
H	4.87330600	2.00961400	3.22527500
H	0.77023900	1.06747100	4.05008000
H	2.92749500	2.14303100	4.73830900
C	5.19211000	0.93602700	0.94153800
C	5.49172800	2.09581700	0.20763800
C	6.19554600	-0.03307100	1.09029400
C	6.72905900	2.24875000	-0.41942900
H	4.75546500	2.89182300	0.14457400
C	7.43506300	0.11917900	0.46500600
H	6.01728700	-0.90112900	1.71388300
C	7.70159200	1.25428200	-0.30188800
H	6.93680600	3.15110700	-0.98675300
H	8.19726500	-0.64394000	0.59187600
H	8.66638900	1.37313200	-0.78538300
Au	-0.19733200	-0.75184800	-0.52696100
H	-4.38370600	-2.63797300	-2.33759000

TS<sub>40-4a</sub>

C	-2.20892200	-0.73323800	-0.60642100
C	-2.80155000	-1.98761800	-1.20493500
H	-2.85308600	-2.76478700	-0.42300800
H	-2.11840300	-2.36308800	-1.97811000
C	-3.03102200	0.32785300	-0.29404600
C	-2.50391300	1.68357000	0.04042000
C	-1.52880800	2.31516300	-0.75323400
C	-2.98498300	2.35299900	1.18110600
C	-1.02992100	3.56507600	-0.39628700
H	-1.18509800	1.82649300	-1.65853700
C	-2.48116800	3.60397600	1.53772000
H	-3.74110200	1.88360400	1.80377300
C	-1.50265400	4.21249600	0.75055500
H	-0.27787700	4.04210300	-1.01764900
H	-2.85450500	4.10229300	2.42727800
H	-1.11334300	5.18876000	1.02298800
C	-4.48995100	0.22069400	-0.27864400
C	-5.29951900	1.04230300	-1.26796400
O	-6.25539300	0.57267800	-1.85066200
O	-4.81579700	2.26557700	-1.46478300
C	-5.50699700	3.05732800	-2.46151400
H	-5.00337800	4.02190900	-2.45724700
H	-5.42798200	2.57776100	-3.43900400
H	-6.55985900	3.16403800	-2.19349700
C	-5.16255400	-0.59794100	0.68801800
C	-4.40726400	-1.13425800	1.77195000
C	-6.56431500	-0.85967200	0.64853100
C	-5.01373100	-1.92060000	2.73981600
H	-3.35449800	-0.89107900	1.85200100
C	-7.15651600	-1.64194900	1.62492900
H	-7.15018100	-0.47577700	-0.17540700
C	-6.38757500	-2.17740600	2.66904300
H	-4.42757300	-2.31515400	3.56332500
H	-8.22154800	-1.84449300	1.57868800
H	-6.86435800	-2.78244700	3.43457200
O	-4.08530400	-1.72086800	-1.76535900
P	2.28735700	-0.85099100	-0.10225500
C	3.04443100	-0.81705700	-1.91702500
C	2.67763200	-2.50166900	0.89068400
C	2.34975200	-3.71201100	0.00233100
H	3.05343300	-3.82546800	-0.82585200
H	2.41729500	-4.62094900	0.61156300
H	1.33470600	-3.65948900	-0.40412100
C	4.13048300	-2.56830000	1.37276400
H	4.34416500	-1.76675200	2.08345000
H	4.28722500	-3.52019000	1.89432500
H	4.85181000	-2.51251400	0.55562700
C	1.74421600	-2.50705700	2.11528100

H	0.68990400	-2.51786600	1.82160000
H	1.94248600	-3.41077900	2.70338100
H	1.91472600	-1.64429200	2.76486700
C	4.49008300	-1.32237100	-2.01754500
H	4.56825400	-2.38082000	-1.75373400
H	4.81886400	-1.22656400	-3.05922800
H	5.18382500	-0.75778800	-1.39847700
C	2.14611500	-1.69710700	-2.81136500
H	1.10504000	-1.36025700	-2.80730700
H	2.51768900	-1.62148400	-3.83999800
H	2.16832500	-2.75203800	-2.53311500
C	2.91961600	0.63617000	-2.40320800
H	1.88280700	0.98533400	-2.35572500
H	3.54387600	1.32036600	-1.83068700
H	3.24128200	0.68668200	-3.44999200
C	2.82684300	0.58208300	1.04138400
C	4.08538300	1.21713100	1.21407300
C	1.75663500	1.00548900	1.85697400
C	4.19414400	2.22171700	2.19613500
C	1.89394200	1.99280900	2.82857900
H	0.78011300	0.55208100	1.72101400
C	3.12888300	2.60859200	3.00230100
H	5.15854500	2.70486400	2.31820100
H	1.03675200	2.27909700	3.43004000
H	3.26541100	3.38553100	3.74835700
C	5.35875900	0.99584600	0.44725100
C	5.69954900	1.87482900	-0.59427100
C	6.31304400	0.05360700	0.85932000
C	6.92607000	1.76826400	-1.25148500
H	5.00452400	2.65979000	-0.87781500
C	7.54210500	-0.05272900	0.20459900
H	6.10481500	-0.58706500	1.70818500
C	7.84774200	0.79548500	-0.86063300
H	7.16552800	2.45437900	-2.05845700
H	8.26594400	-0.79018900	0.53876400
H	8.80419500	0.71326400	-1.36779500
Au	-0.16316900	-0.72402000	-0.39169200
H	-4.55121700	-2.54869200	-1.94443000
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C	2.73296700	0.43499000	1.11786200
C	3.10096200	0.99103600	2.48640000
H	3.72652200	0.24207800	2.99296200
H	2.20366900	1.13344700	3.09401800
C	2.70284900	0.84803800	-0.17116100
C	2.67910000	1.96721700	-1.08463300
C	2.51168600	3.27496000	-0.57993800
C	2.84829600	1.76725800	-2.46819700

C	2.51664200	4.35695000	-1.45331600
H	2.43000600	3.42207800	0.49244100
C	2.84692200	2.85645600	-3.33387400
H	2.97880600	0.76126500	-2.85369300
C	2.67844900	4.14922300	-2.82800400
H	2.40556200	5.36453700	-1.06535600
H	2.97948500	2.70192400	-4.39988200
H	2.68037900	4.99772500	-3.50548000
C	3.42972800	-0.46442500	0.08205300
C	4.93700600	-0.25089100	0.09165400
O	5.46169900	0.70724300	0.64013100
O	5.60983400	-1.20304900	-0.54693200
C	7.05090400	-1.06541700	-0.55935600
H	7.41702600	-1.93264900	-1.10571100
H	7.33585400	-0.13878600	-1.06130700
H	7.43600900	-1.05733200	0.46195500
C	2.91921300	-1.82978100	-0.29427100
C	2.58994300	-2.75060200	0.71048300
C	2.80949300	-2.22280900	-1.63485700
C	2.14507500	-4.03306600	0.38311500
H	2.69091000	-2.46254200	1.75367600
C	2.36311800	-3.50343200	-1.96415000
H	3.09062000	-1.53226200	-2.42437500
C	2.02843300	-4.41139300	-0.95577600
H	1.90096200	-4.73791200	1.17226500
H	2.29118000	-3.79712500	-3.00735200
H	1.69026900	-5.41073800	-1.21228900
O	3.73862700	2.23885900	2.38423700
P	-1.87860300	-0.06152200	0.77258900
C	-2.51744600	1.78149500	1.04672900
C	-2.28342200	-1.31010300	2.23836200
C	-1.90269900	-0.65855800	3.57633400
H	-2.56198900	0.17115500	3.84183600
H	-1.99513100	-1.41153600	4.36718300
H	-0.86754200	-0.30221800	3.58237300
C	-3.75952800	-1.72360200	2.24139400
H	-4.01488200	-2.27554300	1.33424200
H	-3.93283500	-2.39305000	3.09207100
H	-4.44030900	-0.87604600	2.34129400
C	-1.41083900	-2.55588300	2.00967100
H	-0.34291300	-2.31984000	2.03761800
H	-1.61871700	-3.27652600	2.80901000
H	-1.63049900	-3.04503200	1.05716600
C	-3.96444400	1.86966000	1.55299100
H	-4.07516300	1.42366400	2.54528800
H	-4.22941400	2.92927500	1.64615400
H	-4.68235800	1.40758300	0.87926000
C	-1.58905400	2.45703800	2.07625500

