

## Supporting Information

### **$\pi$ - $\pi$ stacking assisted regioselectivity regulation in palladium-catalyzed cyclization reactions: a theoretical study**

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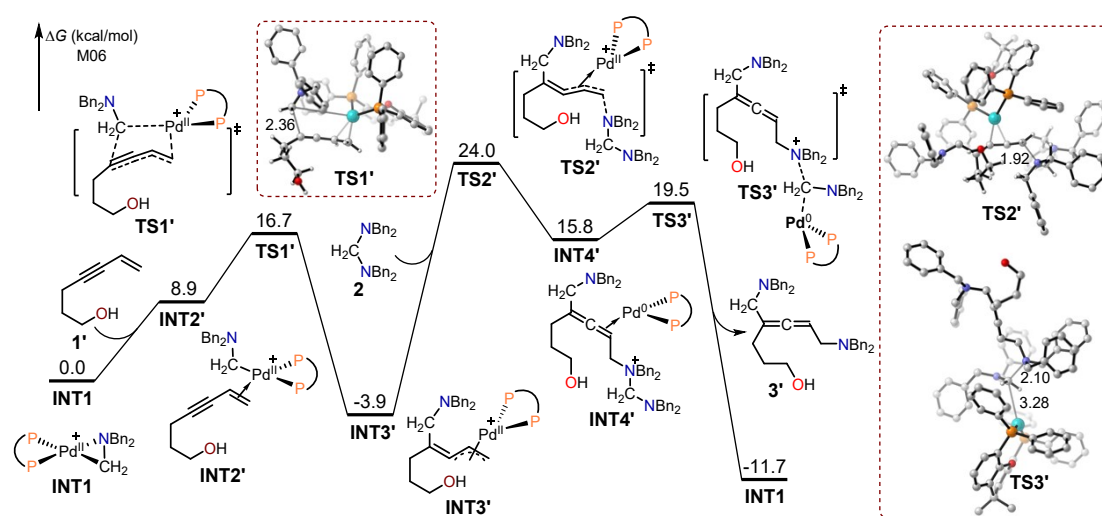
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### 1. The calculated free energy profiles for the production of intermediate **3**, when utilizing hept-6-en-4-yn-1-ol **1'** as the substrate.



**Figure S1.** The calculated free energy profiles for the production of intermediate **3**, when utilizing hept-6-en-4-yn-1-ol **1'** as the substrate.

The calculated free energy profiles for the generation of intermediate **3** using hept-6-en-4-yn-1-ol **1'** as the substrate are presented in Figure S1, with the aminomethyl cyclopalladated complex **INT1** serving as the reference zero point. The binding of the terminal alkene in substrate **1'**, enynols, to the Pd(II) center led to the creation of intermediate **INT2'**, which is 8.9 kcal/mol endergonic. The subsequent migratory insertion of the enyne's triple bond into the Pd(II)-C bond takes place through transition state **TS1'**, resulting in the formation of the  $\pi$ -allylpalladium intermediate **INT3'**, with a free energy barrier of 16.7 kcal/mol. In transition state **TS1'**, the length of the forming C-C bond is 2.36 Å. Intermediate **INT3'** would be intercepted by an aminal leading to the formation of allene-coordinated

Pd(0) intermediate **INT4'** through an S<sub>N</sub>2-type reductive elimination transition state **TS2'**, characterized by an activation free energy of 27.9 kcal/mol. In transition state **TS2'**, the length of the forming C-N bond is 1.92 Å. The following S<sub>N</sub>2-type oxidative addition occurs between Pd(0) and amino cation via transition state **TS3'** with an energy barrier of 3.7 kcal/mol. After release of the allenic 1,5-diamine intermediate **3'**, formation of aminomethyl cyclopalladated complex **INT1** is exothermic by 11.7 kcal/mol in comparison with substrates **1'** and **2**.

## 2. Complete reference for Gaussian 16

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

## 3. B3-LYP and M06 calculated absolute calculation energies, enthalpies, and free energies.

**Table S1.** B3-LYP and M06 calculated absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec-B3-LYP})}^1$	$H_{(\text{corr-B3-LYP})}^2$	$G_{(\text{corr-B3-LYP})}^3$	$E_{(\text{solv-M06})}^4$	IF <sup>5</sup>
<b>INT1</b>	-3027.109473	0.928176	0.783582	-3025.976112	-
<b>1</b>	-500.312248	0.188868	0.137244	-500.080968	-
<b>INT2</b>	-3527.413727	1.119040	0.942451	-3526.058126	-
<b>TS1</b>	-3527.396952	1.117790	0.941423	-3526.0377	-223.1
<b>INT3</b>	-3527.429007	1.119688	0.944885	-3526.074217	-
<b>2</b>	-1232.605335	0.549166	0.459005	-1231.966604	-

<b>TS2</b>	-4760.018624	1.672665	1.437042	-4758.037796	-264.1
<b>INT4</b>	-4760.013064	1.674575	1.436575	-4758.04873	-
<b>TS3</b>	-4760.023258	1.672666	1.425285	-4758.030429	-61.4
<b>3</b>	-1732.949456	0.742253	0.623787	-1732.082023	-
<b>TS4</b>	-4760.029730	1.670402	1.430194	-4758.029331	-200.1
<b>TS5</b>	-3527.375674	1.119259	0.952141	-3526.010973	-332.6
<b>1'</b>	-3027.109473	0.928176	0.783582	-3025.976112	-
<b>INT2'</b>	-3374.984696	1.093453	0.920188	-3373.706063	-
<b>TS1'</b>	-3374.969675	1.092387	0.919278	-3373.692693	-110.2
<b>INT3'</b>	-3375.011045	1.094421	0.926153	-3373.732509	-
<b>TS2'</b>	-4607.591261	1.647388	1.417829	-4605.687348	-272.7
<b>INT4'</b>	-4607.592612	1.649391	1.417716	-4605.700186	-
<b>TS3'</b>	-4607.600836	1.647356	1.406251	-4605.682881	-64.9
<b>3'</b>	-1580.529507	0.716149	0.59903	-1579.732784	-
<b>3-DME</b>	-1887.978889	0.830523	0.694314	-1887.046698	-
<b>TS6</b>	-4915.053918	1.760971	1.499943	-4913.003002	-62.6
HClO <sub>4</sub>	-761.288775	0.031817	-0.002547	-761.2531547	-
<b>INT5</b>	-2523.746025	1.125299	0.959451	-2522.518578	-
<sup>-</sup> ClO <sub>4</sub>	-760.7902275	0.020019	-0.01261	-760.8324357	-
HNBn <sub>2</sub>	-597.2483449	0.269938	0.213608	-596.9369326	-
<b>TS7</b>	-2523.702176	1.120885	0.953815	-2522.474032	-285.7
<b>4</b>	-1135.705789	0.469687	0.385668	-1135.137046	-
<b>TS8</b>	-4915.056385	1.759875	1.501069	-4913.001033	-57.3
<b>INT6</b>	-2523.737286	1.123833	0.95895	-2522.517199	-
<b>TS9</b>	-2523.697545	1.121589	0.956975	-2522.467772	-273.4
<b>5'</b>	-1135.724103	0.470178	0.389378	-1135.15499	-
<b>3'-DME</b>	-1735.563242	0.804512	0.669433	-1734.70397	-
<b>TS6'</b>	-4762.635239	1.735611	1.482829	-4760.659629	-56.7
<b>INT5'</b>	-2371.316051	1.09898	0.934756	-2370.167411	-
<b>TS7'</b>	-2371.277999	1.095269	0.934265	-2370.129793	-240.7

<b>4'</b>	-983.279654	0.444219	0.366248	-982.788770	-
<b>TS8'</b>	-4762.631498	1.735705	1.471804	-4760.64902	-56.9
<b>INT6'</b>	-2371.312899	1.09945	0.934953	-2370.168922	-
<b>TS9'</b>	-2371.275732	1.095169	0.932085	-2370.121173	-149.5
<b>5</b>	-983.300172	0.444354	0.367061	-982.809354	-

<sup>1</sup>The electronic energy calculated by B3-LYP in gas. <sup>2</sup>The thermal correction to enthalpy calculated by B3-LYP in gas. <sup>3</sup>The thermal correction to Gibbs free energy calculated by B3-LYP in gas. <sup>4</sup>The electronic energy calculated by M06 in dimethyl ether solvent. <sup>5</sup>The B3-LYP calculated imaginary frequencies for the transition states.

#### 4. B3-LYP calculated geometries for all the optimized compounds and transition states.

<b>INT1</b>				C	1.52827600	1.54325800	4.39305400
Pd	0.80636600	0.36497100	-0.48960800	C	1.17182500	1.58854800	3.04537600
P	0.25896400	-2.03888700	-0.15960600	C	1.95347900	1.86661200	-1.28525500
P	-0.58670800	1.71521300	0.87389000	C	2.12664500	0.56437600	-3.41926300
O	-2.18664300	-0.80942200	0.65427500	C	0.82628000	1.17074300	-3.89018600
N	2.44640100	0.74310400	-1.96112500	C	-0.40240100	0.53165000	-3.66711100
C	-1.42234200	-2.59893000	-0.67553800	C	-1.59308100	1.10164500	-4.12011100
C	-1.70825100	-3.69409000	-1.50208700	C	-1.57060700	2.31722900	-4.80959700
C	-3.03107600	-4.00415300	-1.82118800	C	-0.35259200	2.95771200	-5.04592600
C	-4.08374100	-3.24495400	-1.30570200	C	0.83669400	2.38600200	-4.58820400
C	-3.84243800	-2.16035600	-0.45416400	C	3.83453500	0.23575900	-1.68588400
C	-2.50579300	-1.86580600	-0.17358500	C	4.33069100	0.38489000	-0.26942200
C	-4.92538500	-1.33654500	0.25561700	C	4.14941100	-0.64669700	0.66162100
C	-4.39647500	0.09760100	0.40617300	C	4.63788300	-0.52188200	1.96366200
C	-3.02266000	0.28361900	0.60877600	C	5.31640800	0.63680800	2.34916400
C	-2.42707900	1.54284500	0.77348900	C	5.51325100	1.66664900	1.42548300
C	-3.27993300	2.65891100	0.80493400	C	5.02801200	1.53702700	0.12317900
C	-4.65351700	2.50597900	0.63147200	H	-0.90162500	-4.29877600	-1.90216600
C	-5.20189500	1.24049300	0.41569000	H	-3.24448400	-4.84946000	-2.46850200
C	-5.13641100	-1.93388500	1.67756400	H	-5.10195900	-3.51578900	-1.56284800
C	-6.26411300	-1.37687800	-0.50226100	H	-2.86631800	3.65067600	0.94643200
C	0.38370900	-2.69724600	1.55779000	H	-5.29986900	3.37807800	0.65422800
C	-0.19072100	-3.92822900	1.91703700	H	-6.27202100	1.14968700	0.26506100
C	-0.06361200	-4.41090400	3.21918800	H	-5.48834700	-2.96893200	1.60576000
C	0.63400300	-3.67058800	4.17800700	H	-5.88406000	-1.35026600	2.22609700
C	1.20389900	-2.44560300	3.83007500	H	-4.20689200	-1.92879600	2.25537200
C	1.07935100	-1.96112000	2.52583000	H	-6.17487300	-0.96103000	-1.51145600
C	1.39333700	-3.13395100	-1.13107200	H	-7.03357000	-0.81623300	0.03611800
C	1.39008700	-3.05926100	-2.53672900	H	-6.63241900	-2.40365300	-0.58255900
C	2.28614400	-3.81206000	-3.29632600	H	-0.74059200	-4.50875600	1.18212300
C	3.21592900	-4.64287500	-2.66422900	H	-0.51228500	-5.36354900	3.48643700
C	3.23200700	-4.72283500	-1.27198900	H	0.72628700	-4.04662100	5.19306200
C	2.32565600	-3.97910300	-0.50984700	H	1.73225900	-1.85555800	4.57345500
C	-0.37491600	3.51161000	0.48195000	H	1.51279700	-1.00203100	2.26416200
C	-0.64804200	3.94121500	-0.83009200	H	0.66700800	-2.42771000	-3.04612200
C	-0.50171400	5.28193600	-1.18219500	H	2.25463800	-3.75422700	-4.38102700
C	-0.06862100	6.21385600	-0.23398400	H	3.91576400	-5.22728600	-3.25436700
C	0.20757100	5.79656500	1.06748500	H	3.94456700	-5.37255100	-0.77160300
C	0.05165600	4.45397800	1.42761400	H	2.34223300	-4.06789300	0.57138800
C	-0.18186300	1.59995000	2.66653900	H	-0.98903400	3.22777400	-1.57669000
C	-1.16853500	1.54830900	3.66083600	H	-0.72385600	5.59763100	-2.19774000
C	-0.80768200	1.48664200	5.00908100	H	0.04917900	7.25798900	-0.50934800
C	0.53808100	1.48849300	5.37817800	H	0.53832500	6.51497600	1.81230700

H	0.25778100	4.14999600	2.44823900	C	-4.57381000	-2.65330300	0.04715600
H	-2.21874100	1.55969200	3.38757800	H	-1.98275700	0.66288900	0.33896600
H	-1.58171700	1.44322600	5.77001000	H	-2.17613200	-0.61543600	-0.97603100
H	0.81505700	1.44820900	6.42784400	H	-0.95010700	-1.62380600	2.77353200
H	2.57856300	1.54548500	4.67115400	H	-1.44408400	0.03856800	2.44322400
H	1.94991500	1.61474800	2.28640100	H	-4.00592000	0.55273000	2.43510700
H	1.38673900	2.57494300	-1.87992700	H	-6.08737900	0.17779900	3.71810500
H	2.61643300	2.30430600	-0.54449200	H	-6.30245100	-1.80865900	5.19816000
H	2.95728200	1.00807600	-3.98447700	H	-4.41447400	-3.41379000	5.39610300
H	2.14911600	-0.51397800	-3.60093800	H	-2.32901100	-3.03925400	4.11523800
H	-0.43238800	-0.41598700	-3.13692500	H	-1.16173500	-3.08729600	0.07427900
H	-2.53574100	0.59121100	-3.94441800	H	-2.19598400	-3.28795400	1.48989100
H	-2.49636600	2.75551700	-5.17123300	H	-2.09266500	-3.98876500	-1.85780200
H	-0.32510900	3.89489200	-5.59437800	H	-4.03407300	-4.56230900	-3.28767100
H	1.78342100	2.88428300	-4.78467500	H	-6.33454800	-3.95215700	-2.56712900
H	3.83241500	-0.81697400	-1.98247600	H	-6.67041300	-2.71575400	-0.42891900
H	4.50734500	0.77137400	-2.36985600	H	-4.73240200	-2.12827600	0.98469500
H	3.64621600	-1.55997700	0.35661400	Pd	0.33725000	0.01740000	-0.61581800
H	4.49919400	-1.33494400	2.67062000	P	0.90161500	1.69704300	1.12529600
H	5.70924900	0.72874100	3.35793300	P	2.11112600	-1.82726000	-0.53391200
H	6.05833400	2.56118400	1.71263200	O	3.23191300	0.92507300	-0.40034700
H	5.20784700	2.33063700	-0.59892900	C	1.95728300	2.84463900	0.13581800
				C	1.73697000	4.22118700	0.00387900
<b>I</b>				C	2.57447200	4.99155900	-0.80440700
C	-3.12057500	-0.74485600	0.00028000	C	3.65057200	4.40436300	-1.47097600
C	-2.43899300	0.47464100	0.00032300	C	3.92018200	3.03468600	-1.34927200
C	-1.04509200	0.51418000	0.00009100	C	3.04716600	2.28782400	-0.55400600
C	-0.31987600	-0.70307700	-0.00010900	C	5.14573100	2.33246400	-1.94863000
C	-1.01876600	-1.92602600	-0.00006000	C	4.75746400	0.88064900	-2.26425600
C	-2.41031900	-1.94684800	0.00006900	C	3.83114900	0.23445800	-1.43638500
H	-4.20732100	-0.75379900	0.00039400	C	3.46044300	-1.11418600	-1.59015900
H	-2.98404100	1.41146300	0.00047500	C	4.07416000	-1.83549700	-2.62518100
H	-0.45203800	-2.85214100	-0.00018200	C	4.99583600	-1.21995000	-3.47039300
H	-2.93727900	-2.89699000	0.00007100	C	5.32693400	0.12345900	-3.29462100
C	1.10532900	-0.70028000	-0.00005200	C	6.26711200	2.31249800	-0.86902600
C	2.32322700	-0.67930700	-0.00028500	C	5.67272900	3.06712300	-3.19477200
C	3.74193300	-0.72224400	-0.00059300	C	1.94697400	1.39962300	2.61744000
H	4.18942600	-1.71646400	-0.00181900	C	2.83992100	2.37512700	3.09284900
C	4.54593400	0.35474500	0.00069700	C	3.56897300	2.15604200	4.26177700
H	5.62562100	0.24270400	0.00047700	C	3.41395400	0.96352800	4.97292200
H	4.14926200	1.36554400	0.00204800	C	2.53403500	-0.01313100	4.50547200
C	-0.29779500	1.82789900	0.00034400	C	1.80922200	0.20253000	3.33184400
H	0.36026000	1.86824500	0.88389200	C	-0.46271000	2.75805500	1.78216000
H	0.36238700	1.86739000	-0.88162400	C	-1.46679000	3.19218800	0.89650600
O	-1.22275400	2.90527000	-0.00128200	C	-2.55431900	3.93521600	1.35947800
H	-0.71429500	3.72893200	0.00230300	C	-2.66381800	4.24544300	2.71726800
				C	-1.67798000	3.81371700	3.60581300
				C	-0.58430800	3.07643200	3.14526100
				C	1.80192700	-3.46964600	-1.33524700
				C	0.78915000	-3.57598100	-2.30181900
				C	0.55431800	-4.78395200	-2.96249300
				C	1.31907600	-5.91051000	-2.65437800
				C	2.32426600	-5.81983000	-1.68928700
				C	2.56811300	-4.60969400	-1.03713300
				C	2.95647500	-2.34083700	1.02606700
				C	4.29184200	-2.03200000	1.31492700
				C	4.87791300	-2.46949000	2.50606200
				C	4.14284100	-3.22907800	3.41598100
				C	2.80890200	-3.54268000	3.13749600
				C	2.21875900	-3.09338400	1.95730800
				H	0.90731400	4.68715000	0.52510900
				H	2.39372400	6.05723900	-0.90774700
				H	4.29150700	5.02850700	-2.08364800

## INT2

N	-1.90968000	-1.31412200	0.93545900
C	-1.79621900	-0.35348300	0.00597500
C	-1.76110600	-1.00437600	2.37302400
C	-3.03117300	-1.23182100	3.16881300
C	-4.09749100	-0.32476500	3.07152100
C	-5.27009200	-0.53341200	3.79669400
C	-5.38983900	-1.64920800	4.63125900
C	-4.33099300	-2.55065400	4.74211100
C	-3.15705700	-2.34058700	4.01430000
C	-2.08191100	-2.73438600	0.55361800
C	-3.27513700	-3.00933300	-0.34571100
C	-3.09373600	-3.69305800	-1.55445500
C	-4.18864500	-4.02314500	-2.35736100
C	-5.47958200	-3.67362900	-1.95631700
C	-5.66872500	-2.98431600	-0.75244000

H	3.82037800	-2.87809300	-2.77909600	C	-6.12830600	-0.21501700	-1.79020800
H	5.45858300	-1.78989700	-4.27036800	C	-5.52935100	1.05825500	-1.17525400
H	6.04534300	0.57966700	-3.96641100	C	-4.29540700	0.96559700	-0.52082300
H	6.55446600	3.33522200	-0.60088700	C	-3.65386600	2.05668200	0.08631900
H	7.15231200	1.79162200	-1.25067000	C	-4.34214400	3.27991300	0.10225600
H	5.93560600	1.80242400	0.04122000	C	-5.58484000	3.39982600	-0.51716400
H	4.92315400	3.10747900	-3.99209900	C	-6.16053700	2.30655000	-1.16656600
H	6.56857600	2.57706500	-3.58617000	C	-6.89568400	-0.98342600	-0.67508100
H	5.96849500	4.09008200	-2.94567900	C	-7.10759200	0.10934300	-2.93248100
H	2.96278800	3.30936300	2.55352700	C	-1.76226200	-2.64406700	0.85728200
H	4.25540800	2.91887700	4.61857700	C	-2.82850500	-3.55721100	0.87827600
H	3.98093100	0.79571600	5.88429400	C	-3.17010800	-4.21942900	2.05885100
H	2.42084300	-0.94956400	5.04292700	C	-2.44951000	-3.98299300	3.23144300
H	1.14725600	-0.57297600	2.96174400	C	-1.39005400	-3.07407800	3.22183600
H	-1.40254400	2.95526100	-0.16121000	C	-1.05330400	-2.40576800	2.04338100
H	-3.31655800	4.26173400	0.65744300	C	-0.05928700	-3.04412300	-1.43444600
H	-3.51202100	4.81932600	3.07961800	C	0.71149100	-2.66815600	-2.54794700
H	-1.75390100	4.05295000	4.66288300	C	1.58485000	-3.57229700	-3.15373100
H	0.17413100	2.75578200	3.85084900	C	1.71726900	-4.86687200	-2.64473700
H	0.18785100	-2.70641000	-2.54260900	C	0.96252100	-5.25158800	-1.53547700
H	-0.22519100	-4.84381900	-3.71743000	C	0.07587000	-4.35120600	-0.93795500
H	1.13448200	-6.85215000	-3.16336300	C	-1.40278100	3.60459700	1.01663400
H	2.92555700	-6.69112500	-1.44527200	C	-1.31224500	4.47382300	-0.08708400
H	3.35871300	-4.55518900	-0.29603000	C	-0.88847900	5.79235400	0.07130900
H	4.88446800	-1.46201200	0.60685200	C	-0.53424100	6.26889400	1.33666300
H	5.91568800	-2.22449900	2.71391900	C	-0.62260000	5.41929700	2.43881500
H	4.60547000	-3.58007200	4.33403100	C	-1.05794300	4.09953200	2.28323800
H	2.23192400	-4.14208200	3.83681500	C	-2.14201800	1.18964900	2.43969400
H	1.18410000	-3.35500700	1.74506200	C	-3.40321800	0.98999400	3.01775400
C	-6.79058700	3.77456000	-2.37123500	C	-3.51410200	0.52136900	4.32904400
C	-6.61769400	2.39091700	-2.45530300	C	-2.36970500	0.26355500	5.08416200
C	-5.34131700	1.82917600	-2.46107400	C	-1.10759800	0.46283800	4.51842000
C	-4.21353100	2.68272300	-2.37553200	C	-0.99492200	0.90768500	3.20141700
C	-4.39976400	4.07816500	-2.29387500	H	-1.98697900	-3.49087900	-3.10562500
C	-5.68149000	4.62007600	-2.29179800	H	-4.02820200	-3.50265800	-4.50096600
H	-7.79353000	4.19209300	-2.37267600	H	-5.91308800	-2.01127500	-3.97866100
H	-7.47415900	1.73015900	-2.52213300	H	-3.89821200	4.14441500	0.58194200
H	-3.52738600	4.72336400	-2.24515300	H	-6.10432200	4.35318900	-0.50209400
H	-5.81413800	5.69655700	-2.23468500	H	-7.11904600	2.43196100	-1.65812700
C	-2.89374800	2.14510800	-2.37511800	H	-7.31480100	-1.91362700	-1.07463100
C	-1.76025800	1.69299800	-2.38987800	H	-7.71746900	-0.37039700	-0.28842300
C	-0.42903400	1.20392200	-2.43009800	H	-6.23596300	-1.23727100	0.16076200
H	0.34799400	1.96530600	-2.49904600	H	-6.61806500	0.65475700	-3.74613400
C	-0.09666000	-0.11987500	-2.77076000	H	-7.94589400	0.71009500	-2.56829700
H	0.86631400	-0.32501000	-3.23060500	H	-7.54214300	-0.80701300	-3.34219800
H	-0.89373000	-0.81578600	-3.02222700	H	-3.39109600	-3.75662800	-0.02850700
C	-5.14152300	0.33509000	-2.55917900	H	-3.99878700	-4.92214100	2.06058600
H	-4.53638000	0.11206800	-3.45430300	H	-2.71741300	-4.49922400	4.14903600
H	-4.55230500	-0.00729500	-1.69141100	H	-0.83636800	-2.87074300	4.13386800
O	-6.39329300	-0.32185700	-2.60856500	H	-0.24684200	-1.67891200	2.05096700
H	-6.21613900	-1.27464300	-2.59309000	H	0.62555300	-1.66228100	-2.94419500
				H	2.16147900	-3.26424200	-4.02178700
				H	2.40022000	-5.57101700	-3.11160200
				H	1.05505200	-6.25753700	-1.13553100
				H	-0.51366800	-4.67394900	-0.08650100
				H	-1.59888100	4.12688700	-1.07434100
				H	-0.83971500	6.44854500	-0.79340600
				H	-0.20386100	7.29623300	1.46138100
				H	-0.36619000	5.78234900	3.43032800
				H	-1.13434000	3.46524700	3.15861500
				H	-4.30233600	1.20779700	2.45079400
				H	-4.49873500	3.69570000	4.76224000
				H	-2.45937500	-0.08752800	6.10830600
<b>TS1</b>							
Pd	-0.52990800	0.58768900	-0.75426900				
P	-1.21156300	-1.79293900	-0.68751700				
P	-1.93090100	1.84750900	0.72856300				
O	-3.65064900	-0.24864900	-0.44202600				
C	-2.69567000	-1.94005400	-1.78254600				
C	-2.80415700	-2.81822900	-2.86924200				
C	-3.95697900	-2.82473400	-3.65570000				
C	-5.02463300	-1.97618200	-3.35775200				
C	-4.96729600	-1.09918900	-2.26791800				
C	-3.78661400	-1.09936500	-1.51998000				