H	-0.54378500	2.45829800	1.75283700
H	-1.90506900	3.50177100	2.17471300
H	-1.64571200	2.00508900	3.06752000
C	-2.34183800	2.49668400	-0.30255300
H	-1.30341600	2.45477900	-0.64791700
H	-2.98451000	2.08366800	-1.07856100
H	-2.60742300	3.55237300	-0.17577000
C	-2.42333700	-0.91641700	-0.84295100
C	-3.67947100	-0.90012700	-1.50370400
C	-1.39044900	-1.70446300	-1.39191700
C	-3.82237700	-1.67576000	-2.67109100
C	-1.56467000	-2.47191500	-2.53974800
H	-0.41759500	-1.72353900	-0.91184900
C	-2.79506500	-2.45745400	-3.18867000
H	-4.78336100	-1.65386000	-3.17516500
H	-0.73729600	-3.06504900	-2.91547100
H	-2.95724200	-3.04153800	-4.08929200
C	-4.91271300	-0.12188100	-1.14448400
C	-5.20346700	1.06842900	-1.83217600
C	-5.88242900	-0.64061400	-0.27340700
C	-6.39453400	1.75754400	-1.59982400
H	-4.49823000	1.44687500	-2.56662000
C	-7.07621300	0.04652300	-0.04219700
H	-5.71687100	-1.59689100	0.20840800
C	-7.33022700	1.25395000	-0.69445600
H	-6.59637900	2.67927900	-2.13722800
H	-7.81355300	-0.37191400	0.63639900
H	-8.25929900	1.78648100	-0.51598100
Au	0.54645600	0.15881400	0.66675200
H	4.55261200	2.07754000	1.87531100
<b>TS<sub>41-42</sub></b>			
C	2.51763500	-0.87811100	-0.64674000
C	2.92905500	-1.44839600	-2.01299400
H	2.83871000	-0.67429000	-2.77992800
H	2.19801000	-2.23326400	-2.24705700
C	3.22479400	-0.61913200	0.52423200
C	3.09717900	-0.97181400	1.91293400
C	2.30128500	-2.06824600	2.31263800
C	3.88572900	-0.30066600	2.87332800
C	2.28164700	-2.46786200	3.64213300
H	1.70882100	-2.59313500	1.56935400
C	3.86111800	-0.70597300	4.20169500
H	4.51577500	0.52541800	2.56050500
C	3.05748100	-1.78490600	4.58798400
H	1.67282400	-3.31267000	3.94807200
H	4.46864600	-0.18969900	4.93776800
H	3.04178700	-2.10081000	5.62668400

C	3.71548700	0.52616600	-0.17465700
C	4.90790400	0.39203100	-1.10561000
O	4.99276300	0.92076100	-2.19062700
O	5.88750900	-0.29485900	-0.49911200
C	7.07343300	-0.49983900	-1.30086500
H	7.76292100	-1.05078700	-0.66283600
H	6.81255500	-1.07470900	-2.19158200
H	7.50212900	0.45955200	-1.59664500
C	3.27962200	1.89994800	0.16263400
C	2.16535300	2.11620100	1.00322000
C	3.96405600	3.03059400	-0.33479700
C	1.76081000	3.40432300	1.33940400
H	1.61000900	1.27327100	1.39946200
C	3.55401000	4.31654900	0.00736900
H	4.80843600	2.90559600	-0.99969800
C	2.45599600	4.51225200	0.84695600
H	0.90096600	3.54238000	1.98758100
H	4.09779100	5.16950700	-0.38652100
H	2.14466200	5.51717900	1.11529400
O	4.24153400	-1.95268100	-2.09766600
P	-2.03846300	-0.57257100	-0.64049000
C	-2.71367100	-1.95292700	0.58777100
C	-2.51934300	-0.86062600	-2.52695500
C	-2.21198700	-2.31539100	-2.91351000
H	-2.88706800	-3.02707600	-2.43258500
H	-2.34616400	-2.42216800	-3.99590700
H	-1.17964800	-2.59605300	-2.68127100
C	-3.99291500	-0.53529400	-2.79572400
H	-4.20106300	0.52177800	-2.61655000
H	-4.21126400	-0.73841800	-3.85076100
H	-4.67672600	-1.13492300	-2.19212600
C	-1.63490800	0.08387000	-3.36015200
H	-0.56940700	-0.12984200	-3.22836600
H	-1.87718100	-0.05621100	-4.41990600
H	-1.80993800	1.13504700	-3.11735300
C	-4.17826600	-2.34928000	0.35241000
H	-4.31894400	-2.81914300	-0.62494500
H	-4.45937600	-3.09142000	1.10903100
H	-4.86657500	-1.51156900	0.43901100
C	-1.82757500	-3.20359500	0.41628000
H	-0.77183300	-2.98720000	0.60599400
H	-2.15403500	-3.95033300	1.14927600
H	-1.91246000	-3.65677000	-0.57217400
C	-2.49691200	-1.40416000	2.00745200
H	-1.44941400	-1.13267800	2.17704800
H	-3.12024800	-0.53605700	2.21573100
H	-2.76148100	-2.18488700	2.73012500
C	-2.54174500	1.22493600	-0.24430500

C	-3.77759100	1.76046600	0.20571600
C	-1.49075500	2.12347300	-0.52155900
C	-3.88615000	3.15934100	0.33354900
C	-1.62886300	3.50315400	-0.39723100
H	-0.53023400	1.73380300	-0.84206500
C	-2.84275400	4.02867700	0.03310800
H	-4.83252700	3.56120400	0.68154600
H	-0.78715100	4.14865500	-0.62660300
H	-2.97947600	5.10019800	0.14207200
C	-5.02120400	1.02529800	0.61782900
C	-5.26803900	0.79609800	1.98177400
C	-6.03892600	0.72742900	-0.30084100
C	-6.46528300	0.21866200	2.40710600
H	-4.52359900	1.09210300	2.71536800
C	-7.23852400	0.15149700	0.12348500
H	-5.90394900	0.96489700	-1.34956300
C	-7.45053700	-0.11634400	1.47670300
H	-6.63289100	0.04544100	3.46594600
H	-8.01278300	-0.07294600	-0.60414100
H	-8.38448400	-0.56140100	1.80585700
Au	0.41160500	-0.72221300	-0.51752800
H	4.32173200	-2.71037700	-1.50247400
<b>42</b>			
C	2.21727500	1.08629700	-1.05582900
C	2.32799100	1.57655100	-2.50649600
H	1.78862200	2.52211600	-2.59910700
H	1.84038100	0.84119900	-3.15782900
C	3.02757500	-0.07916900	-0.67774300
C	3.02279400	-1.33543300	-1.44605700
C	1.84020200	-1.88707100	-1.97512300
C	4.24979000	-1.96845300	-1.73392300
C	1.88337100	-3.03571400	-2.76305300
H	0.88428600	-1.42752400	-1.74114100
C	4.28757100	-3.10868400	-2.53179000
H	5.17238100	-1.55545700	-1.34118700
C	3.10565800	-3.64813200	-3.04611600
H	0.96074200	-3.45525100	-3.15221500
H	5.24178700	-3.57698200	-2.75197800
H	3.13756800	-4.54231000	-3.66090600
C	3.87245300	0.25595000	0.38001900
C	3.64349700	1.63742700	0.59553200
O	2.74036900	2.15780400	-0.19495200
O	4.21212300	2.37303000	1.51183100
C	3.90348500	3.79138600	1.55732900
H	4.52558400	4.18648000	2.35742500
H	4.15441200	4.25796800	0.60284900
H	2.84568000	3.93655200	1.78345700