H	-0.21073400	0.27146100	5.10174200	C	-2.15500200	-3.66572900	-2.14258700
H	-0.00756800	1.05973600	2.77264800	C	-3.27831400	-4.45785100	-2.38152400
C	7.23205900	1.42096700	-4.01089600	C	-4.46772300	-4.23433200	-1.68543100
C	6.54098500	2.44687700	-3.36404000	C	-4.56528900	-3.20902100	-0.73833500
C	5.29457600	2.21820800	-2.77482700	C	-3.43035600	-2.41527500	-0.54899400
C	4.73483600	0.92283000	-2.84286300	C	-5.78533100	-2.94487300	0.15578100
C	5.44188600	-0.10624500	-3.48904400	C	-5.86820100	-1.42853300	0.37656600
C	6.67952500	0.14182000	-4.07959200	C	-4.67049600	-0.70769400	0.45088400
H	8.19932900	1.62340200	-4.46169300	C	-4.61246000	0.68156500	0.61549800
H	6.96111000	3.44428800	-3.30809000	C	-5.82573100	1.36193200	0.81469100
H	4.99983700	-1.09827700	-3.54150000	C	-7.03277800	0.66730600	0.79043300
H	7.20698000	-0.66020000	-4.58797700	C	-7.05387400	-0.70839900	0.54909900
C	3.45112800	0.61880000	-2.21509200	C	-5.54166300	-3.63348600	1.53023200
C	2.21944500	0.81186700	-2.31675300	C	-7.08010100	-3.50565300	-0.45731700
C	0.86049400	1.05691200	-2.48332600	C	-0.29586900	-2.23932600	0.88326200
H	0.37958500	0.54773500	-3.31826000	C	-0.36542100	-3.61978000	1.13942900
C	0.20580900	2.18928400	-1.89897400	C	0.01189800	-4.12533200	2.38306500
H	-0.62348600	2.62530100	-2.45320000	C	0.45291400	-3.26051800	3.38862300
H	0.79701300	2.90590900	-1.33333200	C	0.51279800	-1.88760800	3.14676900
C	4.53761800	3.35127800	-2.11334600	C	0.13960300	-1.37940700	1.90055000
H	3.65351100	3.59513100	-2.72636600	C	0.49938400	-2.13302900	-1.95208800
H	4.15423000	3.02504700	-1.13182100	C	0.37601100	-1.72438400	-3.29296200
O	5.39156400	4.47383600	-1.97811300	C	1.28201500	-2.16425500	-4.25621700
H	4.85367200	5.23118200	-1.70570600	C	2.33600300	-3.00815700	-3.89109900
N	3.43962000	-0.96736700	0.45857500	C	2.47351400	-3.40991200	-2.56283700
C	4.20170000	-0.27178300	-0.36566300	C	1.55773700	-2.97930200	-1.59655800
C	3.25593600	-2.42447400	0.28617300	C	-3.54786700	3.28848300	0.15606500
C	3.71500600	-3.20663700	1.50202600	C	-4.21560900	3.57252100	-1.04940200
C	5.06117200	-3.18335200	1.89624000	C	-4.65299300	4.86502000	-1.33200000
C	5.48603600	-3.91239000	3.00609400	C	-4.42083800	5.89900000	-0.41942200
C	4.56954800	-4.67714600	3.73446000	C	-3.75887800	5.62782300	0.77718500
C	3.22956000	-4.70773500	3.34802200	C	-3.32759000	4.32920000	1.06831700
C	2.80398600	-3.97374500	2.23751800	C	-2.28277400	1.59669500	2.16398100
C	2.56861900	-0.30734600	1.46169700	C	-3.00303100	1.15960800	3.28427200
C	3.16347500	0.93728000	2.07961700	C	-2.43132300	1.21869800	4.55753900
C	2.62285400	2.19802600	1.79558200	C	-1.14036200	1.72070200	4.72666000
C	3.15332400	3.34705300	2.38940200	C	-0.41608800	2.16099300	3.61516100
C	4.23582700	3.24356600	3.26341200	C	-0.97848700	2.09441200	2.33988000
C	4.78361100	1.98883600	3.54901600	H	-1.23496300	-3.86229200	-2.68068600
C	4.24848100	0.84199300	2.96444600	H	-3.22298000	-5.26275800	-3.10813200
H	4.90804600	-0.82400000	-0.97264700	H	-5.32070600	-4.87491800	-1.88083900
H	4.47095600	0.73184500	-0.06227600	H	-5.82778700	2.43519400	0.96554300
H	2.20033600	-2.62157200	0.07708200	H	-7.96501900	1.20263000	0.94233400
H	3.81766000	-2.71383100	-0.60640500	H	-8.00911500	-1.21991000	0.50387900
H	5.78182500	-2.59712800	1.33023200	H	-5.44705000	-4.71700600	1.39905300
H	6.53193400	-3.89126700	3.29876900	H	-6.38202900	-3.43810800	2.20556400
H	4.90196800	-5.24834200	4.59644300	H	-4.62715500	-3.26598900	2.00602300
H	2.51354400	-5.30254900	3.90804500	H	-7.30255700	-3.05152500	-1.42864800
H	1.75907300	-4.00313500	1.93791800	H	-7.93112000	-3.33413200	0.20817100
H	1.61131400	-0.07825700	0.97237400	H	-7.00707100	-4.58896400	-0.59012200
H	2.38125900	-1.06237300	2.23114100	H	-0.71759200	-4.30057100	0.37025800
H	1.77636000	2.27851300	1.11753800	H	-0.04332100	-5.19430900	2.56823500
H	2.71373000	4.31639000	2.17210200	H	0.73980500	-3.65646400	4.35874500
H	4.65111000	4.13476400	3.72514800	H	0.83799800	-1.20664200	3.92792300
H	5.62278400	1.90485600	4.23359900	H	0.17355000	-0.30948800	1.72801800
H	4.67092900	-0.13359100	3.19454500	H	-0.44258500	-1.07202100	-3.58790700
				H	1.16658300	-1.84955900	-5.28978100
				H	3.04493900	-3.34864800	-4.64046900
				H	3.29685900	-4.05170600	-2.26484000
				H	1.68748700	-3.30063900	-0.56930200
				H	-4.40832100	2.77594600	-1.76455300
				H	-5.17455300	5.06589600	-2.26357000
				H	-4.75858500	6.90722100	-0.64088000
<b>INT3</b>							
Pd	-1.15957900	0.86002600	-1.00987700				
P	-0.77772000	-1.54620800	-0.75360900				
P	-2.99288500	1.55055800	0.46419300				
O	-3.46587000	-1.36546500	0.34728400				
C	-2.21625900	-2.61551200	-1.21479600				



H	-3.58300600	6.42345400	1.49574200	C	-0.79774400	-0.21540900	-0.91784200
H	-2.82973200	4.13329800	2.01195900	H	-0.83602500	-1.24368700	-1.30539700
H	-4.01092200	0.77461800	3.16732300	N	-1.41809000	-0.15157900	0.40073400
H	-2.99964800	0.87466800	5.41691700	C	-1.42915700	-1.43077300	1.11448200
H	-0.70005700	1.76978900	5.71849600	H	-2.03742000	-1.28551700	2.01641800
H	0.59175200	2.54801100	3.73999100	C	-2.70019300	0.57002200	0.45558300
H	-0.39536900	2.43028300	1.48492900	H	-2.51888300	1.57996300	0.07334400
C	4.97964200	4.20705300	-2.99673600	H	-2.95778600	0.68104800	1.51589500
C	4.10781100	4.66405700	-2.00820700	H	-1.39321300	0.39768600	-1.61451400
C	3.13333500	3.83126500	-1.44412100	N	0.60862400	0.20981600	-0.94676800
C	3.05698400	2.49049000	-1.88049100	C	1.36876800	-0.50023800	-1.98714800
C	3.92805200	2.04147400	-2.88229000	H	1.11734700	-1.56397900	-1.89379100
C	4.88409000	2.88987000	-3.44160000	H	1.06906700	-0.19528200	-3.00935400
H	5.72389400	4.87780800	-3.41576800	C	0.75677800	1.66473900	-1.08544700
H	4.18031200	5.69462300	-1.66942900	H	0.15146100	2.04125400	-1.93473300
H	3.85192000	1.01390100	-3.22459700	H	1.80408700	1.85307300	-1.34731100
H	5.54780800	2.52069600	-4.21815400	C	2.87136600	-0.34468800	-1.84702100
C	2.07894000	1.50410700	-1.29510000	C	3.50503000	-0.66155500	-0.63614900
C	0.87670300	1.48732300	-1.83333800	C	3.65465400	0.07770200	-2.92690000
C	-0.14011300	1.97366900	-2.63202000	C	4.89016400	-0.55798900	-0.51471800
H	-0.30876800	1.55985400	-3.62617600	H	2.90316200	-0.98697000	0.20685300
C	-1.12918200	2.78451900	-2.01037600	C	5.04358300	0.17935000	-2.80825200
H	-2.01875400	3.05856100	-2.56859800	H	3.17327200	0.32919500	-3.86982500
H	-0.83780700	3.48300700	-1.23063000	C	5.66497200	-0.13814000	-1.60044000
C	2.16733300	4.43510200	-0.44755500	H	5.36771500	-0.80907500	0.42914600
H	2.49182200	5.45955800	-0.22823200	H	5.63600600	0.51047600	-3.65739900
H	1.16493500	4.50203300	-0.89716000	H	6.74465300	-0.05833200	-1.50350500
O	2.09863100	3.66645500	0.76318400	C	0.43199400	2.48011800	0.15183900
H	1.82223900	4.26496500	1.47348600	C	-0.47222800	3.54544500	0.08831400
N	3.89218900	0.30453000	0.10694500	C	1.10187600	2.24077600	1.36033900
C	2.50145200	0.63887300	-0.07581000	C	-0.71628800	4.35023200	1.20622800
C	4.79578200	1.34197600	0.61629300	H	-0.98656700	3.75423900	-0.84797100
C	5.82390500	0.83057500	1.61253000	C	0.86245300	3.03998900	2.47630300
C	5.42453400	0.28784700	2.84194800	C	-0.05056200	4.09809700	2.40458900
C	6.36814700	-0.14593900	3.77066200	H	-1.42430400	5.17220800	1.13623300
C	7.73320100	-0.04325600	3.48421200	H	-0.23529700	4.72133300	3.27570500
C	8.14314900	0.49560200	2.26537100	H	-1.92865000	-2.22414400	0.52807100
C	7.19141800	0.92964900	1.33813900	C	-3.87984100	-0.05047500	-0.28777500
C	4.48244000	-0.67085100	-0.80414500	C	-4.21588700	0.37214600	-1.58231200
C	4.86114600	-2.01493100	-0.18904700	C	-4.65667400	-1.06196500	0.29772300
C	4.20742700	-2.52352000	0.93817900	C	-5.27698900	-0.20858900	-2.27962400
C	4.51199400	-3.79687600	1.42487000	H	-3.64803000	1.17650700	-2.04508900
C	5.47820200	-4.58111800	0.79127600	C	-5.71771400	-1.64778500	-0.39436100
C	6.14316500	-4.07855900	-0.32976500	H	-4.43710400	-1.38568600	1.31244400
C	5.83503600	-2.80530500	-0.81287200	C	-6.02890400	-1.22542900	-1.68865300
H	2.17013600	1.19900200	0.80415100	H	-5.52078600	0.13863300	-3.28049200
H	1.91899600	-0.28549000	-0.11632600	H	-6.30708000	-2.42815000	0.08042300
H	5.32791900	1.84637500	-0.20612300	H	-6.85726100	-1.67770400	-2.22748600
H	4.17241300	2.10612900	1.09267400	C	-0.06254000	-1.93305900	1.54487100
H	4.36355600	0.20109500	3.06514300	C	0.69653900	-1.21445400	2.47967200
H	6.04281900	-0.56340900	4.72012900	C	0.43212000	-3.15464000	1.07720400
H	8.46959900	-0.38154500	4.20799600	C	1.91786100	-1.70810000	2.93488300
H	9.20159100	0.57858900	2.03352300	H	0.32311100	-0.25990300	2.83949600
H	7.51642300	1.35359000	0.39014500	C	1.65945900	-3.65258800	1.52686900
H	3.76886600	-0.86715100	-1.61689200	H	-0.15177900	-3.72753400	0.35965500
H	5.37162800	-0.24029700	-1.28712900	C	2.40420300	-2.93164100	2.45956400
H	3.47070000	-1.90730400	1.44414700	H	2.49122400	-1.14312900	3.66582300
H	3.99598200	-4.17354100	2.30446500	H	2.02799600	-4.60345000	1.15074500
H	5.71962800	-5.56932700	1.17311300	H	3.35504600	-3.31809500	2.81718600
H	6.90920000	-4.67263000	-0.82132600	H	1.80724000	1.41720400	1.41546800
H	6.36296500	-2.41862200	-1.68289200	H	1.39248100	2.84355100	3.40529200

Pd	0.61353200	0.80974500	-0.07464200	H	5.40006200	-0.59277700	4.67868600
P	2.50279900	1.64130100	1.22871700	H	5.03870700	0.73810100	2.63905400
P	0.17655000	2.40310100	-1.98560500	H	-2.63221600	2.91772100	-1.40605500
O	1.75420900	4.09710100	-0.14866000	H	-4.73403600	2.64467100	-2.66945200
C	2.17766100	3.28540700	2.02574100	H	-4.70541000	1.65098000	-4.95358600
C	2.27235800	3.53357300	3.40238900	H	-2.53992200	0.95727500	-5.96299200
C	2.07298700	4.82092600	3.90298900	H	-0.43145200	1.28547800	-4.73146000
C	1.81412500	5.88622300	3.03932500	H	1.95312000	4.04878200	-3.77477900
C	1.72703200	5.68630400	1.65684600	H	3.72771500	3.42209500	-5.37231600
C	1.87758600	4.37442500	1.19678300	H	4.29620000	1.03076400	-5.74157000
C	1.58199800	6.80448800	0.61454200	H	3.07512600	-0.74116800	-4.46551700
C	0.75868500	6.24716900	-0.55396900	H	1.34700400	-0.12437400	-2.84798400
C	0.88252500	4.88693000	-0.86317300	C	-0.10168900	-6.32576800	-0.30962300
C	0.15139100	4.25308200	-1.87781500	C	0.01444400	-5.54284100	-1.45977800
C	-0.65177500	5.06682200	-2.69367300	C	0.42183600	-4.20260300	-1.40521200
C	-0.75691600	6.43387800	-2.44659200	C	0.74573800	-3.64225400	-0.14395300
C	-0.08089500	7.01126600	-1.36984800	C	0.59632400	-4.42924000	1.00632400
C	3.00289500	7.16463500	0.09092600	C	0.17570300	-5.75917800	0.93254200
C	0.93980500	8.06812600	1.21353700	H	-0.41834900	-7.36183600	-0.38568700
C	4.14212100	1.95189900	0.43210600	H	-0.22872500	-5.97802400	-2.42687600
C	5.10598100	2.79129500	1.01787100	H	0.82772700	-3.98944700	1.97227700
C	6.33429700	3.00310400	0.39146200	H	0.07521700	-6.34735300	1.84051800
C	6.61446700	2.38729200	-0.83132600	C	1.28125300	-2.24232900	-0.01153900
C	5.65896900	1.56383200	-1.42720600	C	0.44785900	-1.23876200	0.26396000
C	4.42911600	1.34937600	-0.80064700	C	-0.85486100	-0.77736500	0.52805900
C	2.88171400	0.61282400	2.72025200	H	-1.09395900	-0.59223000	1.57598000
C	1.79401700	0.09446400	3.44488600	C	-1.90135200	-0.51676600	-0.41797200
C	1.99976500	-0.64232100	4.61097800	H	-2.56267500	0.32260900	-0.23869000
C	3.29923500	-0.88931800	5.06290000	H	-1.68426400	-0.69825700	-1.46650100
C	4.38661100	-0.39187000	4.34449700	C	0.39560200	-3.39408900	-2.69573500
C	4.18081800	0.35923300	3.18363200	H	0.00442900	-4.03784100	-3.49864300
C	-1.37203700	2.11625600	-2.97274600	H	-0.30287400	-2.55536700	-2.59108700
C	-2.60548100	2.47880000	-2.40110200	O	1.61685800	-2.78754900	-3.09325200
C	-3.79516900	2.32435400	-3.11336400	H	2.29612300	-3.47985800	-3.18786500
C	-3.77942900	1.77058000	-4.39814200	N	3.76230400	-2.95889200	0.26927600
C	-2.56536200	1.38246000	-4.96333100	C	2.78579700	-2.02304400	-0.27645300
C	-1.36877600	1.56297600	-4.26144600	C	3.99376300	-4.22797700	-0.42000600
C	1.51423100	2.01313800	-3.19652900	C	4.45464700	-4.09187400	-1.86014700
C	2.19963400	3.00133200	-3.91722200	C	5.37129400	-3.10415100	-2.24579600
C	3.20202500	2.64583800	-4.82295900	C	5.82252400	-3.02735600	-3.56418500
C	3.52228400	1.30239400	-5.02869700	C	5.36802300	-3.93777000	-4.52270000
C	2.84213700	0.30915500	-4.31863700	C	4.46024600	-4.93057200	-4.15038700
C	1.85210500	0.66325800	-3.40096800	C	4.00608800	-5.00351800	-2.82853900
H	2.50264200	2.72291300	4.08412400	C	3.82319700	-3.06878700	1.72584600
H	2.13957700	4.99818500	4.97232000	C	5.22955900	-3.31872700	2.24845100
H	1.69166500	6.88161400	3.45222400	C	6.30320900	-2.52388600	1.82083100
H	-1.21464600	4.62668000	-3.50891000	C	7.58427200	-2.72072100	2.33562700
H	-1.38251600	7.05097600	-3.08468700	C	7.81393800	-3.71788000	3.28870800
H	-0.20547800	8.07126900	-1.17684300	C	6.75404400	-4.51658800	3.71884700
H	3.62534300	7.54037600	0.91071100	C	5.47237800	-4.31709000	3.19835100
H	2.93722800	7.94112800	-0.67952600	H	2.92351300	-1.99796700	-1.35991500
H	3.50098400	6.29246000	-0.34391600	H	3.03081900	-1.02875600	0.10614100
H	-0.06740900	7.87122100	1.59572200	H	4.79123800	-4.73247700	0.14149600
H	0.87683900	8.86458000	0.46640900	H	3.12534400	-4.90540600	-0.38279900
H	1.54988000	8.46155500	2.03186500	H	5.72491800	-2.39744400	-1.50124200
H	4.89556300	3.28585200	1.96162500	H	6.53766800	-2.25810400	-3.84437300
H	7.07052200	3.65311100	0.85639000	H	5.72317700	-3.87788000	-5.54764200
H	7.56970900	2.55831000	-1.32005600	H	4.10686800	-5.65034400	-4.88407300
H	5.85708300	1.09802200	-2.38824000	H	3.30814500	-5.78692000	-2.53869000
H	3.68417700	0.72937800	-1.28708000	H	3.45182900	-2.12455900	2.13724500
H	0.78134500	0.27697000	3.09472800	H	3.15939500	-3.85982700	2.11531300
H	1.14687300	-1.02483700	5.16545700	H	6.12484200	-1.75266200	1.07639000
H	3.46233700	-1.47013000	5.96628300	H	8.40641100	-2.09740600	1.99315200

H	8.81271900	-3.87309400	3.68749800
H	6.92394300	-5.29996600	4.45276800
H	4.65033100	-4.94649900	3.53355600
C	-4.16417900	-1.47762400	1.01207100
H	-5.03688000	-2.13534300	1.03766700
N	-3.43005400	-1.75796800	-0.28297300
C	-4.18887200	-1.46330000	-1.54956200
H	-3.95550500	-0.42791900	-1.81117900
C	-2.76671900	-3.10359900	-0.24550800
H	-2.07899900	-3.07045000	0.60379900
H	-2.14599000	-3.15278700	-1.14172900
H	-3.48195800	-1.81607300	1.79602300
N	-4.55436600	-0.09980400	1.21995500
C	-6.01369500	0.09667000	1.33195600
H	-6.48239700	-0.51700300	0.55892800
H	-6.39433200	-0.27098600	2.29811700
C	-3.79407600	0.60914400	2.28654800
H	-4.09943300	1.65776500	2.23801300
H	-2.73492900	0.58294200	2.01868900
C	-6.45984400	1.53499700	1.13960000
C	-5.81287500	2.39575000	0.24299300
C	-7.58263900	2.00938100	1.82996300
C	-6.27672000	3.69686200	0.04197100
H	-4.93492500	2.03814500	-0.28643800
C	-8.05632300	3.30678900	1.62295500
H	-8.09540900	1.35499800	2.53188100
C	-7.40319300	4.15623400	0.72864300
H	-5.75698800	4.35597500	-0.64923100
H	-8.93029700	3.65497200	2.16653900
H	-7.76439100	5.16879200	0.57255800
C	-3.97360800	0.09127100	3.70582500
C	-3.09081800	-0.85448900	4.25028000
C	-5.02757300	0.55351900	4.50974300
C	-3.26884900	-1.34594600	5.54526700
H	-2.23922800	-1.19750300	3.66512000
C	-5.20893600	0.06571400	5.80478200
C	-4.33360600	-0.89044600	6.32430900
H	-2.57113300	-2.07506400	5.94873200
H	-4.47241300	-1.26713400	7.33373600
H	-3.72420300	-2.09004800	-2.31872500
C	-3.62086800	-4.35200700	-0.16752600
C	-4.13501200	-4.81634700	1.05298600
C	-3.85642600	-5.11006900	-1.32398600
C	-4.89823900	-5.98335600	1.10751500
H	-3.93072600	-4.27041200	1.97053200
C	-4.61406100	-6.28099600	-1.27249800
H	-3.44126600	-4.78214400	-2.27408800
C	-5.14396300	-6.71618200	-0.05631600
H	-5.29156000	-6.32615000	2.06037700
H	-4.78736400	-6.85303800	-2.17958100
H	-5.73416500	-7.62702300	-0.01263900
C	-5.70535600	-1.60464000	-1.61687300
C	-6.41971800	-0.53018000	-2.17104100
C	-6.42239600	-2.75097800	-1.24080900
C	-7.80311400	-0.59035800	-2.34152700
H	-5.88435500	0.36543200	-2.47240600
C	-7.80874000	-2.80723200	-1.39835400
H	-5.90937800	-3.60670200	-0.82276300
C	-8.50519500	-1.73050600	-1.94958900
H	-8.33016900	0.25686300	-2.77101700
H	-8.34286800	-3.70278300	-1.09323300
H	-9.58323000	-1.78039400	-2.07305000
H	-5.69958400	1.31566100	4.12307400

H	-6.02856200	0.43980100	6.41213600
<b>INT4</b>			
Pd	0.28395100	0.79177200	-0.26251800
P	1.97705500	2.08350300	0.98731500
P	-0.66520100	2.27069400	-2.04084500
O	0.42625500	4.28139500	-0.20213300
C	1.26304200	3.54920700	1.88411700
C	1.40671100	3.77385000	3.26159200
C	0.88005800	4.92308100	3.85342900
C	0.23043700	5.88526900	3.07842900
C	0.08077900	5.71276400	1.69820800
C	0.57969300	4.52642100	1.14703600
C	-0.49459600	6.76689800	0.74149800
C	-1.22168700	6.02201000	-0.38480000
C	-0.70987700	4.78510800	-0.79510000
C	-1.29583600	3.99686800	-1.79679700
C	-2.39215000	4.54348000	-2.48312000
C	-2.90241800	5.79041900	-2.12648300
C	-2.33758900	6.50994100	-1.07172000
C	0.69402600	7.55899900	0.12254400
C	-1.42381600	7.75643500	1.46589700
C	3.45400000	2.85580700	0.18146600
C	4.13472600	3.94893400	0.74441700
C	5.25440600	4.48930800	0.11108000
C	5.70923200	3.94925900	-1.09443600
C	5.03597500	2.86935800	-1.66631400
C	3.91428100	2.32915100	-1.03358300
C	2.68211500	1.13644500	2.41492200
C	1.80531400	0.31749600	3.14869400
C	2.25511100	-0.38807700	4.26418100
C	3.59576800	-0.30527800	4.65182800
C	4.47787500	0.49091400	3.92179000
C	4.02374800	1.21421200	2.81501300
C	-2.05985700	1.52959900	-3.02323700
C	-3.33037800	1.43972300	-2.42621500
C	-4.40788500	0.87997000	-3.11351100
C	-4.23063600	0.36827800	-4.40309100
C	-2.96999000	0.43170100	-4.99796700
C	-1.89623200	1.01548000	-4.31882000
C	0.65910900	2.45198300	-3.31817300
C	0.85559000	3.62977200	-4.05293400
C	1.86213500	3.70215300	-5.01868600
C	2.67621800	2.59699400	-5.27225700
C	2.48724900	1.41706400	-4.54830700
C	1.49248000	1.34887900	-3.57168200
H	1.93499100	3.05039100	3.87215600
H	0.99712900	5.08090000	4.92173700
H	-0.14716700	6.78194500	3.55762600
H	-2.86213300	3.98364000	-3.28378300
H	-3.75260500	6.19943900	-2.66444000
H	-2.76863600	7.46594200	-0.79489600
H	1.25252700	8.08004200	0.90818100
H	0.32277100	8.30271900	-0.59153800
H	1.38554900	6.89419800	-0.40422600
H	-2.28274900	7.25145700	1.92061900
H	-1.79652500	8.51736400	0.77402600
H	-0.88224100	8.29275800	2.25056100
H	3.79079900	4.38110400	1.67926500
H	5.77080400	5.33373400	0.55950900
H	6.57960800	4.37347300	-1.58736200
H	5.37235300	2.45248400	-2.61137300
H	3.38352000	1.50579200	-1.49858100

H	0.76470300	0.23792000	2.84653300	H	4.08756000	-3.01957100	1.58859600
H	1.56034600	-1.00611700	4.82719300	H	6.02632200	-0.11489900	0.11370800
H	3.95131500	-0.86456300	5.51274300	H	8.30160400	0.50037000	0.88188100
H	5.52598200	0.54343400	4.20058800	H	9.41139700	-0.81720600	2.67802100
H	4.72581400	1.82647100	2.26005600	H	8.22549600	-2.75617100	3.69167000
H	-3.49038200	1.84155100	-1.42873700	H	5.94742800	-3.35557100	2.92362800
H	-5.38571100	0.86105000	-2.64159700	C	-3.69393200	-2.05724400	1.12835200
H	-5.07024700	-0.05932400	-4.94479700	H	-4.35360600	-2.88211500	1.39075200
H	-2.82205200	0.04857200	-6.00417400	N	-2.88873200	-2.59019200	-0.10748300
H	-0.93233700	1.08333100	-4.81170800	C	-3.75111500	-3.00475700	-1.31945100
H	0.22360000	4.49378800	-3.87318000	H	-3.68183200	-2.16860700	-2.01478300
H	2.00579300	4.62366600	-5.57607000	C	-1.99315300	-3.74595400	0.37086700
H	3.45467500	2.65478100	-6.02791800	H	-1.36622500	-3.31554800	1.15146200
H	3.12152600	0.55443300	-4.73561900	H	-1.33747900	-3.96266800	-0.47257400
H	1.36279000	0.43626700	-2.99361300	H	-2.92137900	-1.96774900	1.89669000
C	1.13299200	-6.37681800	0.00343900	N	-4.42815900	-0.84915100	0.95412100
C	1.02573100	-5.74649500	-1.23533400	C	-5.88388600	-0.97255800	1.27275800
C	1.13079200	-4.35349800	-1.35894200	H	-6.26821900	-1.79883400	0.67209900
C	1.36858700	-3.57308000	-0.20382300	H	-6.03323100	-1.24545700	2.32738500
C	1.45631200	-4.21892200	1.03977100	C	-3.76495800	0.38202300	1.42297500
C	1.33952900	-5.60510800	1.14831200	H	-4.47671000	1.19558800	1.25590700
H	1.05272500	-7.45763800	0.07509400	H	-2.91640100	0.59984500	0.76722400
H	0.86218200	-6.34116000	-2.13143300	C	-6.69785200	0.27232100	0.98754800
H	1.63645300	-3.61741500	1.92640300	C	-7.14182600	0.56010500	-0.31078000
H	1.41708600	-6.08062800	2.12232000	C	-7.05651600	1.14158700	2.02677400
C	1.55044700	-2.08321800	-0.28304800	C	-7.91396000	1.69352900	-0.56676000
C	0.55240900	-1.25536600	0.04773500	H	-6.89898800	-0.12575100	-1.11681600
C	-0.81395200	-1.04786700	0.26493700	C	-7.82773100	2.27839100	1.77475000
H	-1.12517100	-0.78864500	1.27851300	H	-6.72876100	0.92733000	3.04146700
C	-1.92579400	-1.46751300	-0.65778100	C	-8.25631600	2.55798200	0.47644200
H	-2.62149600	-0.66487500	-0.90224000	H	-8.25974000	1.89717100	-1.57673000
H	-1.52284200	-1.87036600	-1.58985700	H	-8.09779300	2.93970200	2.59319000
C	0.99042500	-3.74329200	-2.73622700	H	-8.86174100	3.43807600	0.27901200
H	0.20470100	-4.28199200	-3.29001900	C	-3.26531800	0.45000000	2.86607600
H	0.68221700	-2.69148500	-2.65287200	C	-3.75691100	-0.34408200	3.91123800
O	2.23674500	-3.85557400	-3.42525000	C	-2.27709500	1.40174100	3.16625200
H	2.11486600	-3.52478000	-4.32948500	C	-3.27991200	-0.18797800	5.21671700
N	4.14394200	-2.17209000	-0.35917100	H	-4.51891400	-1.09312300	3.72085300
C	2.89970800	-1.57034200	-0.82682800	C	-1.80677700	1.56751400	4.46880700
C	4.56372400	-3.43277600	-0.98122300	C	-2.30720100	0.76986500	5.50125700
C	6.03591600	-3.49953300	-1.36398700	H	-3.67708300	-0.81434500	6.01104200
C	6.62329300	-2.48977200	-2.13784700	H	-1.94170700	0.89414200	6.51661300
C	7.94865600	-2.59049300	-2.55684900	H	-3.20707000	-3.84224100	-1.76475100
C	8.71227300	-3.70933900	-2.21027600	C	-2.65231600	-5.01438500	0.85020600
C	8.13847600	-4.72096800	-1.44064600	C	-3.08359900	-5.15902200	2.17882400
C	6.80952400	-4.61296800	-1.02220800	C	-2.75599400	-6.11645800	-0.01232100
C	4.39032100	-2.08786200	1.07863300	C	-3.64985200	-6.35632600	2.61736000
C	5.82488300	-1.76990700	1.47365400	H	-2.96361100	-4.33760500	2.88060200
C	6.50524200	-0.68432400	0.90544700	C	-3.31818600	-7.31640700	0.42470900
C	7.78622500	-0.34232000	1.33601100	H	-2.37799600	-6.04177900	-1.02860000
C	8.41107300	-1.08156900	2.34550400	C	-3.77552900	-7.43542100	1.73849100
C	7.74509400	-2.16723500	2.91444300	H	-3.97914500	-6.45162600	3.64800200
C	6.46128200	-2.50605500	2.47784000	H	-3.39092600	-8.15858600	-0.25714500
H	2.88990200	-1.68146600	-1.91881100	H	-4.21089600	-8.36934400	2.08180500
H	2.93089700	-0.49609400	-0.61536500	C	-5.22263300	-3.34767100	-1.17868200
H	4.32985600	-4.29212300	-0.33005500	C	-6.10369900	-2.67016300	-2.03792000
H	3.97134700	-3.57055800	-1.89065600	C	-5.74336300	-4.36281900	-0.36082000
H	6.03369100	-1.61426900	-2.39822100	C	-7.46250900	-2.98521700	-2.07581100
H	8.38961900	-1.79682100	-3.15517200	H	-5.71641800	-1.89352000	-2.69263200
H	9.74615800	-3.78814100	-2.53570500	C	-7.10653800	-4.66417300	-0.38422000
H	8.72460500	-5.59238200	-1.16019300	H	-5.09635800	-4.92791600	0.29672300
H	6.36796700	-5.40467000	-0.42018400	C	-7.97105000	-3.98042200	-1.24053700
H	3.74451200	-1.29751700	1.47708700	H	-8.12143100	-2.45100800	-2.75427400

H	-7.48889200	-5.44796600	0.26335000
H	-9.02897500	-4.22494700	-1.26062600
H	-1.87137600	2.02154000	2.36916200
H	-1.04635000	2.31635400	4.67103000

**TS3**

C	-4.96067500	-2.97868400	-1.12260100
C	-5.82096500	-4.07459600	-0.96056200
C	-5.31886000	-5.34763800	-1.24603000
C	-4.01298000	-5.51710100	-1.70451800
C	-3.18649600	-4.41034000	-1.88094400
C	-3.63518100	-3.11316100	-1.58467500
H	-5.95197400	-6.21928400	-1.12341900
H	-3.64194200	-6.51247400	-1.93034800
H	-2.17142400	-4.55688100	-2.23466300
C	-7.27377400	-3.79219200	-0.56067800
C	-7.96222700	-5.03381400	0.03164000
H	-9.00507700	-4.81693700	0.28023800
H	-7.45750200	-5.39081000	0.93582300
H	-7.98401300	-5.84905500	-0.69724300
C	-8.05445000	-3.35693900	-1.83596000
H	-9.09272600	-3.11735700	-1.58034100
H	-8.05580800	-4.16718800	-2.57363200
H	-7.60372700	-2.47412200	-2.29931300
C	-7.26294700	-2.61507800	0.42183200
C	-8.16323900	-2.47065800	1.48159600
C	-6.33929700	-1.58266200	0.20006200
C	-8.15915000	-1.32391400	2.27485400
H	-8.88573500	-3.25233100	1.68818900
C	-6.30634900	-0.40944500	0.98218200
C	-7.24640200	-0.30336500	2.02053900
H	-8.87171000	-1.22385600	3.08827700
H	-7.25157500	0.58380800	2.64483800
O	-5.43061100	-1.71022400	-0.83466800
P	-2.54827700	-1.62353600	-1.80927000
P	-5.06364800	0.93683300	0.67406500
C	-2.84869300	-1.16558200	-3.57527100
C	-2.83858900	-2.11182600	-4.61368100
C	-3.12591800	0.17489000	-3.88172000
C	-3.08661100	-1.72051200	-5.92901100
H	-2.64451500	-3.15816200	-4.39637900
C	-3.37708300	0.56551000	-5.19942000
H	-3.16523500	0.90245600	-3.07464900
C	-3.35515400	-0.38070900	-6.22434600
H	-3.07652700	-2.46198200	-6.72318800
H	-3.60047800	1.60552100	-5.42146600
H	-3.55427900	-0.07976700	-7.24918300
C	-0.84189600	-2.34851200	-1.81371900
C	-0.40265400	-3.06699100	-0.68463300
C	0.08091100	-2.08883200	-2.83939200
C	0.91047100	-3.53085400	-0.59794800
H	-1.09706000	-3.28302600	0.12327600
C	1.40074900	-2.54249000	-2.74462100
H	-0.23053700	-1.54167500	-3.72347800
C	1.81934400	-3.26832800	-1.62877500
H	1.21981200	-4.10906800	0.26913000
H	2.09590000	-2.33567100	-3.55391300
H	2.83934200	-3.63754900	-1.56495900
C	-5.94297800	2.09371900	-0.46850100
C	-7.33754500	2.11227100	-0.62087500
C	-5.16957900	3.00234400	-1.21025600
C	-7.94240100	3.02052300	-1.49291900
H	-7.95493300	1.41626300	-0.06167600

C	-5.77549000	3.91787200	-2.07087900
H	-4.08645300	2.98055800	-1.11395000
C	-7.16483400	3.92629600	-2.21645500
H	-9.02319800	3.01960100	-1.60469900
H	-5.16413800	4.61774100	-2.63451300
H	-7.63818400	4.63192200	-2.89348400
C	-5.05980500	1.84661000	2.28924200
C	-5.62229000	3.12010000	2.45851500
C	-4.40935800	1.24531300	3.38237200
C	-5.53534500	3.77681100	3.69025900
H	-6.13453700	3.60224100	1.63221200
C	-4.33818000	1.89487500	4.61426300
H	-3.96325800	0.25982100	3.26936000
C	-4.89741100	3.16723100	4.77059500
H	-5.97727300	4.76311500	3.80374900
H	-3.84591000	1.40902900	5.45286500
H	-4.83804800	3.67594000	5.72875900
pd	-3.18529900	-0.00135100	-0.29528400
C	-0.30764900	0.94105100	0.76890200
H	-1.04426100	1.69826200	0.52798800
N	-0.10231300	0.66308800	2.04889500
C	0.49098900	-0.64044100	2.44422100
H	1.43053200	-0.47248600	2.97821400
C	-0.64687800	1.53240300	3.12215700
H	-1.55099900	2.00542000	2.73016900
H	-0.97365800	0.85532700	3.91719600
H	-0.16949200	0.13759000	0.05775500
H	0.73891400	-1.16378800	1.51656700
C	0.28169700	2.59072200	3.69113300
C	-0.17367100	3.91393700	3.77317900
C	1.54677900	2.28214500	4.21504700
C	0.61513500	4.90902100	4.35525100
H	-1.16057800	4.16609900	3.39158600
C	2.34111600	3.27742400	4.78666500
H	1.91691200	1.26113100	4.19652500
C	1.87709700	4.59376000	4.86009500
H	0.24222300	5.92756200	4.41196400
H	3.31725000	3.02037400	5.18832200
H	2.49245400	5.36471600	5.31477000
C	-0.44881200	-1.48504300	3.28423200
C	-1.71712600	-1.84187500	2.79879600
C	-0.04765000	-1.94223700	4.54509300
C	-2.55959400	-2.65048800	3.56237000
H	-2.05857600	-1.47381600	1.82992000
C	-0.89043500	-2.75668300	5.30694100
H	0.93053800	-1.66570900	4.93133200
C	-2.14660000	-3.11284500	4.81619400
H	-3.53825400	-2.92148900	3.17555600
H	-0.56501300	-3.10714500	6.28222700
H	-2.80311900	-3.74540100	5.40678800
C	6.76580000	-0.08161500	-4.73206000
C	7.23853100	0.95441100	-3.92801000
C	6.86649700	1.06750300	-2.58220400
C	6.00181400	0.09788200	-2.02743200
C	5.51553800	-0.92980400	-2.85159800
C	5.89253800	-1.02514300	-4.19012500
H	7.07228400	-0.14802800	-5.77194300
H	7.91048100	1.69877100	-4.34850600
H	4.83952200	-1.66435100	-2.42306900
H	5.50841800	-1.83404700	-4.80564600
C	5.56904800	0.14059000	-0.59017400
C	4.29589300	0.27121300	-0.29551800
C	3.04313200	0.45753800	0.05112800

H	2.39608200	-0.40854100	0.18849600	H	1.04397500	5.19035500	-2.14305800
C	2.48784300	1.83179100	0.35024500	C	3.38273800	6.13779900	0.79422700
H	2.35527300	1.95654500	1.43408300	H	2.48751500	4.49508100	1.84914700
H	3.21189800	2.58758900	0.03119900	C	3.40586500	6.88575700	-0.38431100
C	7.40890900	2.22732900	-1.77964600	H	2.55596300	7.12374100	-2.35244100
H	7.54892800	3.09076400	-2.44570500	H	4.02568700	6.40981200	1.62689700
H	6.69038000	2.52211200	-1.00104400	H	4.07155600	7.73937900	-0.47721700
O	8.66074200	1.84178600	-1.20046500				
H	9.04121500	2.62022200	-0.76239700	<b>3</b>			
N	7.22836000	-1.32460400	0.69974400	C	0.74166400	-4.92324400	0.59466700
C	6.59718900	-0.01806400	0.55822400	C	0.71532700	-3.88986000	1.52919700
C	8.26723400	-1.64274500	-0.29238200	C	0.66991100	-2.54576600	1.13533000
C	9.29686000	-2.62501100	0.23873600	C	0.63725900	-2.23437300	-0.24288300
C	9.96825800	-2.37278400	1.44396600	C	0.67288300	-3.28814100	-1.17525300
C	10.94076300	-3.25341300	1.91508100	C	0.72604200	-4.61963500	-0.76841400
C	11.25943900	-4.40360600	1.18658600	H	0.77649400	-5.95751800	0.92711800
C	10.59794500	-4.66511400	-0.01322300	H	0.75265200	-4.10699700	2.59217600
C	9.62179600	-3.78063300	-0.48033200	H	0.63099300	-3.05968500	-2.23683200
C	6.31760200	-2.43532700	0.95841700	H	0.74579300	-5.41303400	-1.51110400
C	5.58620400	-2.35010200	2.28697000	C	0.52469800	-0.83330600	-0.75451000
C	6.22794900	-1.87939000	3.44085100	C	-0.40589600	-0.02606800	-0.28720600
C	5.57079100	-1.87844700	4.67180800	C	-1.34923500	0.78037100	0.13114800
C	4.26284700	-2.36048500	4.77279100	H	-1.13332200	1.45879400	0.95874300
C	3.61435200	-2.83341600	3.62972400	C	-2.75491600	0.84847200	-0.46449900
C	4.27040600	-2.81567400	2.39629600	H	-2.97009600	1.88847100	-0.73360400
H	7.39666800	0.71365500	0.41472400	H	-2.78831900	0.25524400	-1.38156300
H	6.08006400	0.21483100	1.49416100	C	0.69606500	-1.47485000	2.21833200
H	7.84177500	-2.04068300	-1.22885300	H	1.15769900	-0.56002500	1.82441300
H	8.75898800	-0.69949800	-0.55495900	H	-0.32486100	-1.20934600	2.51701200
H	9.71940700	-1.47912500	2.01013000	O	1.33987200	-1.90022400	3.41126000
H	11.45459400	-3.04267600	2.84947100	H	2.28104800	-2.01670000	3.19577500
H	12.01803600	-5.08958700	1.55355300	N	2.64595100	0.41088600	-1.55670600
H	10.83711300	-5.55771700	-0.58522000	C	1.44060100	-0.33562800	-1.89878300
H	9.10877700	-3.98848200	-1.41716300	C	3.89164900	-0.31374700	-1.28916600
H	5.57577900	-2.56625100	0.14803900	C	4.16443600	-0.84609600	0.11676800
H	6.93057100	-3.34522300	0.96079800	C	4.63817900	0.00956200	1.12565100
H	7.24920300	-1.51928700	3.36058500	C	4.93088700	-0.47472800	2.40097900
H	6.08570500	-1.51474500	5.55731800	C	4.77789600	-1.83534400	2.68678600
H	3.76088000	-2.38008800	5.73697500	C	4.32563100	-2.70134800	1.68712800
H	2.60260600	-3.22539700	3.69881100	C	4.01788800	-2.20607800	0.41669200
H	3.76082500	-3.18538200	1.50824000	C	2.43124200	1.65547300	-0.83342400
N	1.15784200	2.11768000	-0.24603800	C	3.45043700	2.73825500	-1.15992800
C	0.70038100	3.52223000	0.03902800	C	3.89437300	3.61596700	-0.16335600
H	-0.19123400	3.68250600	-0.57544100	C	4.78118400	4.65288400	-0.46404200
C	0.93415400	1.65020100	-1.64583200	C	5.24197200	4.82107700	-1.77045600
H	-0.15429800	1.60744500	-1.77448400	C	4.80825600	3.94787200	-2.77183000
H	1.29768600	0.61932100	-1.68339400	C	3.91848700	2.91717900	-2.46868700
H	0.38491500	3.52572200	1.08654200	H	1.75165900	-1.19387400	-2.50312100
C	1.52144200	2.43259500	-2.80527200	H	0.83307900	0.31109500	-2.54336500
C	0.65958100	3.07365000	-3.70622400	H	3.93227500	-1.14888100	-1.99780400
C	2.90075400	2.46409700	-3.05678700	H	4.71343500	0.36398200	-1.55398600
C	1.16059200	3.75370500	-4.81842100	H	4.80198000	1.06045300	0.90080600
H	-0.41551500	3.03121000	-3.54246100	H	5.29658300	0.20422700	3.16687600
C	3.40393800	3.14607300	-4.16424800	H	5.02917300	-2.21885700	3.67258500
H	3.58470200	1.93674700	-2.39976900	H	4.21519200	-3.76295700	1.89130000
C	2.53700700	3.79761700	-5.04522600	H	3.66324400	-2.88954600	-0.35031600
H	0.47686000	4.24115200	-5.50797400	H	1.43466500	2.01801300	-1.11791400
H	4.47483200	3.15200500	-4.34683300	H	2.39138900	1.51614500	0.26073900
H	2.93107600	4.32289500	-5.91070300	H	3.53811900	3.48909100	0.85724700
C	1.67596300	4.67648500	-0.14547200	H	5.11466000	5.32412700	0.32324500
C	1.69855700	5.44554900	-1.31674900	H	5.93558200	5.62359600	-2.00701700
C	2.51858400	5.04888500	0.91443300	H	5.16330800	4.07164400	-3.79189800
C	2.55636500	6.53968500	-1.43643700	H	3.58197300	2.23199400	-3.24191300

N	-3.84350400	0.38535500	0.40832600	C	0.95703200	-3.76503500	1.89487900
C	-4.00298200	1.17074900	1.63595800	C	0.02432600	-4.47209400	2.65258900
H	-4.82343400	0.70643900	2.20001700	C	-0.10498100	-4.21731700	4.02129600
C	-3.80087900	-1.05712400	0.67236300	C	0.70875000	-3.25676100	4.62148100
H	-4.59034200	-1.26627300	1.40690100	C	1.65127000	-2.55413100	3.86461400
H	-2.85049500	-1.36927400	1.14079800	C	4.04008500	-0.97125300	2.63745900
H	-3.11705500	1.11835700	2.29576700	C	5.29722000	-1.44874600	3.03656900
C	-4.04709300	-1.90081500	-0.56590300	C	6.04718300	-0.75464000	3.98801700
C	-5.13202400	-1.62725100	-1.41126200	C	5.54552700	0.41329900	4.56396300
C	-3.22209800	-2.99185500	-0.86093500	C	4.29251500	0.89366600	4.17724200
C	-5.38748200	-2.42977200	-2.52259200	C	3.55091500	0.21353800	3.21096900
H	-5.76569600	-0.77195100	-1.19349400	H	4.51949200	0.68077200	-4.48276000
C	-3.47855200	-3.80047600	-1.97139700	H	5.94991100	-0.88484700	-5.75001600
H	-2.37055000	-3.21011100	-0.22140700	H	6.95777800	-2.83815200	-4.64306600
C	-4.56193300	-3.52224400	-2.80520900	H	3.38604400	-4.77772700	2.15871500
H	-6.23251200	-2.20500500	-3.16872300	H	4.81773500	-6.54114700	1.20207600
H	-2.82429000	-4.64176100	-2.18487700	H	6.32399700	-6.04869100	-0.68248800
H	-4.76186500	-4.14839900	-3.67097000	H	8.77622900	-2.62198200	-1.97728300
C	-4.34719700	2.62691100	1.38013600	H	8.54683100	-3.73566800	-0.60997700
C	-5.37208500	2.97160000	0.48690500	H	7.82492800	-2.11527200	-0.56836900
C	-3.67870100	3.64993000	2.06167800	H	6.32238300	-5.16064800	-3.29897600
C	-5.71873600	4.30668300	0.28383400	H	7.68509900	-5.49717500	-2.21097200
H	-5.88496100	2.18133200	-0.05415700	H	7.90607500	-4.39941400	-3.55676100
C	-4.02699700	4.98889100	1.86479800	H	6.44261700	1.53124700	-2.06514700
H	-2.88048000	3.39659500	2.75649200	H	7.95393100	3.04528500	-0.83210300
C	-5.04815200	5.32080200	0.97429300	H	7.18572500	4.15142500	1.25780200
H	-6.51472400	4.55790100	-0.41264300	H	4.89299200	3.71169800	2.11698400
H	-3.49666100	5.76994600	2.40345600	H	3.38418100	2.18009700	0.89566600
H	-5.31951200	6.36127000	0.81636800	H	1.61639900	0.25313500	-3.64898600

#### TS4

Pd	1.88832000	-0.50528700	-0.24916400	H	0.58771900	1.68794500	-5.37800900
P	3.60467800	0.67518300	-1.57522800	H	1.23344100	4.08460200	-5.55848500
P	2.98218500	-1.86575800	1.41873400	H	2.94571800	5.01754800	-4.01510100
O	5.05436800	-1.68001800	-0.67308200	H	4.00500300	3.57893900	-2.31480700
C	4.69923400	-0.39124200	-2.61782800	H	1.05903400	-3.98901300	0.83637600
C	4.95735300	-0.17364700	-3.97907700	H	-0.59676500	-5.22453800	2.17389000
C	5.76283700	-1.05942000	-4.69464300	H	-0.82607400	-4.77287400	4.61465000
C	6.33385700	-2.16611400	-4.06397800	H	0.62371100	-3.05739700	5.68617400
C	6.12315700	-2.40709700	-2.70193200	H	2.28468200	-1.82335800	4.35507400
C	5.30245900	-1.50437300	-2.01816600	H	5.69239700	-2.36544400	2.61175700
C	6.78478500	-3.53423800	-1.89806300	H	7.02121400	-1.13441900	4.28389900
C	5.80255500	-3.96011600	-0.79795800	H	6.12754000	0.94608500	5.31088200
C	4.98261900	-2.98033600	-0.22478400	H	3.88612700	1.79709000	4.62210600
C	4.07670000	-3.23463200	0.81497500	H	2.58087400	0.60306000	2.91458900
C	4.04901000	-4.53796300	1.33604000	C	-4.00782300	4.39401700	-3.49580100
C	4.85639500	-5.53589100	0.79325400	C	-3.93866200	3.00513700	-3.61116000
C	5.71224400	-5.25272300	-0.27217000	C	-2.98654800	2.26830500	-2.90641100
C	8.06333000	-2.96305000	-1.21827400	C	-2.07389900	2.91352900	-2.03555600
C	7.18800900	-4.71754800	-2.79538400	C	-2.15038300	4.31562200	-1.95173400
C	4.79971600	1.75634700	-0.67721300	C	-3.10182200	5.04585400	-2.66384400
C	6.09725100	2.00579000	-1.15171200	H	-4.75440200	4.95364700	-4.05140300
C	6.95084700	2.86340500	-0.45621300	H	-4.63009700	2.48013000	-4.26648500
C	6.51871200	3.48565100	0.71722900	H	-1.45676700	4.86923900	-1.33667600
C	5.23061500	3.24301600	1.19693700	H	-3.12365400	6.12671500	-2.56079300
C	4.37840900	2.37974600	0.50660700	C	-0.99630100	2.16345500	-1.32373300
C	2.88459300	1.81124700	-2.85161000	C	-0.88408600	0.84327800	-1.24492200
C	1.91073800	1.29684300	-3.72608300	C	-0.16399400	-0.35348400	-1.09612200
C	1.32763400	2.10576600	-4.70033400	H	-0.02478900	-0.87049500	-2.04859500
C	1.69264300	3.45127300	-4.80476300	C	-0.07894100	-1.16161600	0.08576200
C	2.65210900	3.97426500	-3.93790700	H	-0.12118600	-2.24129200	-0.02587100
C	3.25061700	3.15934800	-2.97188200	H	-0.50390200	-0.79558400	1.01765300
C	1.78752500	-2.79736100	2.49043600	C	-2.90369000	0.78405600	-3.12765100
				H	-3.83905700	0.37842100	-3.52864400
				H	-2.10542800	0.54111000	-3.84130700