C	4.78338400	-0.58002600	1.19072800
C	4.37094900	-1.84564200	1.64082900
C	6.06373600	-0.11921000	1.53893800
C	5.22065200	-2.63118100	2.41656500
H	3.38194700	-2.21159100	1.38268400
C	6.91084400	-0.90872200	2.31596600
H	6.39901900	0.85497600	1.19805000
C	6.49299600	-2.16557900	2.75634400
H	4.88773300	-3.60594000	2.75996100
H	7.89915700	-0.54126300	2.57459900
H	7.15381300	-2.77823300	3.36178300
O	3.66596300	1.83017100	-2.89374400
P	-2.20677200	0.70367100	0.14860400
C	-3.18744600	1.01701300	-1.52920800
C	-2.52194400	2.05744100	1.53859100
C	-2.37652000	3.45713700	0.92189600
H	-3.18993500	3.69638200	0.23297200
H	-2.40790200	4.19779500	1.72928300
H	-1.42358400	3.58048300	0.39738300
C	-3.89669600	1.90074700	2.19792000
H	-3.97181300	0.94716100	2.72526400
H	-4.02441800	2.69742600	2.94031700
H	-4.72073500	1.97353900	1.48584500
C	-1.42968600	1.85513800	2.60432200
H	-0.42642100	1.99828700	2.19044300
H	-1.57624000	2.59397600	3.40069400
H	-1.47832300	0.86287900	3.06065400
C	-4.65740800	1.41611200	-1.33795600
H	-4.75260700	2.37781600	-0.82654700
H	-5.11367900	1.53223700	-2.32804000
H	-5.23433000	0.67251600	-0.79264500
C	-2.45921100	2.14417400	-2.28968500
H	-1.41579000	1.89017800	-2.50044900
H	-2.96802200	2.28497900	-3.25023500
H	-2.48209700	3.10005400	-1.76429700
C	-3.05658600	-0.27649500	-2.34959300
H	-2.00729600	-0.55035000	-2.50216800
H	-3.57225000	-1.11596600	-1.88590400
H	-3.50442300	-0.11290100	-3.33656800
C	-2.49317600	-0.99170600	0.97861500
C	-3.68069300	-1.75358400	1.13701100
C	-1.30219100	-1.49591200	1.54224700
C	-3.60065200	-2.96550900	1.85159600
C	-1.25413700	-2.68997300	2.25584400
H	-0.38114000	-0.93581200	1.41560800
C	-2.41816300	-3.43549900	2.41248600
H	-4.51142200	-3.54537400	1.96325200
H	-0.31239900	-3.03058000	2.67492200

H	-2.41017900	-4.37373400	2.95855500
C	-5.05514400	-1.46538000	0.60312800
C	-5.49441200	-2.11850300	-0.56054500
C	-5.98543800	-0.70949900	1.33212000
C	-6.80259800	-1.96211300	-1.02079500
H	-4.81004800	-2.76875800	-1.09789700
C	-7.29583400	-0.55426100	0.87436500
H	-5.69353500	-0.25887500	2.27326800
C	-7.70513200	-1.16949800	-0.30958300
H	-7.11891300	-2.47140900	-1.92618900
H	-8.00011800	0.03554100	1.45355300
H	-8.72464700	-1.05037900	-0.66321200
Au	0.16123800	0.84383500	-0.47017500
H	4.06831900	0.99551900	-3.16796100
<b>TS<sub>21-43</sub></b>			
C	-4.87228600	-1.20701800	0.91042600
C	-4.86621800	-1.32265200	2.31874300
C	-4.36353600	-2.42259400	2.94710000
H	-4.03617900	-3.29279400	2.38950500
H	-4.32770600	-2.48740200	4.02974400
O	-1.88593300	-1.76169000	1.87596500
H	-1.99437500	-1.20778600	2.67995600
C	-5.49327100	-0.17552300	0.13262900
C	-6.05326800	0.99766900	0.70301400
C	-5.57055600	-0.33651600	-1.27458300
C	-6.66136200	1.95166800	-0.09879800
H	-6.01556200	1.14992900	1.77644700
C	-6.18159700	0.62582800	-2.07184700
H	-5.16997700	-1.23932400	-1.72389600
C	-6.72917200	1.77118100	-1.48890800
H	-7.09639500	2.83804500	0.35275100
H	-6.24480500	0.47833800	-3.14550400
H	-7.21793400	2.51688300	-2.10847500
H	-4.50743700	-2.06776900	0.35544500
H	-5.22625000	-0.49561400	2.92400100
C	-2.08410100	-0.89244100	0.84288800
C	-2.01811700	-1.45465600	-0.51359500
C	-1.75564400	-2.84877100	-0.66626300
C	-2.26772800	-0.69122000	-1.69402600
C	-1.73092600	-3.43165200	-1.92728000
H	-1.58193700	-3.44968200	0.21850400
C	-2.22694400	-1.30029500	-2.94584600
H	-2.49591300	0.36163200	-1.60514600
C	-1.96207700	-2.66618800	-3.07651800
H	-1.53468400	-4.49621400	-2.01501200
H	-2.41842300	-0.69794800	-3.82915100
H	-1.94155700	-3.13024300	-4.05724100



C	-2.38496600	0.46587900	1.32472400
O	-2.40939800	0.67944300	2.53918400
O	-2.58466300	1.41230700	0.38979700
C	-2.78478800	2.76538900	0.88784900
H	-1.89933600	3.05639000	1.46097000
H	-3.63970500	2.76277700	1.56765100
C	-3.01234000	3.66239300	-0.31172900
H	-2.15115200	3.64766400	-0.98651200
H	-3.16268100	4.69230400	0.02580500
H	-3.89964200	3.35035500	-0.86882800
P	2.54366400	0.04723400	-0.11142600
C	2.72025900	1.16466200	-1.66155000
C	4.15094100	1.39910300	-2.18110900
C	1.95204500	2.48860000	-1.49079300
H	2.18690400	0.56289500	-2.41068200
C	4.11753600	2.20237600	-3.49591600
H	4.73843700	1.94878100	-1.43747600
H	4.65947100	0.44569700	-2.35484500
C	1.93716200	3.28620500	-2.80681200
H	2.42961900	3.09374500	-0.70968400
H	0.92614800	2.28913900	-1.15859700
C	3.35646200	3.52528200	-3.34005000
H	5.14390300	2.38578400	-3.83200600
H	3.63802700	1.59507100	-4.27593900
H	1.41928600	4.23892300	-2.64966200
H	1.35422100	2.73207800	-3.55559900
H	3.31643300	4.05296700	-4.29898800
H	3.90120400	4.18041000	-2.64605100
C	3.56408000	-1.54805000	-0.41650200
C	2.95199100	-2.75158600	0.32886400
C	5.06660600	-1.42142200	-0.09395400
H	3.44486700	-1.71351600	-1.49631700
C	3.70544400	-4.05181000	-0.00257900
H	2.99585300	-2.57072200	1.41230900
H	1.89256300	-2.85728500	0.07059600
C	5.81179300	-2.72385200	-0.44231400
H	5.19240200	-1.21979200	0.97767500
H	5.51879200	-0.58363400	-0.63198100
C	5.20816000	-3.93253100	0.28345400
H	3.26926200	-4.87891200	0.56835900
H	3.55387700	-4.29072800	-1.06439300
H	6.87135200	-2.61106700	-0.18772000
H	5.76737900	-2.88592500	-1.52803700
H	5.72446800	-4.85099100	-0.01557700
H	5.36602100	-3.82360000	1.36542300
C	3.15369300	0.86135300	1.51583900
C	2.02947400	1.63695100	2.23120800
C	4.41851300	1.73288300	1.37914400