O	-2.56376800	0.09368400	-1.92380100	C	-4.74080700	-2.23263500	-4.52488700
H	-3.35365300	0.08574500	-1.24443400	C	-7.50619400	-1.96384900	-4.55384800
N	0.01194900	3.30230600	0.77051200	H	-7.40956700	-2.21378300	-2.42597500
C	0.17232800	2.95867800	-0.63787200	C	-5.40747200	-2.03950100	-5.73474000
C	-0.03461700	2.15440500	1.67239100	C	-6.79776100	-1.90166800	-5.75334900
C	0.27290500	2.48987700	3.12236200	H	-8.58806100	-1.86014300	-4.55482000
C	1.30280400	3.37923400	3.46427700	H	-7.32147100	-1.74972600	-6.69286400
C	1.59139400	3.65268300	4.80245500	H	-3.14080600	0.39997400	1.35318100
C	0.86473700	3.03011300	5.82143600	C	-5.96719900	1.93290600	0.92094300
C	-0.15793900	2.13961900	5.49196600	C	-7.34691600	1.81398100	0.69568800
C	-0.45476300	1.87894800	4.15207000	C	-5.53346800	2.56936100	2.09217400
C	-0.91278600	4.37989800	1.12588000	C	-8.26741900	2.28640900	1.63284600
C	-0.45425400	5.77177200	0.71386100	H	-7.70473300	1.35780400	-0.22450500
C	0.89615800	6.08118900	0.51024700	C	-6.44973300	3.04765600	3.02964000
C	1.28810300	7.38518600	0.19731600	H	-4.46760200	2.69252200	2.27210000
C	0.33705000	8.40066900	0.08968400	C	-7.82003900	2.90081300	2.80491300
C	-1.01275600	8.10318000	0.29281100	H	-9.33239700	2.18548500	1.44278600
C	-1.40303400	6.79876200	0.59703800	H	-6.09476900	3.53751800	3.93207500
H	1.06885800	2.34376700	-0.72763700	H	-8.53553900	3.27364900	3.53230300
H	0.34780800	3.87367700	-1.20694800	C	-4.35454000	-1.08793300	2.31875000
H	-1.00853300	1.63022900	1.63231300	C	-3.52604100	-1.97034600	3.03409600
H	0.70587500	1.42947600	1.30281700	C	-5.62270400	-0.80808000	2.84436900
H	1.85833300	3.87598000	2.67421800	C	-3.94193400	-2.54600200	4.23401200
H	2.37857400	4.36018700	5.05040200	H	-2.53796600	-2.21153400	2.64601800
H	1.08855300	3.24535600	6.86247200	C	-6.04903100	-1.40021300	4.03784300
H	-0.73527600	1.65704300	6.27577000	H	-6.28758600	-0.11920200	2.34030800
H	-1.26493200	1.19586900	3.90484200	C	-5.21298900	-2.26670400	4.74027900
H	-1.93506500	4.20164700	0.74905200	H	-3.27457700	-3.21860200	4.76609500
H	-0.99516800	4.36581500	2.21804500	H	-7.04049400	-1.17120500	4.41904400
H	1.63839700	5.29354100	0.59581800	H	-5.54711600	-2.72044000	5.66901100
H	2.34047500	7.60717900	0.04062300	H	-3.65778000	-2.34610400	-4.52156100
H	0.64314400	9.41478100	-0.15130000	H	-4.84293700	-1.99725800	-6.66263500
H	-1.76203500	8.88613500	0.21253700				
H	-2.45673300	6.57428500	0.75191300				
C	-5.67032700	-0.92232800	-0.50420100	<b>TS5</b>			
H	-6.45185300	-0.93711500	0.26181900	Pd	-0.99373800	0.91192600	-0.73231200
N	-4.56145300	-0.01316200	-0.09200700	P	-0.93447900	-1.54130400	-0.90085600
C	-3.74443400	-0.46941300	1.06117400	P	-2.84470500	1.62015800	0.61665200
H	-3.04106500	-1.20856100	0.66502100	O	-3.65595300	-1.18340000	-0.08846800
C	-4.96042500	1.42627100	-0.09479400	C	-2.39496400	-2.33263800	-1.70900100
H	-5.34003000	1.62900600	-1.10281800	C	-2.34593600	-3.20847700	-2.80143500
H	-4.03435300	2.00056300	0.00907500	C	-3.52296200	-3.76917600	-3.30044600
H	-6.10384700	-0.45457800	-1.40135200	C	-4.75445000	-3.48877700	-2.70448000
N	-5.24194700	-2.28111000	-0.73398500	C	-4.84280800	-2.63292000	-1.60015900
C	-6.12304800	-3.32489300	-0.16989100	C	-3.64936700	-2.06278900	-1.15218900
H	-6.37491900	-3.00227400	0.84621900	C	-6.12028200	-2.34532300	-0.79896600
H	-7.07422300	-3.42079400	-0.71802600	C	-6.03099900	-0.89916700	-0.28967200
C	-4.63370300	-2.56457200	-2.03316000	C	-4.76801600	-0.38344700	0.02985400
H	-4.33954600	-3.61975200	-2.01894500	C	-4.55593600	0.93163000	0.46521800
H	-3.69589300	-2.00307100	-2.10478400	C	-5.69442100	1.72433500	0.69508400
C	-5.47351300	-4.69423400	-0.10639000	C	-6.96802700	1.22431100	0.43675800
C	-4.41180100	-4.94243700	0.77574800	C	-7.13111600	-0.06377800	-0.07729200
C	-5.93929500	-5.74167400	-0.91006800	C	-6.14923600	-3.30118000	0.42912900
C	-3.83462100	-6.20935700	0.85095100	C	-7.38810100	-2.57815900	-1.63927000
H	-4.05190300	-4.13972000	1.41305600	C	-0.80196900	-2.51233500	0.66155600
C	-5.36108300	-7.01191200	-0.83840200	C	-1.06498100	-3.89250600	0.70356400
H	-6.76351700	-5.56249200	-1.59695500	C	-0.96245600	-4.59406300	1.90471400
C	-4.30638500	-7.24853900	0.04313200	C	-0.60833800	-3.92642900	3.08046700
H	-3.02350000	-6.39332700	1.55160100	C	-0.36169500	-2.55373300	3.05168800
H	-5.73711900	-7.81332900	-1.46839800	C	-0.45992100	-1.85047000	1.84868500
H	-3.85822300	-8.23643200	0.10601900	C	0.44746300	-2.14162800	-1.97395400
C	-5.44027500	-2.30352500	-3.30880700	C	0.65767000	-1.47739300	-3.19560800
C	-6.83401500	-2.16485300	-3.34426100	C	1.65601800	-1.89703400	-4.07387500
				C	2.47101700	-2.98176600	-3.73955300



C	2.27820200	-3.64260500	-2.52557000
C	1.27207200	-3.22871700	-1.64684400
C	-3.20420300	3.43155900	0.50582600
C	-3.71514800	3.93755900	-0.70352600
C	-3.99583100	5.29506000	-0.84277300
C	-3.76118400	6.17227400	0.22089100
C	-3.25215800	5.68046200	1.42173900
C	-2.97673900	4.31661000	1.56761500
C	-2.34009500	1.36399800	2.36961800
C	-3.22571300	0.86298500	3.33378500
C	-2.80805200	0.70003500	4.65682500
C	-1.50867100	1.04543600	5.03077000
C	-0.62097600	1.54762000	4.07439400
C	-1.02559800	1.69839600	2.74707300
H	-1.39519900	-3.44692600	-3.26545100
H	-3.47931100	-4.43920700	-4.15378900
H	-5.64966700	-3.95293100	-3.10381200
H	-5.58286900	2.74104600	1.05296300
H	-7.83802100	1.84851600	0.61630900
H	-8.13103900	-0.41710800	-0.30417300
H	-6.18425900	-4.34452600	0.09656500
H	-7.03514300	-3.10272600	1.04260900
H	-5.26214600	-3.17246200	1.05717200
H	-7.42193700	-1.92376200	-2.51661800
H	-8.28847000	-2.40472000	-1.04288100
H	-7.44013400	-3.61643100	-1.97965200
H	-1.35989500	-4.41840200	-0.19993400
H	-1.16655300	-5.66096400	1.92411400
H	-0.53677500	-4.47440600	4.01577100
H	-0.11129400	-2.02174400	3.96504600
H	-0.29970300	-0.77695300	1.84002500
H	0.03449900	-0.62778500	-3.46294800
H	1.80122300	-1.37355300	-5.01442400
H	3.25042100	-3.30883300	-4.42185300
H	2.90473300	-4.48978300	-2.25985700
H	1.13503800	-3.75731300	-0.70963100
H	-3.90615400	3.26501000	-1.53681300
H	-4.39584800	5.66896200	-1.78106100
H	-3.97644200	7.23123100	0.11144000
H	-3.07199800	6.35396100	2.25487600
H	-2.59176700	3.95059000	2.51324100
H	-4.24203000	0.60182500	3.05674400
H	-3.50290100	0.30893400	5.39459800
H	-1.18959200	0.92788800	6.06268000
H	0.39006900	1.82471900	4.36103800
H	-0.31525300	2.07457600	2.01254500
C	5.34418600	4.85029300	-2.04343200
C	4.34098400	4.79114100	-1.08025700
C	3.53670600	3.65028100	-0.93343600
C	3.75122800	2.55039800	-1.79375300
C	4.76713200	2.61974100	-2.76608800
C	5.56391700	3.75422800	-2.88721200
H	5.95300800	5.74478900	-2.14038200
H	4.17870500	5.64337700	-0.42156900
H	4.90575800	1.77430600	-3.43611600
H	6.34151700	3.79536300	-3.64505500
C	2.87883100	1.32819000	-1.65783300
C	1.62070700	1.75716400	-1.35878300
C	0.46156100	2.24803600	-1.89270400
H	0.30763600	2.05016300	-2.95364600
C	-0.56415900	2.92462100	-1.15223300
H	-1.34936700	3.41193000	-1.72208000
H	-0.28651200	3.41943800	-0.22829400

C	2.47492700	3.66206300	0.18119000
H	2.97028600	3.97918400	1.11434400
H	1.75508200	4.46562300	-0.05980400
O	1.78940800	2.45337900	0.42807700
H	2.87073700	1.23997000	0.69290300
N	3.55884700	0.41795900	0.59628400
C	3.43306700	0.13475200	-0.95274900
C	2.97567000	-0.65453200	1.48561600
C	3.77804600	-1.90935900	1.74777800
C	4.20815800	-2.76652700	0.72421600
C	4.89750600	-3.93991600	1.02726200
C	5.15249400	-4.28755000	2.35629900
C	4.71202900	-3.45293600	3.38339100
C	4.03185500	-2.27246600	3.07753000
C	4.89446100	0.99780200	1.06447600
C	6.17395900	0.26300500	0.72737300
C	6.82526200	0.50104200	-0.49356400
C	8.04069500	-0.11959400	-0.78589600
C	8.63598000	-0.96937800	0.14763100
C	8.01436600	-1.18638900	1.37895300
C	6.79621700	-0.57164900	1.66629400
H	2.76700100	-0.72475400	-1.02991500
H	4.42545000	-0.15033700	-1.30027200
H	2.76044400	-0.15975400	2.43795100
H	2.01068500	-0.90106700	1.03370600
H	4.01276900	-2.52267200	-0.31459500
H	5.23594900	-4.58671600	0.22260100
H	5.68689300	-5.20441900	2.58786800
H	4.89847600	-3.71576600	4.42081700
H	3.69280500	-1.62614500	3.88434000
H	4.92240400	1.99731000	0.62723900
H	4.79168500	1.10842800	2.14818300
H	6.39579100	1.19795900	-1.20781900
H	8.53052600	0.07751200	-1.73534400
H	9.58664000	-1.44552500	-0.07541300
H	8.48042300	-1.82881500	2.12050800
H	6.32649800	-0.74437500	2.62929800

### I'

C	-1.99623500	-0.72720200	0.00031600
C	-0.77522000	-1.70363700	0.00019100
C	0.55107200	-1.08187600	-0.00003900
C	1.65349700	-0.57314900	-0.00015400
C	2.97018300	-0.03130500	-0.00040800
H	3.78484100	-0.75624700	-0.00137500
C	3.26500300	1.27821400	0.00044100
H	4.29652800	1.61674100	0.00017700
H	2.49057800	2.03949700	0.00141500
C	-1.64529700	0.75666000	-0.00021700
H	-1.03945900	1.00200200	0.88551000
H	-1.03971600	1.00141600	-0.88629000
O	-2.87827500	1.46930400	-0.00029200
H	-2.67416100	2.41635000	0.00051800
H	-0.84218000	-2.36713700	0.87262200
H	-0.84243000	-2.36727700	-0.87211200
H	-2.62316400	-0.92323600	-0.87601800
H	-2.62264900	-0.92277100	0.87711800

### INT2'

N	2.45296400	0.27047500	1.06461900
C	2.10174000	-0.10237900	-0.17200500
C	2.36330300	-0.67141000	2.19907900
C	3.72008500	-1.01800200	2.78164400

C	4.61690500	-1.81755500	2.05709700	C	-1.39035000	6.02950200	1.28592800
C	5.86626400	-2.13608300	2.58739000	C	-1.75339600	4.68270700	1.32456000
C	6.23342600	-1.66256600	3.85075400	C	-2.29273900	1.75822900	2.17216000
C	5.34489800	-0.87426900	4.58200200	C	-3.63555100	1.45214700	2.42688900
C	4.09399500	-0.55418700	4.04820900	C	-4.09889700	1.33714500	3.74062400
C	2.87647500	1.65238900	1.38600300	C	-3.23140700	1.53650500	4.81428400
C	3.78464700	2.29683100	0.35716100	C	-1.88875400	1.84200300	4.57109100
C	3.54705800	3.61740400	-0.04104800	C	-1.42245700	1.94251800	3.26138500
C	4.40379600	4.25127200	-0.94475100	H	-1.39340400	-4.39687200	-1.68622800
C	5.49533900	3.56194100	-1.47233500	H	-3.17588200	-4.77651600	-3.36018700
C	5.74243400	2.24268900	-1.08008200	H	-4.94760800	-3.10564200	-3.70112500
C	4.89858800	1.61938400	-0.16060200	H	-3.20519900	4.11784200	-0.88383600
H	2.09493000	-1.16955500	-0.36776400	H	-5.06378500	4.03968900	-2.50351000
H	2.46217200	0.53617700	-0.96918900	H	-6.02445600	1.88516400	-3.20322000
H	1.72568900	-0.22299100	2.97004100	H	-6.80349500	-2.01260700	-1.33588200
H	1.85685400	-1.56770800	1.83333300	H	-7.16969100	-0.28176700	-1.15539500
H	4.33122800	-2.20290900	1.08067200	H	-5.89486400	-1.02964400	-0.17293300
H	6.55150500	-2.75940000	2.01999400	H	-5.37106400	-0.47344000	-4.46369800
H	7.20620400	-1.91313900	4.26369500	H	-6.87381500	0.01406200	-3.65268000
H	5.62158600	-0.50916100	5.56679600	H	-6.50084500	-1.68627900	-3.82651800
H	3.40067500	0.05326900	4.62627600	H	-2.98838000	-3.92188400	1.00997800
H	1.98364700	2.27100200	1.53984900	H	-4.02493800	-4.40089100	3.19792000
H	3.39613800	1.58484900	2.34734600	H	-3.33512600	-3.12168900	5.21600200
H	2.69371500	4.15566600	0.36220000	H	-1.62056900	-1.33108500	5.01622700
H	4.21303500	5.28000900	-1.23823800	H	-0.60279700	-0.82980900	2.82117700
H	6.15599700	4.05010300	-2.18345800	H	1.01374400	-2.89143100	-1.93204700
H	6.57478700	1.69551900	-1.51047700	H	2.68579300	-4.69038600	-2.09885700
H	5.10634300	0.60021300	0.15615000	H	3.05789100	-6.24189800	-0.18819700
Pd	-0.10338000	0.19034300	-0.63999100	H	1.70211000	-5.98899100	1.88192600
P	-0.84537100	-2.03043800	0.16256100	H	-0.01096400	-4.22869100	2.04027500
P	-1.59793300	1.95705500	0.47049000	H	0.42394700	3.47755300	-0.99220400
O	-3.13031400	-0.39102100	-0.52139100	H	1.04717500	5.86792200	-1.08100600
C	-2.14458400	-2.46921900	-1.07570000	H	-0.10565200	7.51243700	0.38817600
C	-2.16602800	-3.64939100	-1.83011400	H	-1.89832500	6.74120200	1.93070400
C	-3.17072700	-3.86194000	-2.77487500	H	-2.54252100	4.36353700	1.99760500
C	-4.17485300	-2.91214200	-2.96550200	H	-4.32965100	1.31739800	1.60391600
C	-4.20609000	-1.72989800	-2.21499500	H	-5.14435000	1.10320800	3.92112400
C	-3.17408600	-1.53846800	-1.29191100	H	-3.59775000	1.46077800	5.83415600
C	-5.33128600	-0.68920700	-2.27798900	H	-1.20795900	2.00937000	5.40162400
C	-4.72269000	0.68664200	-1.97190200	H	-0.37918900	2.19667900	3.08540700
C	-3.66095700	0.76493100	-1.06208700	C	5.26025900	-1.11752500	-3.54410200
C	-3.08408400	1.97707100	-0.64302200	C	3.95655400	-1.85608100	-3.91235600
C	-3.61785200	3.15962800	-1.17724800	C	2.72197600	-1.18094000	-3.50053300
C	-4.66581500	3.11561700	-2.09520900	C	1.67651500	-0.64293300	-3.18850900
C	-5.20806700	1.89278300	-2.48976600	C	0.42778800	-0.03863500	-2.85952200
C	-6.36387700	-1.02415400	-1.16214800	H	-0.45477700	-0.57177200	-3.21348000
C	-6.05174200	-0.70703700	-3.63824800	C	0.28782400	1.31245100	-2.50264200
C	-1.70491300	-2.35127100	1.76394100	H	-0.64756900	1.82516600	-2.70969100
C	-2.68460400	-3.35173300	1.88267600	H	1.17118500	1.94484500	-2.45458800
C	-3.26882400	-3.62464800	3.11943900	C	5.44518800	0.20304300	-4.28112500
C	-2.88055300	-2.90608100	4.25312900	H	5.40335000	0.02872700	-5.36844100
C	-1.91347400	-1.90646600	4.14349500	H	4.63217800	0.89899100	-4.02291500
C	-1.33345600	-1.62757100	2.90428400	O	6.71390800	0.72476800	-3.89721100
C	0.36377600	-3.42794800	0.06526000	H	6.88129100	1.52569800	-4.41666000
C	1.14910700	-3.56900300	-1.09433800	H	3.92560600	-2.02168200	-4.99932000
C	2.10464900	-4.58250300	-1.18698500	H	3.98234100	-2.85697400	-3.46021800
C	2.31141000	-5.45601200	-0.11655200	H	5.29264400	-0.93183900	-2.46404000
C	1.55070600	-5.31379400	1.04439900	H	6.10837300	-1.76851500	-3.78533100
C	0.58113300	-4.31185900	1.13557800				
C	-1.10855500	3.74381800	0.49964700	<b>TS1'</b>			
C	-0.09174600	4.18954600	-0.35774900	Pd	-0.37040900	0.58279000	-0.84757500
C	0.26322300	5.54019500	-0.40361900	P	-0.89657100	-1.82028600	-0.71115200
C	-0.38364900	6.46281400	0.41964200	P	-1.54681300	1.75121900	0.90216900

O	-3.33431400	-0.42173400	-0.02345000	H	-0.93730900	6.39758300	-0.73636500
C	-2.52872700	-2.02264600	-1.55947600	H	-0.05983600	7.29678600	1.41477700
C	-2.76918100	-2.87497100	-2.64518900	H	0.12788200	5.78997200	3.38675200
C	-4.03373000	-2.92405100	-3.23396000	H	-0.53075800	3.43056100	3.21728300
C	-5.07983100	-2.14567900	-2.73546500	H	-3.54629500	0.87801700	2.96771800
C	-4.88874200	-1.29706400	-1.63825600	H	-3.29255500	0.00480800	5.26041600
C	-3.60263200	-1.25069500	-1.09330200	H	-1.03160100	-0.25701800	6.26046400
C	-5.99837600	-0.49337400	-0.94496600	H	0.98388400	0.33594500	4.92399800
C	-5.37248000	0.79588000	-0.39299700	H	0.73777200	1.16476900	2.61254800
C	-4.04363100	0.75706600	0.04602100	C	4.78030400	2.83322700	-3.63334700
C	-3.36633700	1.86805900	0.57328900	C	4.47563200	1.32641900	-3.77832100
C	-4.10485500	3.04984800	0.74103500	C	3.25373100	0.89653100	-3.04541200
C	-5.43828100	3.11424400	0.34089200	C	2.02450700	0.97384800	-2.91022200
C	-6.05732400	2.00583800	-0.23929800	C	0.62950000	1.10666400	-2.80070500
C	-6.52851800	-1.33340400	0.25341300	H	0.04135700	0.58278800	-3.55350600
C	-7.16969900	-0.19616100	-1.89811300	C	0.03594300	2.21394400	-2.12241400
C	-1.17194600	-2.71483700	0.88435200	H	-0.91511900	2.58457300	-2.50121700
C	-2.14859800	-3.71302000	1.03181700	H	0.67726500	2.97392300	-1.68217300
C	-2.28547900	-4.39784300	2.24060000	C	3.76776800	3.73683900	-4.32772000
C	-1.44835800	-4.09768500	3.31745100	H	3.76460800	3.52200000	-5.40960400
C	-0.47867300	-3.10253700	3.18384600	H	2.75492500	3.53240600	-3.94699400
C	-0.34578100	-2.41372600	1.97637600	O	4.15898900	5.07690600	-4.06473500
C	0.17566700	-3.01783100	-1.64566100	H	3.56867400	5.66841400	-4.55513600
C	0.76136900	-2.59223500	-2.85044900	N	3.70516100	-0.74259000	-0.23863200
C	1.57694900	-3.44725400	-3.59293000	C	4.32356500	-0.08765200	-1.18293700
C	1.83813500	-4.74111200	-3.13389800	C	3.51128700	-2.21057700	-0.31487600
C	1.26881900	-5.17436500	-1.93540800	C	4.25278600	-2.93888300	0.78905200
C	0.43889000	-4.32368100	-1.19964900	C	5.65257600	-2.88792300	0.86260700
C	-1.08466000	3.53713200	1.12876500	C	6.33285500	-3.57173200	1.86918400
C	-1.19453300	4.40338600	0.02468700	C	5.62068200	-4.31866400	2.81251800
C	-0.83352900	5.74585100	0.12685300	C	4.22854200	-4.37699800	2.74444700
C	-0.34396500	6.25135100	1.33446200	C	3.54681000	-3.68768800	1.73821800
C	-0.23625300	5.40578800	2.43782200	C	3.04731000	-0.05421400	0.90794300
C	-0.60838900	4.06150900	2.33966000	C	3.69349800	1.25036300	1.30520900
C	-1.42446700	1.07691600	2.61760500	C	3.08152700	2.47033100	0.98809000
C	-2.55187600	0.74644000	3.38143700	C	3.67246100	3.67762600	1.37026100
C	-2.40808500	0.25756300	4.68238500	C	4.88216800	3.67232900	2.06577000
C	-1.13951500	0.10896100	5.24326800	C	5.49918400	2.45861100	2.38560500
C	-0.00814800	0.43921700	4.49190900	C	4.90710400	1.25365400	2.01050000
C	-0.14956900	0.90516800	3.18499300	H	4.84129600	-0.66046500	-1.93979700
H	-1.96875000	-3.49442600	-3.03509600	H	4.59315100	0.94367200	-1.00326200
H	-4.20831900	-3.58131800	-4.08057500	H	2.43882800	-2.41229100	-0.26103500
H	-6.05538800	-2.21392900	-3.20433600	H	3.84668600	-2.52816500	-1.30587900
H	-3.63084800	3.92711600	1.16582200	H	6.21568200	-2.31628100	0.12792900
H	-5.99620800	4.03650900	0.47216900	H	7.41729500	-3.52919500	1.91407300
H	-7.08950400	2.08865500	-0.56168000	H	6.15145600	-4.85477300	3.59387900
H	-6.95950400	-2.27528400	-0.10407000	H	3.67043600	-4.95874800	3.47242600
H	-7.30508000	-0.77851100	0.79168300	H	2.46174600	-3.73860000	1.68760100
H	-5.72653700	-1.57106100	0.95953800	H	1.99712600	0.09520300	0.62128100
H	-6.85158500	0.39781300	-2.76134400	H	3.07840600	-0.77091400	1.73352300
H	-7.96600500	0.34563500	-1.37980900	H	2.13595800	2.47286800	0.45147400
H	-7.61752500	-1.12501400	-2.26302600	H	3.18329800	4.61640400	1.12781600
H	-2.80247800	-3.95952900	0.20082600	H	5.34312500	4.60988000	2.36295600
H	-3.04666400	-5.16684400	2.33979100	H	6.43690600	2.45249500	2.93379700
H	-1.55824700	-4.63023500	4.25799300	H	5.38443200	0.31019000	2.26669900
H	0.16022000	-2.84542600	4.02368500	H	4.35027600	1.07461900	-4.84051300
H	0.38739800	-1.61746900	1.89219300	H	5.35907100	0.76456000	-3.44466100
H	0.57821400	-1.58463100	-3.20679900	H	4.82398700	3.11024800	-2.57253600
H	2.00926900	-3.10124900	-4.52802000	H	5.77226700	3.03330300	-4.05543200
H	2.47667700	-5.40690900	-3.70776700				
H	1.46229400	-6.17994800	-1.57215200				
H	-0.00444600	-4.68419100	-0.27768600				
H	-1.58765300	4.03253400	-0.91577600				
				<b>INT3'</b>			
				Pd	-1.08363400	0.72711600	-1.16621800
				P	-0.39720300	-1.54532800	-0.58873400

P	-2.99118400	1.38482900	0.23231300	H	-4.55619300	2.06790900	-2.12310800
O	-3.06384500	-1.54652600	0.59498400	H	-5.63841800	4.13135400	-2.93059500
C	-1.68919700	-2.85308400	-0.80944700	H	-5.49134100	6.22747300	-1.59601300
C	-1.50566500	-4.02121200	-1.56432600	H	-4.26767700	6.22574000	0.56843000
C	-2.51295700	-4.98444900	-1.62444800	H	-3.19905300	4.16178500	1.39331600
C	-3.70490600	-4.81231100	-0.91828900	H	-3.77453200	0.79981300	3.06191800
C	-3.92100100	-3.67002500	-0.13991800	H	-2.72841600	1.36673100	5.22498800
C	-2.90266000	-2.71223800	-0.12768300	H	-0.62891100	2.69607700	5.29156700
C	-5.14651100	-3.42811800	0.75296800	H	0.42912200	3.44256300	3.16438700
C	-5.43414500	-1.92105000	0.72998000	H	-0.58441700	2.85396300	0.99859800
C	-4.34556700	-1.04562100	0.64014500	C	2.78891700	4.29494900	-1.57086200
C	-4.47556700	0.34696800	0.57841300	C	2.76766100	2.92487300	-2.28725200
C	-5.76708000	0.88405400	0.71179400	C	1.98731900	1.81931300	-1.57752700
C	-6.86794200	0.04116900	0.84491700	C	0.82143900	1.47743100	-2.09504500
C	-6.70441000	-1.34602200	0.82966400	C	-0.23598600	1.71771800	-2.95778400
C	-4.78053200	-3.84133000	2.20832600	H	-0.34579800	1.14759300	-3.88047200
C	-6.36341500	-4.25050600	0.29547700	C	-1.31062400	2.48628300	-2.43960400
C	0.23016000	-1.91594200	1.10286600	H	-2.23434500	2.56644400	-3.00386700
C	0.41162700	-3.24013000	1.53935100	H	-1.07814700	3.30366100	-1.76294300
C	0.89032400	-3.49945500	2.82300500	C	1.46982000	5.05977100	-1.51263400
C	1.18230200	-2.44308300	3.69056800	H	1.68392700	6.10451600	-1.24862800
C	0.98880200	-1.12657400	3.27155000	H	0.98164400	5.05835400	-2.49972600
C	0.51349000	-0.86404700	1.98461100	O	0.60387100	4.48057100	-0.52459500
C	0.89840600	-2.13111300	-1.76640000	H	-0.10100500	5.12068900	-0.34022100
C	0.66006900	-1.94587300	-3.14104200	N	3.98237000	0.98862300	-0.17230600
C	1.57377900	-2.40365500	-4.08821000	C	2.55119700	1.22733100	-0.27517000
C	2.74850700	-3.04132500	-3.67602700	C	4.83748000	2.09340300	0.26893900
C	2.99936400	-3.21976700	-2.31624900	C	6.03027300	1.67223300	1.11088100
C	2.07723000	-2.77127000	-1.36428300	C	5.84369300	1.13589000	2.39237000
C	-3.78143500	2.96736600	-0.31196600	C	6.93591300	0.78631900	3.18326500
C	-4.48019400	2.97831400	-1.53280000	C	8.23661000	0.96968900	2.70319700
C	-5.09549600	4.14232600	-1.98967000	C	8.43415000	1.50486000	1.43093100
C	-5.01421300	5.31940100	-1.23902100	C	7.33462100	1.85530400	0.64260600
C	-4.32433000	5.31883000	-0.02728600	C	4.57128500	0.09600100	-1.16853900
C	-3.71430000	4.14912900	0.43875500	C	5.30392100	-1.12238400	-0.61901100
C	-2.25952300	1.78334300	1.87553100	C	4.90841500	-1.74177200	0.57185000
C	-2.85166800	1.37060000	3.07688900	C	5.52725600	-2.91688900	1.00216000
C	-2.26069800	1.69403900	4.30082200	C	6.55275200	-3.49105800	0.24641600
C	-1.08130900	2.43917600	4.33788500	C	6.96067800	-2.87449100	-0.93841800
C	-0.48666600	2.85807400	3.14395700	C	6.33990300	-1.69803700	-1.36389400
C	-1.06467100	2.52611600	1.91789000	H	2.27090700	1.90429600	0.54176600
H	-0.58143100	-4.17653400	-2.10866400	H	2.02550500	0.28611100	-0.08995800
H	-2.36380500	-5.88088700	-2.21864900	H	5.21405500	2.68692500	-0.58378800
H	-4.46554200	-5.58343600	-0.97236600	H	4.21009500	2.76468100	0.86732000
H	-5.91362200	1.95768500	0.68927000	H	4.83294400	0.98909400	2.76654100
H	-7.86218200	0.46593300	0.94392900	H	6.77662400	0.37407300	4.17620200
H	-7.58114300	-1.98002600	0.90427800	H	9.08879300	0.69841100	3.32013400
H	-4.53880600	-4.90907800	2.24903100	H	9.44130900	1.65179000	1.05058100
H	-5.62557000	-3.65140500	2.87938800	H	7.49409100	2.27826000	-0.34718200
H	-3.91624100	-3.28140700	2.57871800	H	3.76295000	-0.26475900	-1.81840100
H	-6.66732800	-3.99751400	-0.72572000	H	5.25882600	0.65192700	-1.82799200
H	-7.21569500	-4.08606400	0.96116600	H	4.12407100	-1.28531200	1.16814200
H	-6.14337800	-5.32124500	0.33608800	H	5.21275600	-3.38170600	1.93321800
H	0.17440800	-4.06951400	0.87972200	H	7.03787600	-4.40281000	0.58400400
H	1.02983300	-4.52667600	3.14775200	H	7.76835200	-3.30267700	-1.52625500
H	1.54981700	-2.64834900	4.69206700	H	6.66664400	-1.22128400	-2.28624100
H	1.19382800	-0.30013000	3.94581200	H	2.36371900	3.06311700	-3.29636200
H	0.34564500	0.16199900	1.67591500	H	3.80369200	2.58819900	-2.40997700
H	-0.25263600	-1.45571900	-3.47184600	H	3.17385900	4.20023700	-0.55055000
H	1.37055600	-2.26343500	-5.14636400	H	3.50448900	4.92669800	-2.11349500
H	3.46349500	-3.39444100	-4.41361700				
H	3.91524500	-3.69861400	-1.98427800				
H	2.29452100	-2.91829600	-0.31262300				
				<b>TS2'</b>			
				Pd	0.62019100	0.53068800	-0.10349300

P	2.44625600	1.40946100	1.26950100	H	5.00626900	0.57803900	2.67982000
P	0.16878600	2.13648800	-1.99245300	H	-2.68986500	2.50515500	-1.55371700
O	1.56675200	3.85942200	-0.04316000	H	-4.71004500	2.11654400	-2.91394500
C	2.00690900	3.00450200	2.11176000	H	-4.51922600	1.11876600	-5.18943200
C	2.06251000	3.21308100	3.49709600	H	-2.27187700	0.54824000	-6.09270000
C	1.76790100	4.46635700	4.03569100	H	-0.24718000	0.99808700	-4.76684000
C	1.45055100	5.53982300	3.20242000	H	1.91149500	3.99628700	-3.58588600
C	1.39982400	5.38082100	1.81283500	H	3.80093000	3.59145400	-5.12088800
C	1.64727900	4.09841500	1.31288500	H	4.54648200	1.26961900	-5.60534900
C	1.19803300	6.52249100	0.80630100	H	3.39316400	-0.65064400	-4.51524900
C	0.44097600	5.95318900	-0.40046400	H	1.52610300	-0.26015000	-2.96368800
C	0.66316200	4.61614900	-0.75339900	C	0.84996000	-4.62745900	-1.44245600
C	0.00599400	3.97474700	-1.81349700	C	0.88394500	-3.94529700	-0.04612200
C	-0.82461200	4.76526400	-2.62453600	C	1.36441400	-2.50099300	0.00692700
C	-1.02996400	6.11150300	-2.33039100	C	0.49261200	-1.52205400	0.25637400
C	-0.42517600	6.69062800	-1.21312200	C	-0.81496900	-1.07793600	0.51870400
C	2.60101400	6.99856600	0.32877600	H	-1.05535200	-0.86314600	1.56144700
C	0.45689500	7.71659400	1.43331900	C	-1.87843500	-0.86347900	-0.43371200
C	4.08673400	1.83896100	0.53027300	H	-2.51687400	0.00252800	-0.30114400
C	4.98021900	2.72314000	1.15974400	H	-1.64765200	-1.08013700	-1.47346800
C	6.21150900	3.02089800	0.57526800	C	0.35906000	-3.79979100	-2.63647300
C	6.56513800	2.44657200	-0.64859400	H	0.07734600	-4.48522000	-3.45167200
C	5.67994100	1.57765700	-1.28707200	H	-0.53489900	-3.22163600	-2.37971000
C	4.44737900	1.27733000	-0.70248200	O	1.29732100	-2.83717100	-3.10470000
C	2.85683500	0.35548900	2.73549200	H	2.10905400	-3.30721800	-3.36346200
C	1.78756300	-0.23371400	3.43297000	N	3.89071600	-3.06711700	0.20458800
C	2.01598700	-0.99898600	4.57615200	C	2.83530000	-2.19302400	-0.30448900
C	3.32124100	-1.20461300	5.03199200	C	4.31974400	-4.21092600	-0.59441800
C	4.39120800	-0.63696100	4.34015500	C	4.72118100	-3.85737300	-2.01664500
C	4.16183900	0.14234400	3.20250900	C	5.52289200	-2.73735800	-2.28134900
C	-1.31315700	1.77615900	-3.05597100	C	5.92442500	-2.43932700	-3.58378800
C	-2.59131900	2.06646600	-2.54424700	C	5.53084700	-3.25385200	-4.65025500
C	-3.73556200	1.84499000	-3.31131700	C	4.73926300	-4.37578400	-4.40027300
C	-3.62865300	1.29124000	-4.59157800	C	4.33952000	-4.67240300	-3.09233600
C	-2.36898100	0.97301700	-5.09728700	C	3.90483500	-3.30412100	1.64525800
C	-1.21894900	1.22317700	-4.34135600	C	5.30060100	-3.52540700	2.20741100
C	1.58025100	1.90376100	-3.16034600	C	6.34753200	-2.64669800	1.89216400
C	2.23408800	2.97828100	-3.77959800	C	7.61598900	-2.82329700	2.44440000
C	3.30182100	2.74877300	-4.65028400	C	7.85903700	-3.88254500	3.32429100
C	3.72088500	1.44519100	-4.92085700	C	6.82561200	-4.76398400	3.64284100
C	3.07230700	0.36714300	-4.31229600	C	5.55725800	-4.58565200	3.08375900
C	2.01430700	0.59281800	-3.42961900	H	2.94358900	-2.15182300	-1.39145200
H	2.33621600	2.39739800	4.15641500	H	3.03267200	-1.18292800	0.06621500
H	1.80542500	4.61175500	5.11125300	H	5.19770400	-4.62665100	-0.08323600
H	1.25378000	6.51027400	3.64490800	H	3.58096900	-5.03287900	-0.62001500
H	-1.32998400	4.32164100	-3.47473300	H	5.82562900	-2.10078200	-1.45543100
H	-1.67629500	6.71015200	-2.96546200	H	6.55456600	-1.57283500	-3.76762100
H	-0.62497100	7.73231000	-0.98649300	H	5.84840200	-3.02308100	-5.66330100
H	3.17860000	7.38620200	1.17544700	H	4.43996000	-5.02638300	-5.21774400
H	2.49781400	7.79598400	-0.41579500	H	3.74860300	-5.56655900	-2.90358100
H	3.16744600	6.17880500	-0.12409600	H	3.46316300	-2.42135800	2.11999700
H	-0.54154000	7.43677100	1.78569500	H	3.27109500	-4.16170100	1.94034200
H	0.35327900	8.53287600	0.71260600	H	6.15853200	-1.82573000	1.20593100
H	1.02124500	8.12205500	2.27812300	H	8.41765800	-2.13517600	2.18841400
H	4.71271900	3.18441100	2.10589900	H	8.84785700	-4.02116300	3.75285000
H	6.89260500	3.70518700	1.07388900	H	7.00630200	-5.59508200	4.31940200
H	7.52214400	2.68457400	-1.10481400	H	4.75657100	-5.27974000	3.33142800
H	5.93423200	1.14373700	-2.24986400	C	-4.14225700	-1.68223300	1.02214900
H	3.75669200	0.62179700	-1.22151500	H	-5.02096700	-2.33047000	1.05981600
H	0.77082900	-0.08410300	3.07957700	N	-3.37795100	-2.05303500	-0.23978800
H	1.17656500	-1.43784700	5.10901300	C	-4.12149500	-1.85834300	-1.54019000
H	3.50240700	-1.80796000	5.91696300	H	-3.87255500	-0.85067900	-1.88162000
H	5.40981800	-0.80475900	4.67690300	C	-2.73449400	-3.40062000	-0.08510800

H	-2.09283600	-3.30715000	0.79502500	P	-0.29778800	2.05498200	-2.12531100
H	-2.07325500	-3.50635300	-0.94682700	O	0.66891100	3.92470400	-0.07139800
H	-3.48229300	-1.98020900	1.84087000	C	1.34599800	3.09422100	2.03446600
N	-4.52217800	-0.29399200	1.13659300	C	1.39687500	3.25664600	3.42670300
C	-5.98147700	-0.08164700	1.22517300	C	0.84328400	4.38653500	4.03092500
H	-6.44789800	-0.73828300	0.48657200	C	0.26285100	5.39116700	3.25533700
H	-6.37080000	-0.38798900	2.20892700	C	0.20784900	5.28194000	1.86114800
C	-3.76026900	0.47724100	2.15969200	C	0.72621900	4.11194500	1.29403200
H	-4.05458100	1.52312700	2.03957300	C	-0.27284500	6.39413000	0.91837500
H	-2.69959600	0.42212200	1.90164200	C	-0.90179700	5.72948700	-0.31244900
C	-6.41758500	1.34469100	0.94330300	C	-0.38811300	4.49879400	-0.74003400
C	-5.76088000	2.14523200	-0.00056900	C	-0.89164200	3.78956600	-1.84260000
C	-7.54154300	1.86622500	1.59673300	C	-1.88753400	4.41795300	-2.60733000
C	-6.21612600	3.43396100	-0.28410100	C	-2.39314200	5.66124600	-2.23229500
H	-4.88211300	1.75111600	-0.50162300	C	-1.92220200	6.29672500	-1.08214000
C	-8.00661500	3.15101300	1.30762900	C	0.97293600	7.20509000	0.45595200
H	-8.06197200	1.25897000	2.33444900	C	-1.25646600	7.35173200	1.61461800
C	-7.34376900	3.94039700	0.36662400	C	3.63263500	2.45119300	0.44391300
H	-5.68881400	4.04587500	-1.01182200	C	4.28227900	3.51612600	1.09091800
H	-8.88163500	3.53654000	1.82359500	C	5.44481500	4.06994300	0.55331100
H	-7.69855900	4.94325300	0.14645600	C	5.97576600	3.56970100	-0.63818200
C	-3.95572300	0.05396100	3.60761800	C	5.33622600	2.51586200	-1.29160800
C	-3.08345300	-0.85960500	4.21981300	C	4.17103900	1.96356700	-0.75515400
C	-5.01384500	0.57296100	4.37048700	C	2.72192900	0.64043500	2.53547700
C	-3.27603100	-1.26617500	5.54189100	C	1.79626000	-0.18134500	3.20330400
H	-2.22752200	-1.24220000	3.66635100	C	2.18670700	-0.95873900	4.29301200
C	-5.20961100	0.17013100	5.69233200	C	3.51793800	-0.94822400	4.71946300
C	-4.34498100	-0.75588300	6.28005600	C	4.44870400	-0.15009400	4.05495800
H	-2.58586900	-1.97101400	5.99794100	C	4.05351000	0.64563300	2.97560600
H	-4.49499200	-1.06615600	7.31025100	C	-1.61249100	1.41009600	-3.27462400
H	-3.65365800	-2.55185300	-2.24732900	C	-2.95087100	1.39883800	-2.83936500
C	-3.59241300	-4.64186900	0.03374300	C	-3.96539400	0.88463800	-3.64824700
C	-4.16040300	-5.02972600	1.25743300	C	-3.66160100	0.33828200	-4.89927800
C	-3.76692300	-5.47575800	-1.08092500	C	-2.33702200	0.32784400	-5.33500800
C	-4.91678800	-6.19831000	1.35214800	C	-1.32353200	0.86614400	-4.53555200
H	-4.00379300	-4.42293100	2.14565100	C	1.14241100	2.26094300	-3.26820800
C	-4.51784600	-6.64853600	-0.98770200	C	1.44953800	3.47456200	-3.89940300
H	-3.31072300	-5.20635100	-2.03092100	C	2.53957600	3.56567700	-4.76793800
C	-5.10139500	-7.00808700	0.22848800	C	3.32835400	2.44428100	-5.02972100
H	-5.35148800	-6.48291400	2.30605500	C	3.03047800	1.22880500	-4.40856000
H	-4.64266600	-7.28115900	-1.86174600	C	1.95287400	1.14177500	-3.52579400
H	-5.68520100	-7.92078000	0.30474300	H	1.87497900	2.49941700	4.03820200
C	-5.63776000	-1.98987400	-1.60958700	H	0.88584000	4.49665100	5.11069800
C	-6.34057800	-0.93685700	-2.21691500	H	-0.13456300	6.27279500	3.74630500
C	-6.36507700	-3.11435200	-1.18915100	H	-2.28297200	3.92410300	-3.48771200
C	-7.72335200	-0.99501800	-2.39348300	H	-3.16482100	6.13413200	-2.83273200
H	-5.79660300	-0.06060300	-2.55657200	H	-2.34813300	7.25209500	-0.79585900
C	-7.75062900	-3.16798800	-1.35294800	H	1.46123900	7.67495000	1.31711900
H	-5.86080700	-3.95520400	-0.73207400	H	0.67414500	7.99136600	-0.24646700
C	-8.43587500	-2.11152100	-1.95534900	H	1.70475600	6.56157300	-0.04238600
H	-8.24133600	-0.16468600	-2.86479800	H	-2.15648400	6.83102900	1.95860800
H	-8.29307400	-4.04587800	-1.01325100	H	-1.55988500	8.15808700	0.94063600
H	-9.51337900	-2.15965500	-2.08381100	H	-0.78467600	7.83364700	2.47583000
H	-5.67736700	1.31294200	3.92993900	H	3.88081600	3.91493900	2.01766700
H	-6.03196400	0.58730700	6.26704800	H	5.93543100	4.89318600	1.06565400
H	-0.11758100	-3.99082800	0.38691700	H	6.87926000	4.00441100	-1.05687000
H	1.51842800	-4.56126300	0.60339600	H	5.73230300	2.13050700	-2.22688800
H	1.84350400	-5.00892900	-1.69915900	H	3.66674000	1.16317400	-1.28504600
H	0.21053200	-5.51702200	-1.35433900	H	0.76189200	-0.20545200	2.87243100
				H	1.45279400	-1.57612900	4.80453000
				H	3.82804700	-1.56400400	5.55910800
				H	5.48947700	-0.15073100	4.36501300
				H	4.79195600	1.26098300	2.47383500
<b>INT4'</b>							
Pd	0.41490200	0.50652300	-0.29443500				
P	2.09825600	1.66085800	1.11916800				

H	-3.20684900	1.82867500	-1.87398300	H	-1.74624300	-3.92491800	-0.64085900
H	-4.99758700	0.92849600	-3.30968800	H	-3.01325900	-2.02854900	1.95637000
H	-4.45097600	-0.06027300	-5.53035900	N	-4.32639100	-0.60412400	1.17444800
H	-2.08794000	-0.07913700	-6.31152000	C	-5.78119400	-0.46157900	1.40206400
H	-0.30539300	0.87408200	-4.90958600	H	-6.26971800	-1.31232400	0.92020400
H	0.83805000	4.35219400	-3.71531600	H	-6.02644700	-0.51918100	2.47300300
H	2.76742500	4.51494500	-5.24496500	C	-3.50317700	0.44305500	1.80988200
H	4.17063300	2.51661900	-5.71215200	H	-4.09055500	1.36530100	1.75489600
H	3.64191100	0.35155800	-4.60403800	H	-2.61469600	0.62889500	1.19606200
H	1.73729400	0.19900300	-3.02791400	C	-6.37414100	0.82345800	0.85131100
C	1.35044500	-4.63791300	-1.83638500	C	-5.93053200	1.38777200	-0.35131700
C	1.29664900	-3.94927500	-0.43726000	C	-7.42811400	1.44340800	1.53358900
C	1.46178800	-2.43373500	-0.45579100	C	-6.52801200	2.54048400	-0.86298500
C	0.48944500	-1.59620400	-0.08612100	H	-5.10169800	0.92265300	-0.87461100
C	-0.81604700	-1.26348200	0.25417200	C	-8.03722000	2.58968200	1.01889600
H	-1.01788200	-1.06395700	1.30873400	H	-7.77647900	1.02661000	2.47612400
C	-2.03594500	-1.42806500	-0.61432100	C	-7.58817300	3.14277500	-0.18132700
H	-2.61606200	-0.51232000	-0.72324500	H	-6.16322500	2.97221100	-1.79157000
H	-1.75338000	-1.79204400	-1.60233200	H	-8.85474500	3.05552100	1.56198800
C	0.03139900	-5.22050400	-2.33893600	H	-8.05455200	4.03997400	-0.57826100
H	0.20676500	-5.81184100	-3.24915700	C	-3.04834800	0.22451000	3.25237400
H	-0.40309300	-5.89336500	-1.59184500	C	-3.69204600	-0.63177200	4.15621800
O	-0.98233000	-4.23556400	-2.58878900	C	-1.94232300	0.95944300	3.70662400
H	-0.65755600	-3.64674200	-3.28848700	C	-3.24541800	-0.74820800	5.47559300
N	4.05004400	-2.52268500	-0.47952100	H	-4.55131900	-1.21647700	3.84150200
C	2.81521700	-1.89038000	-0.94580100	C	-1.50022300	0.85216200	5.02538700
C	4.56149900	-3.67275400	-1.22558300	C	-2.15021000	-0.00514900	5.91622000
C	6.03242900	-3.59770900	-1.61576500	H	-3.76082100	-1.41726600	6.15948100
C	6.54015800	-2.46830400	-2.27102500	H	-1.80668600	-0.09250200	6.94301800
C	7.86623400	-2.42878600	-2.69797500	H	-3.64971500	-3.50465300	-1.84045700
C	8.70793100	-3.52337400	-2.47782100	C	-3.14013200	-4.97916400	0.59759400
C	8.21236700	-4.65250900	-1.82632800	C	-3.56636800	-5.22930100	1.91175700
C	6.88223500	-4.68607800	-1.39953000	C	-3.36790900	-5.95819500	-0.38323300
C	4.20630900	-2.60442700	0.97151700	C	-4.24380100	-6.40739300	2.22748500
C	5.63556400	-2.47837700	1.47425100	H	-3.35757500	-4.50621700	2.69642900
C	6.43841500	-1.39191500	1.10005400	C	-4.04153500	-7.13923200	-0.06754600
C	7.72121600	-1.24215300	1.62397600	H	-3.00935200	-5.79476600	-1.39637700
C	8.22384800	-2.17646100	2.53532300	C	-4.48845000	-7.36197800	1.23641900
C	7.43418400	-3.26228700	2.91303400	H	-4.56842200	-6.58654600	3.24843100
C	6.14959400	-3.40943100	2.38209100	H	-4.21138100	-7.88619700	-0.83751200
H	2.84250700	-1.92109800	-2.04396800	H	-5.01042200	-8.28171000	1.48409900
H	2.84486200	-0.83028800	-0.67193700	C	-5.56749400	-2.82513200	-1.08532900
H	4.39300900	-4.61538200	-0.67456000	C	-6.40485000	-1.91229700	-1.74738900
H	3.97937500	-3.75391700	-2.15058900	C	-6.16835100	-3.87789400	-0.37512700
H	5.89007900	-1.61116800	-2.42930900	C	-7.79388900	-2.02907600	-1.69186400
H	8.24675900	-1.54457900	-3.20332900	H	-5.96355800	-1.10129000	-2.31894800
H	9.74235100	-3.49267800	-2.80911800	C	-7.55815600	-3.98720700	-0.30709200
H	8.86036000	-5.50557400	-1.64340800	H	-5.56314000	-4.61918300	0.12855300
H	6.50308100	-5.56748800	-0.88633500	C	-8.37669700	-3.06550800	-0.96283800
H	3.61139300	-1.79405100	1.40647800	H	-8.41557800	-1.30600800	-2.21145100
H	3.78337900	-3.54562700	1.37171000	H	-8.00022600	-4.80585500	0.25368600
H	6.05457400	-0.66859600	0.38609500	H	-9.45755900	-3.15868100	-0.91061500
H	8.33322200	-0.39685600	1.31966800	H	-1.42393800	1.62807400	3.02232500
H	9.22528900	-2.06041300	2.94108700	H	-0.64393000	1.43551100	5.35113000
H	7.81725600	-3.99864900	3.61484800	H	1.72734500	-3.93940200	-2.59537800
H	5.53782600	-4.25878700	2.68017900	H	2.07325000	-5.46311100	-1.81384900
C	-3.80229500	-1.92616100	1.20807900	H	0.36380200	-4.21509500	0.06683500
H	-4.57731900	-2.66305900	1.41298600	H	2.09867700	-4.36979500	0.18011200
N	-3.11406700	-2.45244900	-0.09859400				
C	-4.07370000	-2.65729200	-1.29650300				
H	-3.93341200	-1.77529900	-1.92144800				
C	-2.35316000	-3.74304300	0.24454800				
H	-1.68668300	-3.46511000	1.06234800				
				<b>TS3'</b>			
				C	-5.29752600	-0.43324200	-2.76206500
				C	-6.23830900	-1.08586300	-3.57175500
				C	-5.95365500	-1.20864400	-4.93510100