H	3.39930600	-0.01518100	2.13192000
C	2.50198400	2.14063800	3.60610900
H	1.72374400	2.49300900	1.61499000
H	1.14576700	1.00019200	2.34796400
C	4.88480500	2.23106800	2.76056400
H	4.19528600	2.60012300	0.74545600
H	5.22841100	1.18197600	0.89378000
C	3.77412300	2.99188700	3.49557500
H	1.69584700	2.71131800	4.08006600
H	2.69593200	1.27632700	4.25644300
H	5.76893800	2.86565300	2.63462300
H	5.20258300	1.37045900	3.36513400
H	4.11661100	3.29234100	4.49157900
H	3.54637000	3.91892200	2.95107700
Au	0.22405500	-0.50514500	0.05233000
<b>43</b>			
C	-4.30770000	0.92195900	1.12221500
C	-4.68673400	2.38453800	1.05636700
C	-4.69786500	3.20046500	2.11049600
H	-4.43095300	2.85379500	3.10550700
H	-4.98912000	4.24229700	2.01772800
O	-1.97217100	1.44273100	1.51350700
H	-1.85018900	2.32446700	1.12014000
C	-5.36729500	0.00648000	0.52275100
C	-6.01273300	0.27934100	-0.69311300
C	-5.75866300	-1.13705100	1.23562100
C	-7.00221100	-0.57266900	-1.18545900
H	-5.75533200	1.16620700	-1.26197700
C	-6.74772300	-1.99131700	0.74692600
H	-5.29198400	-1.35399500	2.19342100
C	-7.37163100	-1.71296700	-0.46946800
H	-7.49533600	-0.33735200	-2.12424900
H	-7.03771900	-2.86550000	1.32233400
H	-8.14783600	-2.36984700	-0.85010400
H	-4.20650600	0.65625500	2.17975500
H	-4.96999700	2.77907900	0.08202800
C	-2.79398400	0.72679300	0.61114900
C	-2.36642300	-0.74021400	0.67522700
C	-1.56922500	-1.15687300	1.78449200
C	-2.78771400	-1.71403700	-0.24035000
C	-1.21346300	-2.52225300	1.93529900
H	-1.43345800	-0.47053000	2.61592300
C	-2.42007700	-3.05331200	-0.07738700
H	-3.41444500	-1.43101900	-1.07434000
C	-1.62617400	-3.46557400	0.99457300
H	-0.65424000	-2.82775400	2.81431900
H	-2.76907700	-3.78511400	-0.79983100

H	-1.35581700	-4.50994300	1.11080500
C	-2.57623800	1.38714000	-0.77171200
O	-1.99061000	2.45749000	-0.86052000
O	-3.10374300	0.73270000	-1.80387400
C	-2.97666100	1.36742700	-3.11499700
H	-1.91356600	1.52593400	-3.31501500
H	-3.45908100	2.34722800	-3.06429100
C	-3.62807700	0.45094200	-4.12974800
H	-3.11968000	-0.51641600	-4.17334500
H	-3.57421300	0.90978600	-5.12134600
H	-4.68014200	0.27980600	-3.88735900
P	2.63697200	0.12481100	0.12059700
C	3.89524500	-1.17950900	0.75284200
C	5.38073400	-0.77388100	0.71727200
C	3.66341600	-2.55454100	0.09776700
H	3.59739500	-1.25707100	1.80805700
C	6.24747300	-1.86322700	1.37880600
H	5.70986400	-0.63081800	-0.31791700
H	5.53390200	0.17616000	1.23863900
C	4.54540500	-3.63003600	0.75699300
H	3.90493300	-2.49946800	-0.97142000
H	2.60635700	-2.83668300	0.17200500
C	6.02906200	-3.23792700	0.73343400
H	7.30153500	-1.57155700	1.31683300
H	6.00146300	-1.91824600	2.44826200
H	4.39161900	-4.58834900	0.24876400
H	4.22139300	-3.77208200	1.79744000
H	6.62852500	-3.99626800	1.24825100
H	6.38322800	-3.21349000	-0.30652300
C	3.05330000	1.79519000	0.96888800
C	1.78411800	2.64822600	1.16850300
C	4.15298700	2.61637000	0.26598300
H	3.42097700	1.48628300	1.95724900
C	2.09862700	3.93778600	1.94637200
H	1.35844100	2.90685100	0.18852700
H	1.01845500	2.06996700	1.69758900
C	4.46730500	3.89797700	1.06015100
H	3.81087700	2.89842000	-0.73819500
H	5.06632400	2.02870800	0.13912000
C	3.21267100	4.75328900	1.27667300
H	1.18617800	4.53708700	2.03916700
H	2.40343600	3.67319400	2.96839100
H	5.23676800	4.46998000	0.53010700
H	4.89816000	3.62304500	2.03271700
H	3.45446000	5.63327900	1.88229500
H	2.85696700	5.12935600	0.30738400
C	2.67364100	0.38593500	-1.78049900
C	1.68409700	-0.54369900	-2.51113500

C	4.07400200	0.30666000	-2.42081600
H	2.30320000	1.41591100	-1.87846000
C	1.62663700	-0.21126700	-4.01267900
H	1.99455600	-1.58844400	-2.37979600
H	0.68595600	-0.45498700	-2.06750000
C	4.00518900	0.64686100	-3.92141900
H	4.46836200	-0.71043700	-2.30658900
H	4.77537200	0.97973800	-1.92087400
C	3.01588600	-0.26112700	-4.66273700
H	0.94323300	-0.90630900	-4.51347400
H	1.20185000	0.79460900	-4.14033200
H	5.00666100	0.56108200	-4.35705500
H	3.70236800	1.69630400	-4.04090200
H	2.95095400	0.02987200	-5.71665000
H	3.38806000	-1.29492000	-4.64695800
Au	0.46733200	-0.59208900	0.85096400
<b>TS<sub>20-44</sub></b>			
C	-2.40592300	-0.62469300	0.09316000
C	-2.97910400	-1.86613600	-0.45131300
C	-4.04128600	-2.55859700	0.18127500
C	-2.43844300	-2.42830500	-1.63460500
C	-4.50710200	-3.76855800	-0.32261800
H	-4.50105200	-2.14554000	1.07201400
C	-2.91938400	-3.62598600	-2.14719200
H	-1.62355800	-1.90980000	-2.13142700
C	-3.95181800	-4.30428000	-1.48816100
H	-5.30945500	-4.29166200	0.18791700
H	-2.48724600	-4.04108200	-3.05236500
H	-4.32237700	-5.24513300	-1.88344200
C	-2.79483100	-0.35783400	1.53107900
O	-2.04951000	-0.70901300	2.42722000
O	-3.99182000	0.21875500	1.73861900
C	-4.39229500	0.42150700	3.13261000
H	-5.48290700	0.39827900	3.09666600
H	-4.02535700	-0.42099600	3.72117400
C	-3.19595500	1.99159100	-0.49511200
C	-3.42817700	0.81797400	-1.19584300
C	-4.87146600	0.34848600	-1.34421600
H	-4.90424400	-0.70170900	-1.65250900
H	-5.38671500	0.43636500	-0.38520700
O	-5.57266600	1.17979000	-2.25999000
H	-5.36457900	0.89701300	-3.15972800
C	-2.09056400	2.90321300	-0.61572100
C	-1.98810700	3.96323800	0.31675900
C	-1.12730400	2.81765700	-1.64948600
C	-0.96155500	4.89548900	0.22793500
H	-2.73030200	4.04544100	1.10577300