C	-4.78449100	-0.67358700	-5.47479300	C	-3.89678800	-2.66936300	5.11887400
C	-3.87972900	-0.00420000	-4.65430700	H	-4.84924300	-0.85116500	4.47612900
C	-4.10993100	0.12708900	-3.27546000	C	-3.01861900	-4.08624800	3.37289400
H	-6.65273300	-1.71615500	-5.59038000	H	-3.24405300	-3.36205300	1.36271100
H	-4.58260500	-0.77236300	-6.53730000	C	-3.24428500	-3.83952600	4.73094700
H	-2.97311400	0.40721600	-5.08562600	H	-4.08291400	-2.47203500	6.17125100
C	-7.54689400	-1.54628000	-2.91901600	H	-2.51696500	-4.99835100	3.06007300
C	-8.26249400	-2.62150700	-3.75456700	H	-2.91572400	-4.55624100	5.47833600
H	-9.20772200	-2.91076400	-3.28633500	Pd	-3.03790400	0.08458700	-0.05287400
H	-7.64856800	-3.51994000	-3.87960800	C	0.20310400	-0.13822500	0.41185000
H	-8.51687600	-2.23547700	-4.74588700	H	-0.64249500	0.31704400	0.92283300
C	-8.48871000	-0.31268100	-2.79173900	N	0.55718500	-1.36243300	0.78614100
H	-9.42482900	-0.60090700	-2.30048100	C	1.23741900	-2.26502800	-0.16805800
H	-8.72532800	0.08682500	-3.78425800	H	2.17553100	-2.62291100	0.26696700
H	-8.02557500	0.48536000	-2.20363700	C	0.07759600	-1.94440300	2.06475700
C	-7.20952000	-2.04232400	-1.50784500	H	-0.91865800	-1.53532500	2.25473900
C	-7.87412300	-3.09202000	-0.86720600	H	-0.06040900	-3.01325800	1.87550100
C	-6.21933800	-1.35570300	-0.78881100	H	0.32066900	0.09673200	-0.63877200
C	-7.57827800	-3.42853400	0.45323500	H	1.50008400	-1.65826600	-1.04070200
H	-8.63982400	-3.64981900	-1.39468400	C	0.96276800	-1.73748900	3.28108300
C	-5.88928500	-1.67332100	0.54500200	C	0.38236900	-1.26757400	4.46722500
C	-6.60207700	-2.72171000	1.15048500	C	2.32580400	-2.07118900	3.28404100
H	-8.11128200	-4.24037800	0.93924800	C	1.14620200	-1.12341500	5.62836400
H	-6.37556600	-2.99627400	2.17527000	H	-0.67870800	-1.02895300	4.48827500
O	-5.54511300	-0.31788400	-1.40645300	C	3.09222700	-1.91807100	4.44035000
P	-2.91600100	1.01221900	-2.16376300	H	2.80507300	-2.46294500	2.39151500
P	-4.55478900	-0.76894000	1.46867200	C	2.50444400	-1.44397000	5.61671600
C	-3.50540700	2.76388800	-2.23798400	H	0.67799300	-0.76042500	6.53886300
C	-3.93622000	3.36975100	-3.42957300	H	4.14523700	-2.18457800	4.41907500
C	-3.53677200	3.50940600	-1.04922400	H	3.09967600	-1.33393500	6.51876600
C	-4.37291300	4.69491100	-3.43196000	C	0.37586500	-3.44090700	-0.59961700
H	-3.94007300	2.80489000	-4.35724600	C	-0.97692900	-3.27060500	-0.93166100
C	-3.97413900	4.83645700	-1.05234100	C	0.95266200	-4.71000100	-0.72471300
H	-3.24217400	3.03011500	-0.11862400	C	-1.73102700	-4.35370600	-1.38610100
C	-4.39055400	5.43130100	-2.24425600	H	-1.45500100	-2.29745800	-0.81989200
H	-4.70555900	5.15088800	-4.36040600	C	0.19909700	-5.79191100	-1.18630100
H	-4.00440400	5.39788000	-0.12232800	H	1.99967600	-4.85550800	-0.46820900
H	-4.73795600	6.46076300	-2.24810600	C	-1.14464600	-5.61580500	-1.51782100
C	-1.35278500	1.02144000	-3.16105300	H	-2.77791000	-4.20866500	-1.63911000
C	-0.72270600	-0.21051800	-3.42533600	H	0.66179300	-6.77021600	-1.27976900
C	-0.70235300	2.20126900	-3.55217500	H	-1.73342000	-6.45647400	-1.87346100
C	0.51183700	-0.25801200	-4.07255200	C	6.65004100	3.68006700	-1.09791700
H	-1.20805300	-1.13906000	-3.13484100	C	6.32550200	2.29612700	-1.70515200
C	0.54196200	2.15246100	-4.19028400	C	5.98633600	1.19498200	-0.70387800
H	-1.16633000	3.16453600	-3.36689900	C	4.74380000	0.91538000	-0.38627600
C	1.15233300	0.92635600	-4.45367100	C	3.52188300	0.56614200	-0.04859100
H	0.96998800	-1.22018100	-4.28745200	H	3.02588700	-0.21296200	-0.62668200
H	1.02620700	3.07833900	-4.48890400	C	2.80887300	1.07166100	1.18314400
H	2.11380400	0.89013100	-4.95818500	H	2.76008600	0.26756100	1.92825100
C	-5.46736100	0.55152600	2.38525300	H	3.38118500	1.88802800	1.63377200
C	-6.83882900	0.48014400	2.67309800	C	7.81530600	3.71933300	-0.11489800
C	-4.74203500	1.67257000	2.82192200	H	8.01072600	4.76426600	0.16876700
C	-7.46711500	1.50531100	3.38347100	H	7.55464200	3.17320300	0.80590400
H	-7.42105200	-0.37331200	2.34008000	O	8.95743800	3.14263200	-0.74484700
C	-5.36793300	2.69008400	3.54283700	H	9.72716800	3.27863300	-0.17171400
H	-3.68342800	1.74579400	2.58359700	N	7.69583000	-0.72570400	-0.83469400
C	-6.73403600	2.60946000	3.82240200	C	7.12529600	0.37255800	-0.05471100
H	-8.53100500	1.43918000	3.59415700	C	8.51643200	-0.33391600	-1.98777200
H	-4.79250600	3.54916600	3.87757900	C	9.55978100	-1.37721200	-2.35004400
H	-7.22563300	3.40517000	4.37516700	C	10.44574400	-1.86696400	-1.37969300
C	-4.10327100	-1.98422300	2.79406900	C	11.43009200	-2.79407200	-1.71842300
C	-4.32921700	-1.74904300	4.15818000	C	11.54539300	-3.24693600	-3.03626100
C	-3.43459500	-3.16290900	2.41471100	C	10.66893400	-2.76736400	-4.00958400



C	9.68185600	-1.83997600	-3.66498000	C	-1.31059400	0.29968200	0.10410600
C	6.79003200	-1.83314300	-1.11726800	H	-1.54737600	1.04027500	0.87081800
C	6.39397500	-2.65100200	0.10245600	C	-2.37355900	0.10432400	-0.95606500
C	7.23438400	-2.76616800	1.21632000	H	-2.46174300	1.02938000	-1.53833400
C	6.88107900	-3.57582200	2.29830800	H	-2.06072700	-0.69144600	-1.65817300
C	5.68564300	-4.29721300	2.27887300	C	1.45345300	-3.76194300	-1.22864900
C	4.84434500	-4.19844500	1.16681700	H	1.02981000	-4.62965800	-1.75947400
C	5.19366500	-3.37474500	0.09444700	H	1.37620000	-2.89599700	-1.90317100
H	7.94775400	1.05252300	0.18245700	O	2.80693800	-4.00932400	-0.85685800
H	6.75117100	-0.04864100	0.88294000	H	3.38441100	-3.85552700	-1.61881100
H	7.90670200	-0.12052900	-2.88425900	N	3.18608200	0.40860300	0.16949600
H	9.01428200	0.60562900	-1.71993900	C	2.18261500	-0.32240400	-0.61678300
H	10.35414700	-1.51693900	-0.35504100	C	4.25521000	-0.39364200	0.76972200
H	12.11102000	-3.16300900	-0.95582300	C	5.15696300	-1.04728000	-0.26384700
H	12.31327400	-3.96898000	-3.30007100	C	5.71902400	-0.28365700	-1.29728300
H	10.74900200	-3.11560900	-5.03588400	C	6.57663400	-0.86676000	-2.22965800
H	9.00046800	-1.46869000	-4.42787900	C	6.88812200	-2.22699000	-2.14441200
H	5.87582000	-1.50038400	-1.64323900	C	6.33420800	-2.99668900	-1.12028600
H	7.31679400	-2.49763700	-1.81342500	C	5.47287200	-2.40882200	-0.18820700
H	8.17093800	-2.21747600	1.22142500	C	2.62197200	1.41513500	1.06901300
H	7.54882500	-3.65391100	3.15239500	C	3.60160000	2.52502800	1.40800700
H	5.41815000	-4.94058400	3.11267800	C	4.23897500	3.24560500	0.38710900
H	3.92222300	-4.77475300	1.13411900	C	5.11149100	4.28985500	0.68965800
H	4.54029600	-3.30926800	-0.77426800	C	5.36188800	4.63270200	2.02205400
N	1.39929400	1.49889100	0.96939600	C	4.73409200	3.92298700	3.04561000
C	0.73944700	1.92647200	2.25480700	C	3.86129500	2.87561600	2.73731500
H	-0.23297000	2.34136800	1.97160900	H	2.71813200	-1.10380400	-1.16511600
C	1.15841400	2.39737300	-0.19919500	H	1.77152200	0.37598900	-1.35513800
H	0.09362300	2.30258000	-0.43831500	H	4.85798200	0.29831200	1.37084800
H	1.71337100	1.95654200	-1.03336000	H	3.88335600	-1.16029200	1.47126700
H	0.55479000	1.00181000	2.80979900	H	5.47102700	0.77160000	-1.36431300
C	1.48599100	3.87399000	-0.09247800	H	7.00545100	-0.25951900	-3.02299800
C	0.45243000	4.81163600	-0.22845100	H	7.55784200	-2.68143700	-2.87003100
C	2.79953300	4.34046600	0.05940800	H	6.57071500	-4.05510900	-1.04268800
C	0.71854600	6.18227700	-0.19151800	H	5.03126200	-3.01809400	0.59535300
H	-0.56969500	4.46888000	-0.37657200	H	1.75392800	1.84839800	0.55582700
C	3.06605100	5.70819200	0.10843500	H	2.23023400	0.97717700	2.00525600
H	3.61934000	3.63287600	0.13279000	H	4.04524200	2.97481600	-0.64743600
C	2.02674100	6.63404800	-0.01408900	H	5.59587700	4.83984200	-0.11331400
H	-0.09521800	6.89334400	-0.30416000	H	6.04254000	5.44643900	2.25818900
H	4.08848300	6.05378100	0.23458200	H	4.92508800	4.17918400	4.08458600
H	2.23805500	7.69913500	0.01799600	H	3.37573300	2.32293600	3.53894300
C	1.46302300	2.88578500	3.18827800	N	-3.69624900	-0.15981900	-0.37499200
C	1.16712800	4.25561200	3.20420500	C	-4.76687100	0.01286300	-1.36433100
C	2.37583300	2.38849900	4.13252300	H	-4.59836300	-0.61975100	-2.25830400
C	1.78670100	5.11033000	4.11652400	C	-3.76146500	-1.47865300	0.26441000
H	0.45076400	4.66068500	2.49693000	H	-2.83206900	-1.60075700	0.83287400
C	3.00340200	3.24271800	5.04003500	H	-3.77848300	-2.29492800	-0.48485900
H	2.58426300	1.32259700	4.17472700	H	-5.69103500	-0.35028800	-0.89902600
C	2.71257800	4.60808600	5.03249300	C	-4.94255600	-1.63131500	1.20380700
H	1.54199100	6.16875800	4.11215200	C	-5.17470200	-0.68184500	2.20989800
H	3.70706300	2.83811700	5.76235600	C	-5.79797900	-2.73500300	1.11360000
H	3.19408700	5.27338000	5.74376900	C	-6.23372100	-0.83605200	3.10334600
H	5.48451300	2.42566900	-2.39558500	H	-4.51886600	0.18156400	2.27943200
H	7.18246600	1.97852200	-2.30434700	C	-6.85872300	-2.89495300	2.00943000
H	6.87271500	4.36061500	-1.92920200	H	-5.63171400	-3.47675800	0.33505700
H	5.76443100	4.07826100	-0.58750600	C	-7.07954000	-1.94516900	3.00698000
<b>3'</b>				H	-6.39981300	-0.09163300	3.87802600
C	0.65645300	-3.50097300	0.04530700	H	-7.51325300	-3.75847300	1.92292200
C	1.15232400	-2.28905500	0.86294300	H	-7.90511900	-2.06522600	3.70354000
C	0.99800800	-0.95093900	0.14056400	C	-4.96417500	1.45343000	-1.79597500
C	-0.16011500	-0.32970900	0.13440300	C	-5.04155100	1.79300500	-3.15139000
				C	-5.11260800	2.46833200	-0.83925800

C	-5.26978800	3.11337000	-3.54800000
H	-4.92264300	1.01610500	-3.90382800
C	-5.33637200	3.78746100	-1.23130600
H	-5.04393700	2.21195100	0.21400300
C	-5.41740800	4.11484200	-2.58815500
H	-5.32629400	3.35769800	-4.60569200
H	-5.44997000	4.56274800	-0.47768400
H	-5.59216700	5.14336900	-2.89284500
H	0.59349600	-2.25895900	1.80537300
H	2.20222800	-2.45537400	1.11609700
H	0.71271100	-4.39714300	0.67719800
H	-0.39838700	-3.35881100	-0.22309800

### 3-DME

C	-0.34811000	-3.03429900	-4.15756400
C	-0.40951200	-3.14049200	-2.76900100
C	-0.03644400	-2.07813600	-1.93540500
C	0.41787100	-0.86989500	-2.51874700
C	0.47506200	-0.78258900	-3.92275700
C	0.09674600	-1.84668200	-4.73855800
H	-0.64230200	-3.87520900	-4.78021100
H	-0.73376700	-4.06373200	-2.30227300
H	0.79719900	0.14624900	-4.38475200
H	0.14824400	-1.74474400	-5.81946800
C	0.80693200	0.33288900	-1.71627800
C	0.04040000	0.76836100	-0.73759000
C	-0.72701800	1.25324200	0.20720600
H	-0.55038900	0.94762000	1.24035000
C	-1.86999000	2.23923600	-0.03118300
H	-1.74872100	3.08578200	0.65355300
H	-1.80788000	2.62670900	-1.05092400
C	-0.11445400	-2.26860600	-0.43460500
H	0.73014600	-1.75104400	0.03940700
H	-1.03120900	-1.79294900	-0.04845500
O	-0.10664200	-3.65454400	-0.12371400
H	-0.10711000	-3.72383500	0.85161100
N	3.25501500	1.11742500	-1.29230200
C	2.05865900	1.16537100	-2.11738800
C	4.24071700	0.05001000	-1.49405000
C	4.15358100	-1.18708300	-0.60399300
C	4.90618300	-1.25848500	0.57766300
C	4.84949800	-2.38699600	1.39816100
C	4.03502900	-3.46633900	1.04736400
C	3.28216600	-3.41119700	-0.12879400
C	3.35075200	-2.28219600	-0.94783000
C	3.15301900	1.66449700	0.05095500
C	4.40060300	2.41660800	0.49931700
C	4.81665500	2.36585100	1.83518900
C	5.92113300	3.10211700	2.27055800
C	6.63149400	3.89616200	1.36879100
C	6.22871600	3.94823200	0.03169300
C	5.12161400	3.21569500	-0.39756200
H	2.35520800	0.86902400	-3.12781300
H	1.74638800	2.21560800	-2.16952600
H	4.17512600	-0.25130800	-2.54540000
H	5.23580900	0.49284200	-1.35228800
H	5.54794100	-0.42425000	0.85155500
H	5.44765800	-2.42589300	2.30539700
H	3.99827200	-4.35119100	1.67848400
H	2.62707700	-4.23170600	-0.40518400
H	2.77106400	-2.25579400	-1.86608400
H	2.30589600	2.36201700	0.05123100
H	2.90805300	0.89722400	0.80461400

H	4.26990200	1.74307100	2.54045800
H	6.22931300	3.04983700	3.31180000
H	7.49430100	4.46625700	1.70321000
H	6.77834600	4.56168700	-0.67800900
H	4.80797200	3.24578700	-1.43750600
N	-3.22910000	1.70940200	0.16067200
C	-3.50084700	1.23540100	1.52028400
H	-4.52961500	0.84944700	1.51755800
C	-3.61633100	0.72649700	-0.85722300
H	-4.59628400	0.33145500	-0.55617600
H	-2.92890600	-0.13755200	-0.88775800
H	-2.85927400	0.38246100	1.81217600
C	-3.73423500	1.31944400	-2.25009900
C	-4.46689800	2.49585800	-2.46417400
C	-3.15092900	0.67966100	-3.34944000
C	-4.61613800	3.01652400	-3.74904700
H	-4.90799600	3.00356000	-1.61078900
C	-3.30293300	1.19685800	-4.63873400
H	-2.56982400	-0.22654600	-3.19824500
C	-4.03606600	2.36620700	-4.84245800
H	-5.18686100	3.92964700	-3.89929200
H	-2.83982800	0.68669000	-5.47933900
H	-4.15322300	2.77169300	-5.84416900
C	-3.38974300	2.32353600	2.57288700
C	-4.02593800	3.55999500	2.39005400
C	-2.68797400	2.09924500	3.76242400
C	-3.96179500	4.54476600	3.37488300
H	-4.56033000	3.74327600	1.46208700
C	-2.62592400	3.08191500	4.75410200
H	-2.18764900	1.14516400	3.91595600
C	-3.26271400	4.30813300	4.56239000
H	-4.45898100	5.49863700	3.21777000
H	-2.07590900	2.88974100	5.67173400
H	-3.21371200	5.07590600	5.33001200
O	-3.78573700	-4.64144900	2.69227400
C	-2.63606900	-3.95886600	2.24062300
H	-2.38869400	-4.22466700	1.20062900
H	-2.78088300	-2.86563500	2.27896000
C	-4.92664600	-4.36931100	1.90672000
H	-5.75400400	-4.94454000	2.33027000
H	-5.18815400	-3.29888600	1.92603400
H	-4.77935800	-4.67067900	0.85749100
C	-1.48866600	-4.35717100	3.15946700
H	-1.71046500	-4.05560100	4.19398500
H	-1.36057900	-5.45011000	3.14477200
O	-0.31174800	-3.70672900	2.69714100
C	0.83362900	-3.98489500	3.48683500
H	1.67837600	-3.47712700	3.01612800
H	0.70366200	-3.60952800	4.51227000
H	1.03706600	-5.06530400	3.52942200

### TS6

C	6.24333300	-1.16697900	-1.67217000
C	7.42336000	-0.98472800	-2.40761700
C	7.48235500	-1.52914500	-3.69417100
C	6.41046500	-2.25213400	-4.21582800
C	5.25871900	-2.43977200	-3.45509900
C	5.14234900	-1.89555700	-2.16600700
H	8.37516900	-1.40089500	-4.29600800
H	6.47563600	-2.67516100	-5.21396000
H	4.43147100	-3.00479800	-3.87130900
C	8.59239300	-0.26950000	-1.72040300
C	9.61525100	0.27241100	-2.73347700

H	10.45354400	0.75134800	-2.21932900	Pd	3.33861600	-0.28391000	0.22494900
H	9.16794800	1.00010100	-3.41919700	C	0.52507500	1.64273000	0.19539500
H	10.04303900	-0.54218700	-3.32494800	H	0.80805900	2.14766500	1.10772600
C	9.31254800	-1.29062500	-0.79120200	N	0.21142300	2.40498800	-0.85121200
H	10.13733100	-0.80251000	-0.25990100	C	0.28297400	1.85649400	-2.22929400
H	9.72095700	-2.11744000	-1.38305200	H	-0.66471600	2.06462900	-2.73509600
H	8.62664700	-1.70835900	-0.04813700	C	-0.02456100	3.86949000	-0.72536000
C	8.00153800	0.84307800	-0.84653300	H	0.28861300	4.15850100	0.28034600
C	8.62494600	2.07266700	-0.61391800	H	0.66548100	4.34710900	-1.42935100
C	6.79388000	0.58289800	-0.18146400	H	1.07556800	0.72437600	-0.01701300
C	8.07568100	2.99841700	0.27235700	H	0.37146400	0.77115300	-2.13636000
H	9.55555300	2.31120400	-1.11673400	C	-1.44353600	4.33403400	-0.99430500
C	6.20828400	1.49706800	0.71866100	C	-2.32042600	4.59831700	0.06759500
C	6.88613600	2.70790700	0.93598700	C	-1.89237300	4.55223400	-2.30502300
H	8.57854100	3.94449700	0.44999900	C	-3.62774300	5.02356000	-0.17566500
H	6.46868500	3.43644800	1.62271700	H	-1.97478500	4.49039700	1.09322000
O	6.15376400	-0.62154900	-0.40367900	C	-3.20009400	4.97378300	-2.55054200
P	3.60121700	-2.11815400	-1.15334800	H	-1.20815400	4.41640100	-3.13810000
P	4.59981900	1.12003500	1.56875400	C	-4.07570700	5.20189700	-1.48651800
C	3.93151800	-3.68055700	-0.22254400	H	-4.29602300	5.22507500	0.65655200
C	4.77652600	-4.69203500	-0.70654800	H	-3.53120400	5.13623900	-3.57238300
C	3.29942500	-3.86233100	1.01768400	H	-5.09410700	5.52931400	-1.67339400
C	4.97640700	-5.85999700	0.03156400	C	1.44222000	2.41008300	-3.03954400
H	5.28492800	-4.56758700	-1.65785900	C	2.76614000	2.21257900	-2.61559700
C	3.49295100	-5.03424700	1.75069200	C	1.20903500	3.08394500	-4.24431700
H	2.66478900	-3.07368400	1.41263000	C	3.83023700	2.69612800	-3.37747300
C	4.33347100	-6.03481600	1.25920000	H	2.97140900	1.65525700	-1.69955400
H	5.63670800	-6.63273200	-0.35266600	C	2.27479400	3.56626800	-5.00908200
H	2.99613600	-5.15921800	2.70897600	H	0.18949100	3.22109300	-4.59782900
H	4.49294500	-6.94385900	1.83255500	C	3.58659700	3.37794300	-4.57369600
C	2.35673600	-2.62248500	-2.43221200	H	4.84974300	2.52848100	-3.04115000
C	1.87427800	-1.63129600	-3.30736100	H	2.07752500	4.08691400	-5.94179500
C	1.82913900	-3.91766300	-2.52851800	H	4.41632100	3.75273000	-5.16618100
C	0.89928500	-1.93117700	-4.25777200	C	-3.41608000	-4.98243400	-0.41594000
H	2.27925600	-0.62319400	-3.25430800	C	-4.17467200	-4.29159600	0.52810800
C	0.84414300	-4.21482400	-3.47673600	C	-4.05244800	-2.90655300	0.69421100
H	2.18889000	-4.70138800	-1.86983600	C	-3.13457200	-2.20000900	-0.11632700
C	0.37631100	-3.22612100	-4.34255300	C	-2.37916800	-2.90857800	-1.06669100
H	0.55056100	-1.15660600	-4.93600900	C	-2.51142000	-4.28696800	-1.21843200
H	0.45383800	-5.22708000	-3.54343800	H	-3.53146200	-6.05790800	-0.52217300
H	-0.38386000	-3.46087900	-5.08233700	H	-4.86597700	-4.82019900	1.17399100
C	5.12365500	0.30671700	3.14317400	H	-1.69498900	-2.37469500	-1.72128300
C	6.37636200	0.52555700	3.73758300	H	-1.91318100	-4.80566300	-1.96221900
C	4.21749200	-0.56225800	3.77218100	C	-2.98819300	-0.70846200	-0.06267700
C	6.71007400	-0.10699300	4.93671900	C	-4.05194500	0.06942600	-0.15073000
H	7.09620100	1.18544600	3.26298400	C	-5.08625800	0.85904600	-0.27515300
C	4.54853000	-1.18627700	4.97572900	H	-5.57574700	1.23314800	0.62623100
H	3.25655500	-0.75893400	3.30334800	C	-5.66183500	1.32755200	-1.61465900
C	5.79694100	-0.96085200	5.55925000	H	-5.55178300	2.41630700	-1.67114300
H	7.68531000	0.06688300	5.38325400	H	-5.07595800	0.89247000	-2.42799200
H	3.83712800	-1.85686100	5.45009800	C	-4.90758500	-2.21678500	1.74278100
H	6.06031000	-1.45349400	6.49112200	H	-4.30287900	-1.44553400	2.24633700
C	4.05169400	2.80779900	2.11783800	H	-5.73871100	-1.68813900	1.25029600
C	4.03454500	3.21315600	3.46015500	O	-5.40144900	-3.16023500	2.67395300
C	3.57889300	3.70345700	1.13989900	H	-6.21331700	-2.78807500	3.07332000
C	3.56392700	4.48192300	3.81573300	N	-0.97952200	0.57464500	1.08706400
H	4.39883700	2.54450700	4.23318700	C	-1.60155500	-0.05011700	-0.13451000
C	3.12164900	4.97283500	1.49397600	C	-0.18641400	-0.34525700	1.97159300
H	3.58802400	3.41174700	0.09215500	C	-0.82557800	-1.60900700	2.51328000
C	3.10955600	5.36630000	2.83696400	C	-1.62644100	-1.59896900	3.66517300
H	3.57019500	4.78104700	4.86066400	C	-2.13738400	-2.78759000	4.18712700
H	2.78650400	5.66102200	0.72192600	C	-1.83608000	-4.00775300	3.57899900
H	2.75984500	6.35737300	3.11292500	C	-1.01819300	-4.03391500	2.44930300

C	-0.52078700	-2.84252900	1.92016800
C	-1.97608600	1.44805500	1.78707200
C	-1.59793300	2.11349000	3.10111600
C	-2.42564600	1.87277700	4.21084300
C	-2.20678700	2.50258400	5.43668900
C	-1.14446700	3.39454300	5.58355600
C	-0.31974600	3.66020100	4.49000000
C	-0.55102100	3.03587400	3.26264400
H	-0.87105300	-0.77161300	-0.50803600
H	-1.67324200	0.77004100	-0.85185600
H	0.69989600	-0.63281600	1.39227400
H	0.16445600	0.28016900	2.79691600
H	-1.82866900	-0.66094500	4.17212500
H	-2.76460000	-2.76306300	5.07343600
H	-2.23579800	-4.93157700	3.98640800
H	-0.77476100	-4.97787100	1.97117200
H	0.11523000	-2.87363700	1.03932200
H	-2.27262900	2.19995900	1.04763400
H	-2.86458100	0.83942500	1.97242400
H	-3.26287800	1.18693000	4.10894400
H	-2.86639000	2.29419400	6.27425700
H	-0.96551100	3.88320200	6.53683700
H	0.50728700	4.35781600	4.58096900
H	0.09897800	3.29674200	2.43596000
N	-7.07143700	1.00946400	-1.84684200
C	-8.00178400	1.68438500	-0.93748400
H	-9.00787700	1.33333500	-1.20269700
C	-7.33885800	-0.42934700	-1.96526600
H	-8.42588300	-0.53773800	-2.07504900
H	-7.06148600	-0.98248900	-1.04917800
H	-7.85410300	1.39649900	0.12071400
C	-6.65375100	-1.06665600	-3.16016000
C	-6.83717400	-0.53801300	-4.44645700
C	-5.86046400	-2.20900200	-3.00764400
C	-6.24560400	-1.14329100	-5.55428900
H	-7.44411000	0.35500300	-4.56936100
C	-5.26826500	-2.81955400	-4.11682100
H	-5.70176200	-2.62706800	-2.01655600
C	-5.46030800	-2.28915600	-5.39260200
H	-6.40158700	-0.72612100	-6.54584000
H	-4.65485700	-3.70533300	-3.97600000
H	-5.00435900	-2.76388500	-6.25750000
C	-7.96582400	3.19804000	-1.05128100
C	-8.05132900	3.81967800	-2.30556800
C	-7.89624400	4.00086400	0.09296600
C	-8.07297000	5.21040800	-2.40998100
H	-8.09676800	3.20111200	-3.19743900
C	-7.92150900	5.39498800	-0.00636000
H	-7.83411400	3.53149000	1.07277800
C	-8.01043800	6.00404100	-1.25940700
H	-8.14999600	5.67735200	-3.38850200
H	-7.87837500	6.00262700	0.89380200
H	-8.03933000	7.08731800	-1.34025500
O	-9.87586900	-4.08340200	1.38702400
C	-8.76124500	-3.30390600	1.75405700
H	-7.82039000	-3.86865700	1.65525200
H	-8.67725700	-2.40277200	1.12174100
C	-9.80273100	-4.55912000	0.05871100
H	-10.70467200	-5.14900500	-0.12099600
H	-9.76485300	-3.73150200	-0.66774100
H	-8.91850900	-5.19735600	-0.09564100
C	-8.96516200	-2.89539100	3.20663200
H	-9.89424200	-2.31623800	3.30779400

H	-9.05197200	-3.79157000	3.83821300
O	-7.84892200	-2.10474200	3.60893500
C	-7.94273500	-1.66415300	4.95504400
H	-7.04108600	-1.08495800	5.16834900
H	-8.82604000	-1.02593300	5.09842000
H	-8.00183600	-2.51232600	5.65221400

#### HClO<sub>4</sub>

Cl	-0.14963900	0.00527700	0.00010300
O	-0.41775400	0.76082300	-1.22576800
O	-0.41467900	0.76264100	1.22559100
O	1.54033500	-0.24923600	-0.00146900
O	-0.63071300	-1.36714700	0.00168000
H	1.92635700	0.65364700	-0.00202100

#### INT5

C	2.08330100	2.34113700	-0.02810400
H	2.59480100	2.99801700	0.67925300
H	2.82866400	1.88590800	-0.67704500
N	1.07223800	2.99161200	-0.80437800
C	0.61530200	4.30829400	-0.30388000
H	0.56139200	4.25319600	0.78629600
H	1.35303900	5.09382000	-0.53990700
C	1.38746500	3.06806300	-2.26154300
H	2.38776000	3.50697100	-2.40687800
H	0.66760900	3.77486700	-2.68110200
C	-0.74357100	4.71617300	-0.84382500
C	-1.85178300	3.86167600	-0.73700600
C	-0.91885500	5.97727800	-1.42458600
C	-3.10542400	4.26081100	-1.20058500
H	-1.73253900	2.87545300	-0.29498900
C	-2.17390600	6.38226900	-1.88640100
H	-0.06858100	6.64957300	-1.51614400
C	-3.26809000	5.52455100	-1.77645400
H	-3.95710900	3.59134200	-1.11263800
H	-2.29202600	7.36445200	-2.33511600
H	-4.24397300	5.83536600	-2.13817900
C	1.28376200	1.75960600	-3.01234800
C	0.02381600	1.23775300	-3.34538500
C	2.42965300	1.05962700	-3.40713200
C	-0.08398600	0.03546800	-4.04213400
H	-0.87252300	1.78509000	-3.06210100
C	2.32532900	-0.14867900	-4.10248900
C	1.06828300	-0.66302200	-4.41988100
H	-1.06488000	-0.35203900	-4.30369100
H	0.98336600	-1.59563900	-4.97057600
H	3.41340000	1.46774300	-3.18367600
H	3.22453700	-0.67982100	-4.39992300
C	1.61938100	-4.42305200	2.44285100
C	1.94436800	-4.12613200	1.11901800
C	1.44055300	-2.98945600	0.47200900
C	0.58538000	-2.12010900	1.18798800
C	0.25201400	-2.43930300	2.51549800
C	0.76166000	-3.57544700	3.14311300
H	2.01894400	-5.31539400	2.91597300
H	2.59765100	-4.79399100	0.56213500
H	-0.43295800	-1.79007000	3.05481300
H	0.48241100	-3.79897200	4.16876800
C	-0.04303100	-0.89432400	0.58287800
C	-1.35851400	-0.76337600	0.59007400
C	-2.65502400	-0.60158800	0.55486100
H	-3.16281600	-0.14314000	1.40552200
C	-3.55466200	-0.95335200	-0.61437700

H	-3.79917100	-0.02016800	-1.13573800
H	-3.01030700	-1.59231700	-1.33443700
C	1.85162600	-2.73894600	-0.96623900
H	2.04982700	-3.69896600	-1.46022200
H	1.05409700	-2.24475300	-1.52764700
O	3.00117800	-1.88879200	-1.06653400
H	3.78117600	-2.41545100	-0.77715500
N	1.57516600	1.14256800	0.85580900
C	0.74176700	0.22912900	-0.07513000
C	2.78797500	0.31519600	1.39198400
C	4.15341400	0.96988400	1.41587200
C	5.00293500	0.79123100	0.30931900
C	6.29689000	1.31255300	0.31142500
C	6.76683600	2.00816000	1.42796000
C	5.94068700	2.16833100	2.54196100
C	4.64383400	1.65101500	2.53908900
C	0.66487400	1.64730400	1.98681100
C	1.31600100	2.22539600	3.22254400
C	1.74427300	3.55878100	3.31218200
C	2.28637900	4.05735500	4.49720100
C	2.40236200	3.23354700	5.61886200
C	1.96354000	1.90972700	5.55209900
C	1.42133500	1.41492700	4.36545100
H	1.46028800	-0.13865000	-0.80769100
H	0.05191900	0.90387800	-0.57460600
H	2.49400100	-0.02386600	2.38365400
H	2.84057100	-0.54767500	0.73040200
H	4.64775400	0.22396200	-0.54828800
H	6.94007800	1.16748200	-0.55198700
H	7.77556100	2.41099000	1.43474800
H	6.30784200	2.69021300	3.42099500
H	4.02206100	1.76467300	3.41998100
H	-0.01808300	2.35117000	1.50885400
H	0.07459000	0.77927700	2.27623600
H	1.65252500	4.22597400	2.46176600
H	2.60907800	5.09315200	4.54603300
H	2.81859000	3.62498000	6.54243700
H	2.03216100	1.26594200	6.42401500
H	1.06397400	0.38812500	4.32999300
N	-4.81340000	-1.54042400	-0.16369300
C	-5.86713100	-1.42954000	-1.18389800
H	-5.56838300	-1.91761500	-2.13152500
C	-4.63895600	-2.92273300	0.30458200
H	-3.73675500	-2.93486900	0.92956100
H	-4.44171400	-3.61201500	-0.53878500
H	-6.73019800	-1.98864200	-0.80555300
C	-5.81393700	-3.43671200	1.11393900
C	-6.29934900	-2.70477000	2.20732600
C	-6.40854300	-4.66652400	0.81062100
C	-7.35297500	-3.19344100	2.97855300
H	-5.84823100	-1.74466600	2.44341800
C	-7.46162700	-5.16161400	1.58423200
H	-6.04441400	-5.24259200	-0.03746700
C	-7.93670400	-4.42571500	2.66993000
H	-7.71972800	-2.61468100	3.82224300
H	-7.91239900	-6.11806600	1.33383900
H	-8.75777300	-4.80665800	3.27085800
C	-6.27413100	0.00559600	-1.45804300
C	-6.33286100	0.49858900	-2.76686900
C	-6.62242400	0.85938800	-0.40060000
C	-6.73711300	1.81208600	-3.02036700
H	-6.06611000	-0.15304300	-3.59624200
C	-7.02220100	2.17228400	-0.64901300

H	-6.57698300	0.48331000	0.61751500
C	-7.08173100	2.65322500	-1.96148600
H	-6.78282500	2.17534200	-4.04354800
H	-7.29933600	2.81864800	0.17982700
H	-7.40419800	3.67270500	-2.15567700
O	6.50866000	-3.78735000	-3.70208000
C	5.50048800	-3.80795800	-2.71973300
H	4.73910100	-3.03095200	-2.90557400
H	4.98309700	-4.78170400	-2.69334600
C	6.02578500	-4.07579500	-4.99896000
H	6.88190200	-4.03476500	-5.67610000
H	5.57467900	-5.07892800	-5.04978000
H	5.27445300	-3.33845500	-5.32502900
C	6.18378500	-3.55111700	-1.38316500
H	6.89180300	-4.36082000	-1.16014500
H	6.74837100	-2.60807700	-1.42671500
O	5.17993100	-3.48830500	-0.37045600
C	5.71906100	-3.31672900	0.93564000
H	4.87594900	-3.30992300	1.62990400
H	6.39167900	-4.14676100	1.18949200
H	6.27162800	-2.37006300	1.01764500

#### -ClO<sub>4</sub>

Cl	0.00021000	0.00004900	0.00016700
O	-0.62838000	-1.35875700	0.06939900
O	-0.13361300	0.54132600	-1.39044600
O	1.45175700	-0.10147700	0.35919400
O	-0.69021000	0.91880400	0.96149900

#### HNBn<sub>2</sub>

N	-0.09823200	2.55428300	0.36715100
C	-1.13836500	2.08523200	-0.55922500
H	-1.98635800	2.77738600	-0.46202100
H	-0.74918900	2.21195600	-1.57634100
C	1.28935800	2.19660700	0.07127500
H	1.91032300	2.77206900	0.77221700
H	1.51947200	2.58756200	-0.92810000
C	-1.65779800	0.66478200	-0.37659600
C	-2.50768400	0.36830800	0.69923900
C	-1.32259600	-0.36642400	-1.26189500
C	-2.99333100	-0.92435900	0.89736200
H	-2.80044500	1.16234900	1.38489400
C	-1.80837700	-1.66147400	-1.07164600
H	-0.66771200	-0.15589400	-2.10369500
C	-2.64317400	-1.94526400	0.01041900
H	-3.65246700	-1.13303900	1.73635500
H	-1.53357400	-2.44870000	-1.76896400
H	-3.02302000	-2.95265300	0.15908700
C	1.71488200	0.73168200	0.13499500
C	2.33676200	0.12112500	-0.96007400
C	1.53540900	-0.02217500	1.30306300
C	2.76168800	-1.20866100	-0.89859700
H	2.49259400	0.69436800	-1.87224700
C	1.95255300	-1.35042200	1.37019600
C	2.56803000	-1.94950800	0.26729700
H	3.24147700	-1.66392100	-1.76145300
H	2.89465900	-2.98474600	0.31934500
H	-0.33998200	2.30399700	1.32318700
H	1.05744500	0.43202200	2.16901800
H	1.80027700	-1.91943600	2.28378600

#### TS7

C	3.52443700	1.53067700	0.77612300
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H	3.91421400	2.31035000	1.45669500	C	1.81048900	2.00202300	3.54643000
H	4.37230600	0.91922900	0.47286800	C	2.31941100	3.31037500	3.56336400
N	2.95248900	2.12248600	-0.43874200	C	2.57430900	3.96554300	4.76963700
C	2.40870700	3.48616600	-0.22660600	C	2.31902000	3.32793200	5.98466300
H	1.82172300	3.47589800	0.69344500	C	1.80073400	2.03201200	5.98575900
H	3.22579300	4.21233600	-0.06626000	C	1.54972300	1.38089800	4.77770800
C	3.97196600	2.17967800	-1.52586500	H	2.58000700	-1.26115500	-0.10266700
H	4.92816500	2.56242800	-1.12948800	H	1.63469700	0.17416800	-0.75464100
H	3.61428400	2.92215200	-2.24284500	H	3.91988800	0.46310900	3.22490500
C	1.51988400	3.96923900	-1.35617400	H	2.70151400	-0.79330700	3.07379900
C	0.32749500	3.29643400	-1.66251500	H	3.12109200	-2.81972300	1.73833800
C	1.84682100	5.11990300	-2.08280800	H	4.83593900	-4.38328900	0.88978400
C	-0.51844200	3.76715200	-2.66591700	H	7.19670500	-3.63579600	0.64353400
H	0.05778800	2.40541800	-1.09996500	H	7.82463000	-1.31461600	1.28162600
C	1.00467500	5.59201100	-3.09334300	H	6.10644900	0.24814600	2.12621900
H	2.76502900	5.65581500	-1.85272800	H	0.98567300	1.88940300	1.53875600
C	-0.18032900	4.91743600	-3.38558700	H	0.81002400	0.43813800	2.49945100
H	-1.45184800	3.25141800	-2.87604500	H	2.50779200	3.83829300	2.63431800
H	1.27452900	6.48723300	-3.64638900	H	2.96438800	4.97941100	4.75798800
H	-0.84090400	5.28695400	-4.16481000	H	2.51388200	3.84023500	6.92234200
C	4.20674200	0.88165500	-2.27104900	H	1.58669100	1.52977400	6.92495900
C	3.39863800	0.55565800	-3.37110600	H	1.13571900	0.37472400	4.79131000
C	5.25931100	0.01948800	-1.93727000	N	-4.09002700	0.29978700	0.17712500
C	3.63649400	-0.60006000	-4.11419000	C	-5.09445400	0.90708500	-0.71312200
H	2.59342900	1.22945300	-3.65595700	H	-5.04969500	0.46631500	-1.72787400
C	5.48811600	-1.15043600	-2.66681400	C	-4.39692200	-1.11168900	0.46665800
C	4.67888200	-1.46133200	-3.76018500	H	-3.53964600	-1.51436100	1.02142400
H	3.02442000	-0.81979000	-4.98534200	H	-4.47453900	-1.70745300	-0.46210200
H	4.87167900	-2.35583200	-4.34626400	H	-6.07500700	0.64211500	-0.30339100
H	5.92422000	0.26957300	-1.11459400	C	-5.65187200	-1.29090300	1.29753500
H	6.31093800	-1.80377100	-2.39076500	C	-5.78627900	-0.63909000	2.53220400
C	0.31690500	-5.51550700	1.29858800	C	-6.68268700	-2.13266200	0.86490100
C	0.96478000	-5.06172500	0.15112800	C	-6.92408200	-0.82810800	3.31521300
C	1.01572000	-3.69730600	-0.16127500	H	-4.99494100	0.02500100	2.87010600
C	0.40072800	-2.77147400	0.70778800	C	-7.82275100	-2.32777800	1.64924500
C	-0.26320600	-3.24053000	1.85257000	H	-6.59422600	-2.63601600	-0.09554400
C	-0.30598100	-4.59978700	2.15062100	C	-7.94571400	-1.67580700	2.87631900
H	0.29049000	-6.57786800	1.52192400	H	-7.01562100	-0.31567700	4.26919600
H	1.42971700	-5.77898000	-0.52214700	H	-8.61507800	-2.98298400	1.29766900
H	-0.74106700	-2.52230500	2.51304600	H	-8.83225000	-1.82306700	3.48675000
H	-0.81796800	-4.94271600	3.04468400	C	-4.97507000	2.41487200	-0.80899600
C	0.42652800	-1.30965800	0.38819800	C	-4.92343100	3.05155000	-2.05494900
C	-0.63427300	-0.52533800	0.55755400	C	-4.94916200	3.20186900	0.35190300
C	-1.68558400	0.23162300	0.71035200	C	-4.85535400	4.44476900	-2.14437500
H	-1.83697300	0.77110000	1.64711300	H	-4.95109100	2.45277300	-2.96324700
C	-2.74297800	0.46599000	-0.35393400	C	-4.87603100	4.59164200	0.26567400
H	-2.64568300	1.50616200	-0.68729800	H	-4.98769700	2.71381500	1.32178400
H	-2.53930400	-0.17832200	-1.23063400	C	-4.82982100	5.21797200	-0.98337500
C	1.73818600	-3.28315300	-1.43523500	H	-4.82547200	4.92325200	-3.11966500
H	2.82471800	-3.31659000	-1.30244600	H	-4.86232500	5.18909900	1.17340800
H	1.48428500	-3.96374100	-2.25532600	H	-4.77776300	6.30114600	-1.04925300
O	1.44577500	-1.94532500	-1.86930500	O	-0.74580700	-2.17639500	-3.42126200
H	0.52779200	-1.93577400	-2.25489800	C	-2.12227500	-2.54722200	-3.31695300
N	2.63795700	0.60573000	1.53196100	H	-2.74083900	-1.66307300	-3.10794700
C	1.62407500	-0.78402200	-0.25044100	H	-2.45994600	-2.98187000	-4.26680200
C	3.43278100	-0.20997300	2.50550600	C	-0.46958400	-1.38400900	-4.57525300
C	4.47496100	-1.15087300	1.93311800	H	0.59694600	-1.15205400	-4.55244400
C	4.14179100	-2.47212500	1.59874900	H	-0.70483100	-1.94096400	-5.49100800
C	5.11192000	-3.35958500	1.12827200	H	-1.04894500	-0.45088500	-4.56259000
C	6.43838500	-2.94268600	0.99642000	C	-2.27521500	-3.56847100	-2.19852600
C	6.79012700	-1.63882000	1.35183800	H	-1.73018700	-4.49101900	-2.45748600
C	5.81646300	-0.75503800	1.82156500	H	-1.84276200	-3.17937900	-1.26186800
C	1.50333000	1.24952400	2.25546000	O	-3.65561600	-3.81279400	-2.05729000

C	-3.93963100	-4.87247100	-1.15969200
H	-5.02637800	-4.96909600	-1.11377600
H	-3.50793600	-5.82120000	-1.51260400
H	-3.55279700	-4.66288400	-0.15091600

**4**

C	5.70703500	2.02217700	0.10585700
C	6.13125300	0.70576500	0.27378500
C	5.24660300	-0.36224800	0.09262300
C	3.90946600	-0.10589200	-0.26641100
C	3.49079300	1.22533100	-0.42916700
C	4.37790800	2.28034800	-0.24622600
H	6.40432300	2.84220600	0.25425300
H	7.16187900	0.50120400	0.55785000
H	2.46078000	1.42089000	-0.71443700
H	4.03645400	3.30328500	-0.37980000
C	2.99342700	-1.25496200	-0.46400900
C	1.69124600	-1.15195100	-0.62254900
C	0.39210600	-1.09027700	-0.77542400
H	-0.03334600	-0.99035300	-1.77665900
C	-0.62098400	-1.18754600	0.34697100
H	-1.18110400	-2.12191000	0.22173400
H	-0.10085900	-1.24840900	1.32026400
C	5.72676900	-1.79059100	0.26582600
H	6.29568900	-2.10436400	-0.62946000
H	6.40139900	-1.86820600	1.12465200
O	4.67418700	-2.70663700	0.50885500
C	3.67164900	-2.62016900	-0.49034200
H	4.11795000	-2.79531400	-1.48586700
H	2.95402400	-3.41836200	-0.29081400
N	-1.59835000	-0.09302900	0.30473600
C	-2.79744700	-0.40399900	1.09318100
H	-2.54003500	-0.66272800	2.13901000
C	-1.00355200	1.18601500	0.70920900
H	-0.02396100	1.24887000	0.22059800
H	-0.80798400	1.21794800	1.79884600
H	-3.39258700	0.51580000	1.14045200
C	-1.83592600	2.38941900	0.30900300
C	-2.28148300	2.53721200	-1.01278200
C	-2.14103200	3.39286500	1.23544600
C	-3.01115900	3.66164200	-1.39625500
H	-2.05457200	1.75718600	-1.73416800
C	-2.86886800	4.52323600	0.85405600
H	-1.80528600	3.28861800	2.26509800
C	-3.30638800	4.66037600	-0.46344500
H	-3.34924200	3.76139200	-2.42464800
H	-3.09723100	5.29164000	1.58816200
H	-3.87519700	5.53678900	-0.76265000
C	-3.64390600	-1.51041800	0.49298100
C	-4.10541200	-2.56941700	1.28308600
C	-4.01367800	-1.46976800	-0.85937100
C	-4.92514000	-3.56329800	0.74189900
H	-3.82128500	-2.61600500	2.33234100
C	-4.82817900	-2.46188100	-1.40368400
H	-3.64995800	-0.65536100	-1.47914900
C	-5.28860600	-3.51218900	-0.60399000
H	-5.27338100	-4.37825400	1.37126300
H	-5.10681300	-2.41588000	-2.45352500
H	-5.92366900	-4.28506100	-1.02894700