C	-0.10679200	3.75529800	-1.73852300
H	-1.20163100	2.03457100	-2.39559600
C	-0.02018900	4.79395200	-0.80177500
H	-0.89862500	5.70646700	0.94619100
H	0.61399500	3.69501000	-2.54796500
H	0.77141800	5.53255600	-0.88549300
C	-3.87397700	1.74303700	3.67283400
H	-4.24024100	2.58554000	3.07820300
H	-4.22855200	1.87921700	4.69934300
H	-2.78124500	1.75753900	3.68740500
P	2.09959200	-0.36872500	-0.10467900
C	2.55464000	-1.97861700	0.84136600
C	4.01721800	-2.45118800	0.76016000
C	2.04878300	-1.94641400	2.29771300
H	1.94045800	-2.71052200	0.29722000
C	4.17408600	-3.82861600	1.43258700
H	4.67694300	-1.73170600	1.25817700
H	4.34460300	-2.52071000	-0.28222400
C	2.22057100	-3.32390600	2.96236100
H	2.61800300	-1.20196400	2.86964300
H	0.99670600	-1.64102200	2.33296800
C	3.67202600	-3.81715500	2.88274400
H	5.22539800	-4.13458900	1.39127000
H	3.60921100	-4.57528800	0.85719100
H	1.88921100	-3.26854400	4.00520400
H	1.56053100	-4.04704000	2.46336500
H	3.75711500	-4.81791000	3.32016200
H	4.31378500	-3.15842600	3.48454600
C	2.87331100	-0.53170200	-1.85451500
C	2.02579000	0.21028400	-2.90706900
C	4.35120200	-0.10918100	-1.95977500
H	2.80129500	-1.60951700	-2.05768000
C	2.57381800	-0.01232500	-4.32788100
H	2.02888500	1.28618700	-2.67913000
H	0.98230800	-0.11921900	-2.84787100
C	4.89507900	-0.34516100	-3.38117800
H	4.44212600	0.95828700	-1.71936400
H	4.96693400	-0.65012000	-1.23643700
C	4.05293000	0.38071100	-4.43769500
H	1.97109600	0.55410000	-5.04724300
H	2.45869300	-1.07281300	-4.59215300
H	5.93907400	-0.01637700	-3.42943500
H	4.89820900	-1.42341500	-3.59216400
H	4.42975500	0.15949000	-5.44211600
H	4.15262500	1.46644400	-4.29920200
C	2.81510400	1.21393700	0.71239500
C	1.81955600	1.82931400	1.71773900
C	4.21165300	1.06990200	1.34900000

H	2.89498200	1.90202600	-0.14114400
C	2.33377200	3.18014600	2.24492700
H	1.67463600	1.13955400	2.55899000
H	0.83900200	1.95998200	1.24735100
C	4.71987000	2.43046800	1.86044800
H	4.15501100	0.37291200	2.19356400
H	4.92819600	0.65086200	0.63830800
C	3.73748500	3.06359000	2.85423900
H	1.62715700	3.57664100	2.98308100
H	2.35577200	3.90105500	1.41526800
H	5.70465600	2.30067000	2.32280700
H	4.86350100	3.10620800	1.00564200
H	4.09781800	4.04943200	3.16830600
H	3.69022400	2.44565800	3.76160400
Au	-0.33696000	-0.35285000	-0.14587200
H	-2.77425500	0.58699500	-2.03280400
H	-3.93482300	2.25352200	0.25872000
<b>44</b>			
C	2.54838500	-1.03560800	0.18962900
C	2.34722000	-1.58695900	1.57280000
C	2.25198600	-2.97211000	1.82800900
C	2.29432500	-0.71585600	2.68730300
C	2.13875200	-3.45282100	3.13251300
H	2.27759600	-3.67391200	1.00722000
C	2.16269400	-1.20081600	3.98363800
H	2.33170100	0.35922900	2.54291500
C	2.08971000	-2.57722200	4.21639500
H	2.09165500	-4.52514700	3.29641800
H	2.12019100	-0.50283300	4.81436000
H	1.99738900	-2.95825300	5.22862500
C	2.40537100	-1.99585700	-0.97749400
O	1.70035200	-2.98970200	-0.97566500
O	3.13547100	-1.61693200	-2.04542600
C	3.07391500	-2.46759000	-3.23001700
H	4.04252100	-2.31700800	-3.71018500
H	2.98397100	-3.50476400	-2.90379600
C	2.54581900	1.05202200	-0.75084700
C	3.49358000	0.16945600	0.03074600
C	4.91404000	0.00281400	-0.54723100
H	5.38916200	-0.88216000	-0.09694500
H	4.87815800	-0.15411700	-1.62434100
O	5.67246200	1.18375600	-0.33788900
H	6.03424300	1.16960400	0.55714600
C	2.26225900	2.45745000	-0.46517800
C	1.58327600	3.21994900	-1.44620000
C	2.67189000	3.10653100	0.72063100
C	1.33641800	4.57416500	-1.25482100

H	1.27459400	2.73724400	-2.36961000
C	2.41655400	4.45978600	0.91078200
H	3.21361300	2.55814300	1.48310300
C	1.74839800	5.19822600	-0.07270000
H	0.83301700	5.14734300	-2.02706200
H	2.75145800	4.94793500	1.82067900
H	1.56168300	6.25710000	0.07704200
C	1.92702500	-2.06668800	-4.14215600
H	2.01238000	-1.01898900	-4.44621100
H	1.95048800	-2.68327700	-5.04627200
H	0.96328100	-2.22281400	-3.65068800
P	-1.87601100	0.08764000	0.13117400
C	-2.34025200	-1.57853800	0.97599900
C	-3.77127500	-1.68030100	1.53720200
C	-1.98586200	-2.78839700	0.09033300
H	-1.64639700	-1.57558200	1.82860700
C	-3.95611700	-3.00669300	2.29996300
H	-4.50184600	-1.62997800	0.72219000
H	-3.98326600	-0.84425800	2.21148300
C	-2.18957600	-4.10568000	0.86016000
H	-2.62643400	-2.79322200	-0.80143100
H	-0.94892100	-2.72467900	-0.25714500
C	-3.61034400	-4.22047600	1.42785500
H	-4.98801700	-3.07276400	2.66221900
H	-3.31278300	-3.00186100	3.19088000
H	-1.96922000	-4.94921400	0.19684400
H	-1.46032500	-4.15535100	1.68069900
H	-3.71380800	-5.14375800	2.00817600
H	-4.32926300	-4.29121000	0.59952400
C	-2.41718000	1.48244100	1.33633700
C	-1.46069300	2.68755200	1.25234900
C	-3.88129400	1.94086500	1.18648600
H	-2.29524200	1.01466200	2.32331900
C	-1.82118200	3.76350300	2.29115700
H	-1.51020600	3.12343100	0.24469500
H	-0.42582900	2.35999700	1.40006300
C	-4.23323200	3.01046400	2.23787800
H	-4.02927700	2.36699700	0.18566200
H	-4.56988700	1.09633900	1.27836600
C	-3.28288500	4.21217100	2.16621400
H	-1.14368900	4.61709600	2.17806600
H	-1.64950700	3.35906100	3.29857500
H	-5.27094700	3.33056600	2.09350300
H	-4.18179700	2.56186300	3.23945600
H	-3.52638100	4.93512600	2.95220000
H	-3.42476600	4.73250300	1.20862500
C	-2.74648700	0.35552600	-1.56118600
C	-1.90640400	-0.21114000	-2.72442900

C	-4.20131100	-0.14461800	-1.64728000
H	-2.75010300	1.45119900	-1.65029600
C	-2.53534800	0.14166500	-4.08406200
H	-1.83502600	-1.30239400	-2.62733100
H	-0.88158000	0.17546100	-2.67491000
C	-4.82376300	0.21846500	-3.00870900
H	-4.21697300	-1.23465700	-1.52877800
H	-4.80873500	0.27285500	-0.84063300
C	-3.99317400	-0.32786000	-4.17684500
H	-1.93699800	-0.30102000	-4.88827600
H	-2.49369300	1.23077400	-4.22651400
H	-5.84815600	-0.16744000	-3.05173200
H	-4.89925900	1.31159400	-3.09128400
H	-4.43042800	-0.01648800	-5.13153600
H	-4.02342600	-1.42617500	-4.16298400
Au	0.58905300	0.03988400	-0.13813800
H	3.63616100	0.58316300	1.02936200
H	2.49621000	0.78464900	-1.80625000
TS <sub>44-45</sub>			
C	2.65474900	-0.90256200	0.14621300
C	2.75557500	-0.71676500	1.64918200
C	3.51414900	-1.66316500	2.36050000
C	2.22147500	0.37153900	2.35133900
C	3.71235500	-1.52952300	3.73310300
H	3.93506000	-2.51864000	1.84309800
C	2.42880100	0.50902400	3.72712200
H	1.64576000	1.12818000	1.82752500
C	3.17134300	-0.44234400	4.42331600
H	4.29217800	-2.27866200	4.26355000
H	2.00684900	1.36284000	4.24902800
H	3.32977400	-0.33905400	5.49223300
C	2.13758200	-2.25910400	-0.30874900
O	1.72916000	-3.10467000	0.46037400
O	2.21497500	-2.42953500	-1.64599100
C	1.89796500	-3.75611900	-2.16898800
H	2.58915300	-3.88433000	-3.00466700
H	2.11952200	-4.49080500	-1.39357400
C	2.70016300	0.51513900	-1.17946800
C	3.81986200	-0.27608500	-0.62256400
C	4.74761900	-1.02772400	-1.58829300
H	5.28634900	-1.81582100	-1.04054700
H	4.17604600	-1.50346100	-2.38315300
O	5.62752800	-0.11902900	-2.22324300
H	6.29984000	0.16572500	-1.59054100
C	2.55069100	1.98221900	-1.04158700
C	1.80716000	2.65948200	-2.02980300
C	3.19149500	2.73842700	-0.04327000

C	1.71541300	4.04939200	-2.02453900
H	1.32699400	2.09056800	-2.82141900
C	3.08280400	4.12666300	-0.03243000
H	3.77023900	2.24697800	0.73122900
C	2.34719700	4.78735900	-1.02130100
H	1.15809100	4.55515000	-2.80686300
H	3.58491400	4.69700300	0.74289800
H	2.27830700	5.87069300	-1.01545500
C	0.45201100	-3.84319000	-2.62168300
H	0.23112800	-3.09400200	-3.38729700
H	0.26549300	-4.83344100	-3.04935900
H	-0.22813400	-3.70405000	-1.77761000
P	-1.92207900	0.18469700	0.17714800
C	-2.27643800	-1.18152100	1.48357900
C	-3.62391300	-1.08210500	2.22296300
C	-2.03797100	-2.59205100	0.91116800
H	-1.47834100	-0.98106700	2.21190000
C	-3.71327800	-2.15884200	3.32179100
H	-4.45376000	-1.21660100	1.52007800
H	-3.74129100	-0.09275800	2.67606100
C	-2.14699200	-3.65624800	2.01740900
H	-2.78199600	-2.80552500	0.13272000
H	-1.04858300	-2.65165000	0.44475100
C	-3.48671200	-3.56838300	2.76018100
H	-4.69041500	-2.09077500	3.81252900
H	-2.96071900	-1.94842300	4.09417100
H	-2.01332700	-4.65034800	1.57709100
H	-1.32140500	-3.51774700	2.72836000
H	-3.52120200	-4.30655500	3.56859300
H	-4.30453400	-3.82191300	2.07099500
C	-2.32346100	1.87779300	0.98981400
C	-1.44080300	2.99843500	0.40585100
C	-3.81067000	2.28235900	0.93747000
H	-2.03711400	1.72114500	2.03924800
C	-1.68202800	4.33606900	1.12650800
H	-1.66445900	3.11651000	-0.66396700
H	-0.38256400	2.72589100	0.47407000
C	-4.04112000	3.61439500	1.67589100
H	-4.11882700	2.40171200	-0.10923800
H	-4.44772000	1.50702700	1.37123700
C	-3.16268900	4.73658200	1.10925100
H	-1.06518200	5.11288300	0.66135700
H	-1.34025900	4.24789200	2.16728600
H	-5.10081200	3.88400200	1.60930900
H	-3.82065100	3.47790500	2.74351800
H	-3.31267700	5.65994900	1.67885700
H	-3.47021400	4.95320000	0.07663900
C	-2.97677500	0.02753700	-1.42005000

C	-2.27348900	-0.82491200	-2.49419700
C	-4.42406400	-0.45629800	-1.20007800
H	-3.00790600	1.06495700	-1.78182000
C	-3.06669100	-0.81208100	-3.81281200
H	-2.17682000	-1.85781000	-2.13659400
H	-1.25604100	-0.45437300	-2.66336700
C	-5.21103300	-0.44014100	-2.52431000
H	-4.40836600	-1.48004800	-0.80746800
H	-4.93780100	0.16153600	-0.45941600
C	-4.51623900	-1.27252900	-3.60920200
H	-2.56099000	-1.44712100	-4.54890000
H	-3.06190000	0.20690700	-4.22444200
H	-6.22566100	-0.81199200	-2.34458400
H	-5.31632800	0.59784100	-2.86883800
H	-5.07027000	-1.20558100	-4.55154300
H	-4.52408100	-2.33174300	-3.31693100
Au	0.44192700	0.02952600	-0.26677100
H	4.42450900	0.30159200	0.07746800
H	2.31152400	0.09474700	-2.10562100
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C	3.38020600	0.61077300	-0.56297100
C	2.64549400	-0.57779100	-1.12308000
C	2.62453800	-0.84069500	-2.48963300
C	1.96551200	-1.47363200	-0.25252800
C	1.96148000	-1.96607300	-3.00935600
H	3.14195200	-0.16899100	-3.16793700
C	1.30858200	-2.61465800	-0.77454600
H	2.11728000	-1.38466600	0.81946900
C	1.30578400	-2.85176000	-2.16604200
H	1.97624700	-2.14695500	-4.07980500
H	0.92027000	-3.36815300	-0.09570700
H	0.81878900	-3.73712500	-2.56142600
C	2.45874400	1.74502000	-0.20816000
O	1.25086300	1.71599000	-0.39756900
O	3.07675600	2.78623300	0.36744900
C	2.24617000	3.91878400	0.74913400
H	1.75771200	4.30530100	-0.15000900
H	1.46768700	3.55985400	1.42845800
C	4.62160300	0.38083300	0.36475300
C	4.82315900	0.83194200	-1.04067600
C	5.45445200	2.17403500	-1.38328700
H	5.16132300	2.46877300	-2.40339300
H	5.10231700	2.94788400	-0.70301900
O	6.86296300	2.12898000	-1.23269100
H	7.23516300	1.57934500	-1.93428500
C	4.97838500	-0.96513800	0.90809900
C	4.86492600	-1.17148500	2.29304000

C	5.42135600	-2.03043000	0.11065100
C	5.17583800	-2.40537700	2.86365000
H	4.54272500	-0.35041500	2.92907100
C	5.73158100	-3.26631600	0.67971100
H	5.53993700	-1.90060700	-0.96063600
C	5.60799500	-3.45981000	2.05673500
H	5.09033200	-2.53967000	3.93788700
H	6.08151300	-4.07591800	0.04603800
H	5.85730000	-4.41984500	2.49818500
C	3.14771100	4.94704000	1.40219200
H	3.91789900	5.29664600	0.70935200
H	2.55106200	5.81026300	1.71187700
H	3.63828200	4.53474600	2.28813600
P	-2.62558900	-0.08802500	-0.01985800
C	-2.96528800	1.21946400	-1.38458900
C	-4.44323400	1.57897200	-1.62582300
C	-2.09463600	2.47789400	-1.20913800
H	-2.60272900	0.68413100	-2.27374500
C	-4.57307300	2.51448200	-2.84383800
H	-4.85855700	2.07668400	-0.74231600
H	-5.04123500	0.67888600	-1.80066100
C	-2.23862700	3.40316600	-2.43105600
H	-2.41470300	3.02379500	-0.31194800
H	-1.04501700	2.20707000	-1.06163700
C	-3.70453100	3.77093400	-2.69829700
H	-5.62565400	2.78708000	-2.97811300
H	-4.27560800	1.96737700	-3.74921600
H	-1.63776600	4.30624000	-2.27591600
H	-1.82086500	2.89861600	-3.31353700
H	-3.78314800	4.38945900	-3.59894400
H	-4.08364400	4.38169400	-1.86696500
C	-3.83898400	-1.54605400	-0.32787600
C	-3.21640200	-2.89550900	0.08204900
C	-5.22704800	-1.37219300	0.32106900
H	-3.95623900	-1.54031300	-1.42037300
C	-4.14800200	-4.06918600	-0.26674500
H	-3.02096700	-2.89406200	1.16409300
H	-2.24766700	-3.02644500	-0.41244100
C	-6.15416700	-2.54826300	-0.04035200
H	-5.11594700	-1.33341200	1.41245300
H	-5.69070800	-0.43085800	0.01372800
C	-5.53992200	-3.89734500	0.35416200
H	-3.69115800	-5.00774400	0.06631900
H	-4.24216100	-4.13749300	-1.35946800
H	-7.12287800	-2.40701200	0.45137700
H	-6.34861200	-2.53501800	-1.12161600
H	-6.19654100	-4.71752600	0.04483300
H	-5.46129000	-3.95609000	1.44864200

C	-2.89538300	0.56098300	1.76721300
C	-1.59509900	1.13406400	2.36530700
C	-4.06245300	1.55417700	1.93753200
H	-3.14097600	-0.35880400	2.31608700
C	-1.79022900	1.51681700	3.84276000
H	-1.28483300	2.01684600	1.79206800
H	-0.78526900	0.40125900	2.27233400
C	-4.25033500	1.92150700	3.42171900
H	-3.84864100	2.46778800	1.37014800
H	-4.99288900	1.14176800	1.53916100
C	-2.96259300	2.48889400	4.03199000
H	-0.86267400	1.95227800	4.23142500
H	-1.97521000	0.60555700	4.42837400
H	-5.07084700	2.64150900	3.51406800
H	-4.55690500	1.02598300	3.97967500
H	-3.10925600	2.70264500	5.09614100
H	-2.72377700	3.44733000	3.55023700
Au	-0.35959400	-0.85585300	-0.27803500
H	5.12977500	0.04814300	-1.73259800
H	4.71282200	1.17695900	1.09855700
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C	-0.56383100	0.46602100	0.21613900
C	0.50236800	1.52569500	0.10189100
C	0.77695000	2.39174800	1.16640400
C	1.21149400	1.68580800	-1.09590200
C	1.74322000	3.39174600	1.04268700
C	0.22259600	2.28966800	2.09543500
C	2.17616300	2.68402500	-1.22375500
H	1.00929800	1.01823200	-1.92830300
C	2.44636600	3.53950500	-0.15336100
H	1.94142600	4.05725200	1.87823200
H	2.71972600	2.79191800	-2.15805700
H	3.19915000	4.31648600	-0.25188300
C	-1.85227600	0.88617200	-0.45129100
O	-2.09619900	2.02447700	-0.79194300
O	-2.72133700	-0.13673700	-0.65067400
C	-3.97036400	0.22000800	-1.28945000
H	-4.48215700	0.96547300	-0.67291300
H	-3.74851600	0.68909300	-2.25268900
C	-0.19297400	-1.04257700	0.19021600
C	-0.59180500	-0.39687300	1.48090300
C	-1.84665600	-0.79849400	2.23364800
H	-2.14397300	0.01910700	2.91084300
H	-2.67086900	-0.96898200	1.54107000
O	-1.67650700	-2.01981700	2.94314100
H	-0.96219300	-1.89812500	3.58198800
C	1.17457000	-1.56015700	-0.11516500

C	1.30620200	-2.52673100	-1.12501000
C	2.33411700	-1.14954600	0.56075200
C	2.54982700	-3.06662700	-1.45149300
H	0.41864900	-2.86241500	-1.65568300
C	3.57899500	-1.68758000	0.23526000
H	2.27379700	-0.39740000	1.34061300
C	3.69410600	-2.64833500	-0.77111600
H	2.62269400	-3.81596000	-2.23481000
H	4.46266300	-1.35322200	0.77164500
H	4.66479200	-3.06695600	-1.02064500
C	-4.78407200	-1.05042000	-1.44600900
H	-4.99976200	-1.50428400	-0.47434500
H	-5.73566200	-0.82108600	-1.93570500
H	-4.25151400	-1.78411300	-2.05802900
H	0.23691900	-0.15775200	2.14747000
H	-0.97910600	-1.64064200	-0.26051400
<b>TS<sub>21-47</sub></b>			
C	-5.62009600	0.56018200	0.47174700
C	-4.28726300	0.63391900	0.30859500
C	-3.36086300	-0.32653200	0.96423800
H	-3.86559300	-0.99712100	1.65735200
H	-2.53776400	0.18023300	1.49062700
O	-2.75945500	-1.16319600	-0.10464800
H	-1.55136200	-0.70735100	-0.27563600
C	-6.64952900	1.44535300	-0.08090800
C	-6.35701300	2.55398000	-0.89840300
C	-7.99678000	1.17505100	0.21882000
C	-7.37732100	3.35711300	-1.39638500
H	-5.32671500	2.79067600	-1.14630000
C	-9.01941100	1.97962200	-0.28002400
H	-8.23979800	0.32330600	0.84893000
C	-8.71257700	3.07373200	-1.08955400
H	-7.13459600	4.20821700	-2.02570700
H	-10.05298300	1.75291500	-0.03690000
H	-9.50612100	3.70365600	-1.47989100
H	-6.00319100	-0.24735200	1.09651300
H	-3.83447200	1.40781700	-0.30738700
C	-1.40861400	-1.92389800	0.20033500
C	-1.31019700	-2.99041900	-0.84968500
C	-1.74388200	-4.29726800	-0.56942800
C	-0.85014100	-2.68990500	-2.14253700
C	-1.69487500	-5.28109800	-1.55500200
H	-2.13866700	-4.54446700	0.41045500
C	-0.81175200	-3.67364500	-3.12841300
H	-0.52535300	-1.67983700	-2.37696600
C	-1.22815800	-4.97349800	-2.83443800
H	-2.03074300	-6.28719500	-1.32453000

H	-0.45592100	-3.42586500	-4.12356300
H	-1.19319000	-5.74216200	-3.60020500
C	-1.40498000	-2.46314800	1.62589100
O	-2.41153200	-2.71966300	2.24775300
O	-0.15326800	-2.67919100	2.05611700
C	-0.00779600	-3.33959100	3.35530900
H	0.96229200	-3.83400400	3.28573100
H	-0.79539500	-4.08995500	3.44675000
C	-0.05654500	-2.33782900	4.49540800
H	0.71549000	-1.57100900	4.38054600
H	0.12141200	-2.85855900	5.44156100
H	-1.03602000	-1.85715100	4.55321100
P	2.32313500	0.89727900	0.05326500
C	3.79090100	-0.31680100	0.29478400
C	5.15123700	0.31286500	0.64740900
C	3.90403000	-1.30318800	-0.88418700
H	3.45023400	-0.88438400	1.17268600
C	6.19583400	-0.78442600	0.92710300
H	5.50089300	0.94276600	-0.17779500
H	5.06028300	0.95664800	1.52802000
C	4.95927200	-2.38486800	-0.59404800
H	4.18897600	-0.75968800	-1.79416100
H	2.93199400	-1.77078300	-1.08318200
C	6.32038600	-1.76823900	-0.24382600
H	7.16233200	-0.31542900	1.14125500
H	5.90767700	-1.33258900	1.83488700
H	5.04757100	-3.04797900	-1.46150500
H	4.61413100	-3.00862400	0.24221600
H	7.04090800	-2.55617700	-0.00001200
H	6.71925300	-1.24202700	-1.12228300
C	2.30261500	2.08996700	1.55655000
C	0.86593200	2.55578000	1.86849800
C	3.25040900	3.30042700	1.43944600
H	2.64556900	1.45064700	2.38210900
C	0.82230700	3.42474500	3.13705000
H	0.47703100	3.13361500	1.01767800
H	0.20660700	1.68804800	1.98642200
C	3.20686700	4.15594300	2.71954500
H	2.94192000	3.92217700	0.58910200
H	4.27802300	2.98112200	1.24462600
C	1.78128500	4.61917500	3.04378300
H	-0.20416800	3.76718100	3.30861700
H	1.09426200	2.80555900	4.00317100
H	3.87334400	5.01693200	2.59940300
H	3.60378800	3.56964400	3.55967800
H	1.77053400	5.18672500	3.98032500
H	1.43404200	5.30521500	2.25876700
C	2.43647300	1.94133500	-1.55547500

C	1.74499000	1.23954700	-2.74223600	H	3.62144800	4.98846400	-3.29335400
C	3.85622400	2.40197600	-1.94233500	H	-0.14019000	6.08129200	-1.51676200
H	1.84230600	2.82928500	-1.29778500	H	1.67384700	6.52580000	-3.15789300
C	1.71713300	2.15029800	-3.98222700	C	2.12334600	2.68780100	1.58534200
H	2.27969200	0.31121400	-2.98292500	O	3.19644500	2.83328500	2.11838300
H	0.72314000	0.95454700	-2.46724000	O	0.92609800	2.91954500	2.14645800
C	3.81306600	3.31658200	-3.18101800	C	0.93723000	3.48110400	3.49793500
H	4.47347900	1.52449400	-2.16966000	H	-0.01032800	4.01818800	3.56590500
H	4.33951600	2.92642100	-1.11378600	H	1.76567200	4.18919800	3.56334900
C	3.12156100	2.63349700	-4.36754800	C	1.05009400	2.39165100	4.54959000
H	1.25207600	1.61342600	-4.81644400	H	0.23527200	1.66690600	4.45648500
H	1.07658500	3.01869000	-3.77447300	H	0.99151900	2.84139700	5.54579200
H	4.83424000	3.61061300	-3.44706800	H	2.00705300	1.87088200	4.46905500
H	3.27828200	4.24229300	-2.92762800	P	-2.46920100	-0.87391900	0.07068200
H	3.06459100	3.31965500	-5.21920500	C	-3.95279400	0.32599100	0.27077400
H	3.72503600	1.77633800	-4.69696100	C	-5.30604600	-0.33386300	0.59788100
Au	0.32259700	-0.47877900	0.07158000	C	-4.06186300	1.29873400	-0.91889200
<b>47</b>				H	-3.63931100	0.90288100	1.15201000
C	5.15971400	-1.21982000	0.37849600	C	-6.37692300	0.74477700	0.85224800
C	4.05408200	-0.75148500	-0.22357400	H	-5.62521300	-0.97232900	-0.23308600
C	3.09632900	0.15840600	0.46444900	H	-5.22029400	-0.97261100	1.48260400
H	3.42249000	0.38937800	1.48354800	C	-5.14173200	2.36244000	-0.65250200
H	2.08035400	-0.29368900	0.51460500	H	-4.32379700	0.74264300	-1.82795700
O	2.95964500	1.37526200	-0.29803900	H	-3.09477400	1.78067800	-1.10702100
H	0.94055500	1.68098300	0.07534500	C	-6.49736100	1.72176400	-0.32470500
C	6.16211600	-2.14285900	-0.16585600	H	-7.33752400	0.25651100	1.04860100
C	6.05846500	-2.72999600	-1.44127200	H	-6.11731700	1.30057000	1.76375200
C	7.28424800	-2.45537300	0.62177900	H	-5.22599000	3.01902800	-1.52513300
C	7.04566100	-3.59122100	-1.90872200	H	-4.82345600	2.99629700	0.18670800
H	5.20101500	-2.51435000	-2.07157900	H	-7.23620200	2.49717100	-0.09660800
C	8.27349900	-3.31857100	0.15401100	H	-6.87065100	1.18571000	-1.20836400
H	7.37959500	-2.01111500	1.60937100	C	-2.44030400	-2.05600500	1.58126100
C	8.15750100	-3.88921500	-1.11381800	C	-1.00023700	-2.48556300	1.92558100
H	6.95051200	-4.03413500	-2.89575000	C	-3.35732000	-3.28865200	1.44113000
H	9.13288900	-3.54428000	0.77806300	H	-2.81821300	-1.42129100	2.39455600
H	8.92569200	-4.56231600	-1.48223700	C	-0.96785000	-3.34863900	3.19857700
H	5.35948600	-0.88302400	1.39641700	H	-0.57827200	-3.05693800	1.08664600
H	3.80188500	-1.02677700	-1.24511000	H	-0.36522800	-1.60163600	2.05707000
C	1.98193000	2.24040300	0.10893900	C	-3.32406300	-4.13746000	2.72650500
C	1.88134900	3.43134700	-0.82226300	H	-3.01231400	-3.90507700	0.60119500
C	2.90374400	3.68240600	-1.74521500	H	-4.38714700	-2.99389400	1.22060300
C	0.78552900	4.30285300	-0.74128300	C	-1.89634200	-4.56532500	3.08725600
C	2.82385000	4.79606600	-2.58244600	H	0.06206800	-3.66621100	3.39421200
H	3.75404600	3.01334800	-1.79692300	H	-1.27337400	-2.73236200	4.05543700
C	0.711171900	5.41133500	-1.58207500	H	-3.96715500	-5.01395600	2.59252700
H	-0.00591600	4.11616400	-0.02095300	H	-3.75578100	-3.55729200	3.55345300
C	1.73145800	5.66054500	-2.50467700	H	-1.89589400	-5.12781500	4.02677600
				H	-1.51403200	-5.24701500	2.31496500



C	-2.49047900	-1.90377100	-1.54922900
C	-1.79742900	-1.16949000	-2.71500100
C	-3.88706400	-2.40750500	-1.96870600
H	-1.87242000	-2.77111800	-1.27874100
C	-1.70703900	-2.07707400	-3.95451500
H	-2.36140900	-0.26218500	-2.96727100
H	-0.79378500	-0.84527000	-2.41626800
C	-3.78166800	-3.31732700	-3.20756100
H	-4.52442800	-1.54862500	-2.21000800
H	-4.37352300	-2.94909700	-1.15312500
C	-3.08375800	-2.60900000	-4.37510600
H	-1.24145900	-1.52088200	-4.77526900
H	-1.04087900	-2.92227800	-3.73234300
H	-4.78617500	-3.64329500	-3.49843600
H	-3.22398700	-4.22572800	-2.94138400
H	-2.98065700	-3.29248500	-5.22444100
H	-3.70843900	-1.77378500	-4.72076300
Au	-0.50239200	0.50021500	0.12591200

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C	-2.93049100	0.68094900	-0.13501100
C	-1.90419900	0.07940600	-0.75308800
C	-0.52982000	0.66612700	-0.82878400
H	-0.46380200	1.58842500	-0.23836900
H	-0.28170100	0.91378300	-1.87722400
O	0.40297600	-0.30731200	-0.35196700
H	1.91421100	0.22149800	-1.67366200
C	-4.32125200	0.21220400	-0.04239100
C	-4.80040100	-0.92299000	-0.72321100
C	-5.22459800	0.92732900	0.76345200
C	-6.12514100	-1.32845000	-0.59102300
H	-4.13341900	-1.48923300	-1.36604600
C	-6.55224500	0.52289800	0.89586200
H	-4.87427200	1.80900900	1.29456200
C	-7.00864600	-0.60876500	0.21952200
H	-6.47315700	-2.20788300	-1.12575100
H	-7.22919800	1.09196700	1.52682100
H	-8.04244400	-0.92684100	0.31835300
H	-2.73376400	1.62671900	0.37075000
H	-2.02682600	-0.88124300	-1.24941500
C	1.75225900	-0.00790800	-0.60786900
C	2.60313300	-1.20624600	-0.21530500
C	2.22825800	-2.00217000	0.87337100
C	3.77862000	-1.50253400	-0.91327300
C	3.01899900	-3.08808800	1.25035900
H	1.31237000	-1.77085300	1.40569400
C	4.56978700	-2.58671600	-0.53194700
H	4.07496900	-0.88392600	-1.75599800

C	4.19118500	-3.38270400	0.55091700
H	2.71853100	-3.70482100	2.09275200
H	5.47778500	-2.81236800	-1.08406200
H	4.80456300	-4.22944400	0.84577600
C	2.21901900	1.22522600	0.19361500
O	1.65697400	1.67625100	1.16608800
O	3.35727700	1.71768300	-0.33720900
C	3.96989700	2.83369000	0.35697200
H	5.03385600	2.74786500	0.12419900
H	3.82070200	2.70256300	1.43121900
C	3.39735500	4.15936700	-0.12043600
H	3.50681300	4.26451300	-1.20391200
H	3.92823400	4.98789500	0.36019000
H	2.33841500	4.23566000	0.13841500