**TS8**

C	5.76758700	2.17452400	-2.01031000
C	6.71207400	3.19530200	-2.19119700

C	6.26536200	4.41483100	-2.70861600
C	4.92837000	4.59767100	-3.05986100
C	4.01593800	3.55770700	-2.89912100
C	4.41070300	2.32134300	-2.36338600
H	6.96493700	5.23064500	-2.85249000
H	4.59959900	5.54925800	-3.46713500
H	2.97879200	3.71241400	-3.17734700
C	8.17938100	2.87384100	-1.88491300
C	9.01859000	4.14591400	-1.67532300
H	10.06643600	3.89268500	-1.49011400
H	8.65307100	4.74484700	-0.83423500
H	9.00775100	4.76893400	-2.57432200
C	8.76892600	2.08765600	-3.09294200
H	9.81138400	1.81494000	-2.89383000
H	8.73747400	2.70480100	-3.99784200
H	8.20603700	1.16942500	-3.28578500
C	8.20349300	1.95773600	-0.65571500
C	9.20957200	1.97548900	0.31443900
C	7.18899600	0.99600400	-0.53294800
C	9.21622100	1.05005700	1.35744200
H	10.00536300	2.70959700	0.25549700
C	7.16002000	0.04969300	0.51211700
C	8.20615400	0.09613700	1.44894900
H	10.01070000	1.07149000	2.09754400
H	8.21751000	-0.61419100	2.26880800
O	6.18039400	0.96638200	-1.47900600
P	3.21404400	0.91762400	-2.14818700
P	5.79140500	-1.19742100	0.67318000
C	3.32722600	0.03957400	-3.77158100
C	3.38700700	0.72111700	-4.99853000
C	3.37818500	-1.36239600	-3.77207300
C	3.48065800	0.01331700	-6.19685400
H	3.36988600	1.80688700	-5.01999500
C	3.47300400	-2.07045300	-4.97244100
H	3.36784800	-1.89047700	-2.82165900
C	3.52202000	-1.38377100	-6.18606800
H	3.52763800	0.55244300	-7.13906500
H	3.52130600	-3.15594800	-4.95763500
H	3.60140200	-1.93235900	-7.12053800
C	1.56948900	1.77277200	-2.20934400
C	1.24963800	2.68073800	-1.18108700
C	0.58643700	1.47189900	-3.16475000
C	-0.00654300	3.28528400	-1.12576700
H	1.99331800	2.92908700	-0.42818500
C	-0.67697300	2.06950300	-3.10083200
H	0.80628900	0.77799200	-3.96962500
C	-0.97648200	2.98049500	-2.08728300
H	-0.22463800	4.00076600	-0.33685200
H	-1.42182700	1.82623800	-3.85375900
H	-1.95274900	3.45595400	-2.04763200
C	6.45963600	-2.69799000	-0.17496300
C	7.83007800	-2.92136100	-0.37724500
C	5.54369000	-3.66253700	-0.62659000
C	8.27159600	-4.08373000	-1.01304900
H	8.55614200	-2.18697100	-0.04297600
C	5.98633100	-4.82950000	-1.25027200
H	4.47880900	-3.48591700	-0.49357600
C	7.35277100	-5.04089100	-1.44755000
H	9.33561300	-4.24049600	-1.16769100
H	5.26570900	-5.56841700	-1.59078300
H	7.69937700	-5.94428500	-1.94163000
C	5.88073100	-1.63807700	2.47156800
C	6.25946200	-2.90681100	2.93272700

C	5.48554600	-0.66877500	3.41216000	H	-8.72075000	-0.92213800	-0.48448700
C	6.24285500	-3.19964000	4.30047800	N	-5.64240700	2.74363300	0.95545500
H	6.57500400	-3.66965200	2.22828400	C	-5.72926400	1.29000200	0.83654500
C	5.48451400	-0.95798300	4.77595000	C	-6.21647500	3.50858200	-0.15535700
H	5.18606700	0.32097000	3.07532300	C	-7.72347300	3.38643100	-0.28793200
C	5.85924200	-2.22861900	5.22479400	C	-8.31563700	3.35736700	-1.55622600
H	6.54076100	-4.18807300	4.63991600	C	-9.70538000	3.35722200	-1.69628700
H	5.19099200	-0.19222500	5.48935000	C	-10.52283300	3.36669600	-0.56434800
H	5.85365600	-2.45624500	6.28704600	C	-9.94023400	3.37615200	0.70586200
Pd	3.88995200	-0.36118500	-0.34939900	C	-8.55208900	3.39141400	0.84219800
C	0.94443400	-0.71185000	1.00184300	C	-4.32424500	3.23274500	1.36001200
H	1.62462200	-1.51022400	0.72487300	C	-4.36610500	4.60442900	2.01055300
N	0.93659000	-0.31310900	2.26615900	C	-5.21940800	4.84898400	3.09633700
C	0.38764000	1.01072900	2.62485400	C	-5.23255500	6.09383900	3.72374300
H	-0.32066200	0.88075100	3.44817500	C	-4.39019000	7.11614200	3.27586900
C	1.68483400	-1.05289800	3.32515500	C	-3.53846100	6.88466200	2.19568700
H	2.11619900	-1.93521900	2.84856000	C	-3.53051300	5.63583500	1.56833600
H	2.51895400	-0.40987800	3.62170100	H	-6.76601800	1.01117700	0.63508000
H	0.71904000	0.02576800	0.24287500	H	-5.45676400	0.86380400	1.80817900
H	-0.18638900	1.36120000	1.76251500	H	-5.97397600	4.56067100	0.03955900
C	0.87487300	-1.44486400	4.54618900	H	-5.74290400	3.26038200	-1.12124500
C	0.40503700	-2.75604000	4.70386000	H	-7.68372700	3.34370600	-2.44161300
C	0.63686600	-0.52007200	5.57472400	H	-10.14789400	3.35230200	-2.68932100
C	-0.31713900	-3.12682100	5.83994500	H	-11.60462700	3.37187600	-0.66976000
H	0.62804600	-3.50638400	3.94969600	H	-10.56922000	3.38164900	1.59227300
C	-0.09069400	-0.88569700	6.70824500	H	-8.09724700	3.40717500	1.82796800
H	1.04016000	0.48641500	5.49835700	H	-3.92363400	2.50623600	2.07947100
C	-0.57532500	-2.18853100	6.84071500	H	-3.60629700	3.25426800	0.51795300
H	-0.66465600	-4.15043600	5.94681200	H	-5.87850900	4.05578700	3.43849100
H	-0.26573700	-0.15671800	7.49441400	H	-5.90063300	6.26904200	4.56287800
H	-1.13466700	-2.47526500	7.72654700	H	-4.40283200	8.08694100	3.76370200
C	1.44348800	2.03817900	3.00356100	H	-2.88631800	7.67583300	1.83521500
C	2.67110200	2.11827600	2.33060000	H	-2.87029100	5.46244800	0.72034700
C	1.15572300	2.97118300	4.00795800	N	-0.71273000	-1.88528900	0.36181600
C	3.59026100	3.11692100	2.66059500	C	-0.42316700	-3.21818500	0.98618900
H	2.92642300	1.39853400	1.55077900	H	0.37720200	-3.66952600	0.39152000
C	2.07264800	3.97373000	4.33190500	C	-0.53446300	-1.81969400	-1.11852400
H	0.20509700	2.92123300	4.53477800	H	0.53731800	-1.96902200	-1.29674900
C	3.29339400	4.04773000	3.65952300	H	-0.76142200	-0.79025100	-1.40869700
H	4.53801600	3.16612500	2.13094200	H	-0.01294100	-2.99019200	1.97376700
H	1.83309100	4.69141500	5.11130700	C	-1.30825700	-2.77679000	-2.00492600
H	4.00970800	4.82399200	3.91285600	C	-0.61623900	-3.76390500	-2.72055100
C	-6.43200300	-0.25535600	-4.16109500	C	-2.69262900	-2.65499300	-2.19346900
C	-6.86942900	-0.97262500	-3.04647900	C	-1.29108600	-4.62864500	-3.58508300
C	-6.36925900	-0.71375200	-1.76273700	H	0.46292300	-3.85049700	-2.60903100
C	-5.40333800	0.30605600	-1.60368500	C	-3.36962400	-3.52031100	-3.05243600
C	-4.95106500	1.00422700	-2.73324000	H	-3.24348800	-1.86904200	-1.68671700
C	-5.46128300	0.73400600	-4.00318600	C	-2.67269200	-4.51287600	-3.74628900
H	-6.83738900	-0.47537100	-5.14485600	H	-0.73769700	-5.38489300	-4.13503700
H	-7.61806600	-1.75295300	-3.16492000	H	-4.44093400	-3.40494900	-3.19023200
H	-4.19162500	1.77072200	-2.60474900	H	-3.20120200	-5.18173400	-4.41977900
H	-5.09968300	1.29128300	-4.86314100	C	-1.55695800	-4.21507600	1.18448300
C	-4.83459900	0.63002200	-0.25020000	C	-1.81281500	-5.23779900	0.26123800
C	-3.57526700	0.35761000	-0.00064500	C	-2.32176200	-4.17081000	2.36157000
C	-2.33018200	0.05603500	0.29178900	C	-2.81892700	-6.17566100	0.49680400
H	-1.55321800	0.80073500	0.11646400	H	-1.22572500	-5.30400200	-0.64831000
C	-1.94196500	-1.26451200	0.91891100	C	-3.33354300	-5.10259300	2.59581200
H	-1.73809800	-1.13337000	1.99224900	H	-2.11482600	-3.41004700	3.11051700
H	-2.78335100	-1.95980600	0.84306800	C	-3.58638700	-6.10786900	1.66079500
C	-6.87508800	-1.54438100	-0.59451700	H	-2.99950400	-6.96195200	-0.23067800
H	-7.16851300	-2.53703900	-0.96828000	H	-3.91512400	-5.04899500	3.51195000
H	-6.07484600	-1.69573100	0.13684300	H	-4.36878700	-6.83916000	1.84317700
O	-7.94546500	-0.93724800	0.11621000	O	-10.12880000	-1.34682200	-1.62153800



C	-11.17140700	-2.06545700	-0.96785100
H	-11.73623400	-1.40199100	-0.29671500
H	-11.87189100	-2.47425500	-1.71035600
C	-10.61353600	-0.27255700	-2.41710200
H	-9.74275100	0.21405900	-2.86071500
H	-11.27361700	-0.64559000	-3.21306800
H	-11.16089100	0.45896800	-1.80750800
C	-10.54253500	-3.19789800	-0.16743400
H	-9.98680200	-3.86843600	-0.84544000
H	-9.82398300	-2.78742600	0.55971900
O	-11.59676400	-3.88112600	0.47361300
C	-11.15064000	-4.95699800	1.27104900
H	-12.03597200	-5.41138300	1.72266600
H	-10.62471000	-5.71734100	0.67109700
H	-10.47385700	-4.61661900	2.07104900

## INT6

C	4.08370300	-0.65142500	-1.49359200
H	4.73223300	-1.28387800	-2.10348600
N	4.77657300	-0.05605900	-0.43359100
C	4.43848300	1.32838800	-0.05846600
H	4.60715800	1.43331700	1.01786300
C	6.20460000	-0.43031500	-0.22251800
H	6.35413600	-1.41790400	-0.66919200
H	6.84261300	0.27330900	-0.77278900
H	3.56077800	0.05802600	-2.13695400
H	3.36272100	1.46926400	-0.20472600
C	6.63345100	-0.46082100	1.23238100
C	6.54432600	-1.63828700	1.98883200
C	7.16287500	0.68657000	1.84006400
C	6.94780300	-1.66428000	3.32462600
H	6.18335800	-2.55486600	1.52757400
C	7.56455700	0.66545200	3.17718000
H	7.27189900	1.59946300	1.25968300
C	7.45375200	-0.50866900	3.92377100
H	6.88118700	-2.58879600	3.89116400
H	7.97499600	1.56303700	3.63098500
H	7.77380500	-0.52796900	4.96153200
C	5.19700700	2.43469400	-0.78762400
C	5.58401800	2.33441500	-2.13026000
C	5.47350700	3.62548300	-0.10073200
C	6.22430900	3.39698500	-2.77170500
H	5.40092400	1.41935300	-2.68829300
C	6.10588800	4.69299100	-0.74078000
H	5.18750400	3.71827200	0.94474800
C	6.48378600	4.58124200	-2.08016000
H	6.52128200	3.29766500	-3.81201100
H	6.31092500	5.60690300	-0.19050800
H	6.98211400	5.40729400	-2.57879100
C	-4.24436000	-1.28293100	-3.62983400
C	-4.26665700	-1.75379200	-2.31603100
C	-3.39578200	-1.25360300	-1.33813600
C	-2.47751900	-0.24135500	-1.70340100
C	-2.44860800	0.21139700	-3.03209800
C	-3.32490400	-0.29807600	-3.99016300
H	-4.93300500	-1.68823700	-4.36578100
H	-4.97724500	-2.52777700	-2.03409000
H	-1.73521800	0.98313100	-3.30739900
H	-3.28772000	0.07348100	-5.01031600
C	-1.51330600	0.35279600	-0.71784300
C	-0.22073600	0.23578200	-0.90368300
C	1.08818500	0.13297200	-0.99489500
H	1.64462000	0.91396400	-1.51256800

C	1.84508700	-0.94453400	-0.25905400
H	2.39509900	-0.54304700	0.59689500
H	1.15242100	-1.69554900	0.11693900
C	-3.48014000	-1.82001300	0.06985600
H	-3.84012700	-2.85859800	0.01291700
H	-2.48752300	-1.84665100	0.53103400
O	-4.29771300	-1.05494800	0.94569500
H	-5.22334800	-1.09661600	0.61620700
N	-2.66686100	2.43269200	0.22050600
C	-2.00868100	1.16897600	0.50971700
C	-4.04924100	2.33978100	-0.26758600
C	-4.89297200	3.54133700	0.12262700
C	-4.96920000	3.95370200	1.46099600
C	-5.77589400	5.02958600	1.82852800
C	-6.52181100	5.71135700	0.86192700
C	-6.45262800	5.31069600	-0.47235500
C	-5.64035900	4.23326500	-0.83709700
C	-1.86530900	3.42303300	-0.49521900
C	-0.60863600	3.85269600	0.23977100
C	-0.63449400	4.12614800	1.61457100
C	0.51065200	4.57680500	2.27175000
C	1.69975400	4.76884300	1.56288200
C	1.73681400	4.50268900	0.19281300
C	0.59002200	4.04068900	-0.45877900
H	-2.71024500	0.55065500	1.07494900
H	-1.13744300	1.36946800	1.13976700
H	-4.09737600	2.20970400	-1.36243700
H	-4.47609100	1.43163400	0.17166700
H	-4.38755300	3.42412700	2.21080400
H	-5.82649400	5.33675700	2.86986900
H	-7.15011500	6.55011900	1.14877300
H	-7.02424900	5.83842200	-1.23116800
H	-5.58598500	3.92694500	-1.87997800
H	-1.59007800	3.08144800	-1.51082800
H	-2.50945500	4.30027400	-0.63361300
H	-1.56206900	3.98312600	2.16133000
H	0.47247900	4.78895400	3.33706900
H	2.58670600	5.13387400	2.07443100
H	2.65383600	4.65986600	-0.36910200
H	0.61945200	3.84351800	-1.52897700
N	2.89696800	-1.68151000	-1.07911700
C	3.54346400	-2.81627500	-0.24608600
H	3.81471400	-3.58998900	-0.96613000
C	2.34409900	-2.17557500	-2.42378700
H	3.22644600	-2.38828900	-3.03318000
H	1.83201900	-1.31276900	-2.85454900
H	4.45209400	-2.36917200	0.15011200
C	1.44067000	-3.38222300	-2.42055700
C	1.95183900	-4.62851800	-2.81459800
C	0.07370400	-3.27213000	-2.12602900
C	1.12390100	-5.75023800	-2.87996100
H	3.00045400	-4.72172000	-3.08967300
C	-0.75378000	-4.39300100	-2.18986800
H	-0.35302700	-2.30735200	-1.87100600
C	-0.23053800	-5.63455000	-2.55950500
H	1.53295700	-6.70664800	-3.19199300
H	-1.81181900	-4.28815100	-1.96912200
H	-0.87877900	-6.50415300	-2.61668800
C	2.76432000	-3.39098600	0.91710000
C	1.94604000	-4.52178100	0.78086600
C	2.93063500	-2.82487000	2.19241400
C	1.29436500	-5.05912700	1.89200900
H	1.82431600	-4.99250400	-0.18828200

C	2.27419900	-3.35913100	3.30040800	H	-3.63505300	-1.54165100	-2.33915700
H	3.59286900	-1.97237600	2.32215200	H	-5.23731000	0.72049500	-2.56400500
C	1.45053800	-4.47694500	3.15117000	H	-5.61177200	-0.93406100	-2.09118300
H	0.66874800	-5.93883100	1.77227400	H	-5.96345100	-0.38104900	0.98119500
H	2.41507900	-2.91002100	4.27917700	H	-7.98110800	0.33840100	2.21672600
H	0.94283200	-4.89877700	4.01373600	H	-9.72714600	1.69654400	1.07889500
O	-6.95947900	-1.29139500	0.10937500	H	-9.42842300	2.32963000	-1.30981700
C	-7.80927200	-1.60664200	1.21173600	H	-7.40671700	1.61176100	-2.54030700
H	-7.92069000	-0.73672900	1.87494000	H	-4.32939400	1.48048900	0.41704600
H	-8.80725100	-1.88864100	0.84802500	H	-2.69005500	0.90739900	0.20398000
C	-7.46719500	-0.23260600	-0.69451700	H	-1.38837500	1.69405400	-1.93162000
H	-6.75679900	-0.08238100	-1.51030800	H	-1.04761900	3.57777400	-3.48361300
H	-8.44844100	-0.49839100	-1.11090600	H	-2.79882300	5.32608500	-3.73545500
H	-7.56476300	0.69767500	-0.11733900	H	-4.89918900	5.16104100	-2.41120300
C	-7.18705000	-2.76743100	1.97618200	H	-5.24970600	3.26015400	-0.87062000
H	-7.08510900	-3.64010100	1.30838600	C	2.95021900	0.33126400	1.01859800
H	-6.17734100	-2.49009400	2.32119500	H	3.67390000	0.26823900	1.84276100
O	-8.04295300	-3.04955800	3.05935700	N	1.57278100	0.41607800	1.59938800
C	-7.58190700	-4.11512900	3.86349800	C	1.43030800	1.65321800	2.42546100
H	-8.30943400	-4.24845800	4.66767000	H	2.06913100	1.55151300	3.31600800
H	-7.50549000	-5.05291300	3.29014700	C	1.17728500	-0.84385100	2.28247700
H	-6.59634200	-3.89442300	4.30360200	H	1.13357400	-1.60879200	1.50000600

## TS9

C	-4.26984700	-5.27582800	0.94682100	H	2.98648400	-0.62123100	0.48393900
C	-2.93059500	-5.36278300	0.56551500	N	3.28210100	1.42852400	0.12776600
C	-2.27410700	-4.26157300	0.01667900	C	4.27510700	2.37058000	0.67753400
C	-2.95083700	-3.03576800	-0.15013400	H	4.03854300	2.50798800	1.73898600
C	-4.29749100	-2.96219000	0.24076400	H	5.29180200	1.94738000	0.64717200
C	-4.94968900	-4.07012100	0.78133200	C	3.56708200	1.02862600	-1.27358400
H	-4.77194900	-6.13936100	1.37243500	H	3.57088500	1.94766800	-1.86721000
H	-2.38982800	-6.29793500	0.68904300	H	2.71783300	0.43055100	-1.62000600
H	-4.81863800	-2.02050900	0.13455100	C	4.28064400	3.72972800	-0.00188900
H	-5.99060500	-3.98382800	1.07899500	C	3.09564200	4.35340600	-0.41525500
C	-2.27338000	-1.85111400	-0.74633700	C	5.49168900	4.41392300	-0.17025500
C	-0.96852100	-1.60589200	-0.69075700	C	3.12103900	5.62913700	-0.98026000
C	0.07882900	-0.70711300	-0.88608700	H	2.15062800	3.82953000	-0.30223700
H	0.82487400	-0.93821700	-1.64554500	C	5.52003500	5.69302400	-0.72980900
C	0.19046300	0.47006600	-0.15829900	H	6.42062900	3.94366400	0.14535000
H	-0.59931500	0.75571500	0.52187400	C	4.33355400	6.30436900	-1.13767400
H	0.82717700	1.26940300	-0.51621600	H	2.19277700	6.09775400	-1.29613600
C	-0.86099600	-4.38607600	-0.45880000	H	6.46892900	6.20826500	-0.85021400
H	-0.36631500	-5.26177100	-0.02661000	H	4.35317000	7.29767700	-1.57689400
H	-0.80759600	-4.45634900	-1.55491600	C	4.86001900	0.26282700	-1.51682600
O	-0.14482100	-3.20068200	-0.03478500	C	6.04885800	0.94873800	-1.80800700
H	0.75929100	-3.23292700	-0.45641000	C	4.89667900	-1.13918700	-1.46194300
N	-4.11562100	-0.09463800	-0.92760400	C	7.24399800	0.25762600	-2.01509400
C	-3.11124600	-0.88879200	-1.63235200	H	6.03436300	2.03308600	-1.88553600
C	-5.36450100	0.05858300	-1.69144500	C	6.09109900	-1.83294600	-1.66906600
C	-6.54776500	0.55050700	-0.87259300	C	7.26975300	-1.13622400	-1.94147300
C	-6.72586000	0.20226700	0.47322700	H	8.15295400	0.80752100	-2.24278700
C	-7.86205700	0.61454200	1.17232500	H	8.19791200	-1.67559900	-2.10750700
C	-8.84247900	1.37747900	0.53515500	H	1.84205000	2.45736500	1.81363600
C	-8.67454800	1.73200100	-0.80476300	C	2.02565900	-1.35435500	3.44324400
C	-7.53338100	1.32582200	-1.49837400	C	3.28325200	-1.94983900	3.24386100
C	-3.60504000	1.16190200	-0.33766000	C	1.51727300	-1.31966200	4.74944000
C	-3.35463700	2.32466900	-1.29288900	C	4.02076800	-2.45192900	4.31693400
C	-2.17063900	2.43988100	-2.03969300	H	3.69550500	-2.03232500	2.24187400
C	-1.97200800	3.50915300	-2.91583600	C	2.24864000	-1.82601200	5.82622800
C	-2.95339100	4.49175900	-3.05705000	H	0.52422500	-0.91628000	4.92418400
C	-4.13193700	4.39767600	-2.31468000	C	3.50848100	-2.38566900	5.61434600
C	-4.32782900	3.32519400	-1.44262000	H	4.99330600	-2.90210100	4.13782500
H	-2.42492300	-0.27486200	-2.22870900	H	1.82913900	-1.78830900	6.82760100
				H	4.08141800	-2.77820600	6.44935500

C	0.02791000	2.04738100	2.85017600
C	-0.45401300	1.73707700	4.12939300
C	-0.78230400	2.82617800	2.00776300
C	-1.72245800	2.15146800	4.54087700
H	0.18190800	1.19372600	4.82145400
C	-2.05131000	3.24205800	2.41335100
H	-0.41209800	3.13074500	1.03179800
C	-2.52839600	2.89784500	3.68033300
H	-2.07312300	1.90348300	5.53876400
H	-2.65816900	3.84494800	1.74378700
H	-3.51257800	3.22687500	4.00132300
H	3.98172800	-1.69841500	-1.27709100
H	6.10222100	-2.91956500	-1.63030200
O	2.33229100	-3.72075000	-1.03093400
C	2.53886600	-4.27007400	-2.34012800
H	3.61451800	-4.37919000	-2.52575200
H	2.07593900	-5.26391600	-2.41150200
C	2.98837000	-4.48264600	-0.01229600
H	2.74390100	-4.02320200	0.94744300
H	2.64462000	-5.52548200	-0.01878400
H	4.07461500	-4.46246200	-0.16132100
C	1.92876700	-3.33767100	-3.37811000
H	0.86580600	-3.14521500	-3.14040500
H	2.45325900	-2.36747300	-3.36843700
O	2.06371300	-3.98412900	-4.61690900
C	1.61611500	-3.20190100	-5.71000700
H	1.77042600	-3.79874800	-6.61108000
H	0.54640400	-2.95703500	-5.61918400
H	2.18723400	-2.26508700	-5.79506300

**5'**

C	4.41607900	1.86714800	-1.47753100
C	4.75664600	0.54426100	-1.18313600
C	3.88029300	-0.27119300	-0.47370000
C	2.61095000	0.19916400	-0.06469300
C	2.29955400	1.54153600	-0.34633900
C	3.18897700	2.36317800	-1.04042400
H	5.10591600	2.50125800	-2.02732800
H	5.72123100	0.14803700	-1.49441800
H	1.36148200	1.96739600	-0.01582100
H	2.91323500	3.39559900	-1.23843500
C	1.71157200	-0.72353800	0.65780900
C	2.07276200	-2.04346200	0.73433800
C	1.37937000	-3.09937400	1.46980700
H	0.51913600	-2.80266000	2.05844300
C	1.75891200	-4.38663500	1.48292600
H	1.21070400	-5.12123500	2.06477400
H	2.61495000	-4.73389500	0.91543900
C	4.29119800	-1.64172800	-0.01231500
H	4.99242700	-2.11503300	-0.70522800
H	4.78062700	-1.58077500	0.97581400
O	3.18148700	-2.53043500	0.08328200
N	-0.83647900	-0.23186800	0.46939300
C	0.40470400	-0.21533000	1.27818900
C	-1.21247400	-1.54946600	-0.04841200
C	-2.68173900	-1.65211600	-0.42217200
C	-3.67910800	-1.27922300	0.49064000
C	-5.02814700	-1.41975100	0.16832400
C	-5.40388900	-1.93916000	-1.07421000
C	-4.42049800	-2.31315500	-1.99015200
C	-3.06935000	-2.16728400	-1.66432300
C	-0.98705600	0.82476200	-0.53089800
C	-1.21266900	2.21265300	0.04974700

C	-1.82949200	2.39808000	1.29367400
C	-2.08789000	3.68211800	1.77701400
C	-1.73982300	4.80360300	1.02140400
C	-1.12778500	4.63088200	-0.22174900
C	-0.86390400	3.34594400	-0.69900100
H	0.19215300	-0.79370800	2.18269300
H	0.54285400	0.81566200	1.61636700
H	-0.59534600	-1.85800700	-0.91116600
H	-1.01114000	-2.27940300	0.74124400
H	-3.38587600	-0.87091700	1.45384500
H	-5.78888000	-1.12552800	0.88702400
H	-6.45564500	-2.04866400	-1.32527300
H	-4.70191300	-2.71406200	-2.96052200
H	-2.30558300	-2.45755900	-2.38267500
H	-0.15182800	0.85553500	-1.25164800
H	-1.87598900	0.56575700	-1.11883700
H	-2.10167800	1.52362300	1.87629500
H	-2.56473700	3.80648100	2.74614900
H	-1.94137800	5.80280000	1.39839700
H	-0.85100500	5.49611500	-0.81884600
H	-0.38342800	3.21825500	-1.66719000

**3'-DME**

C	1.93663300	-0.76867400	-0.95025000
C	1.33485000	0.07549300	0.18863200
C	0.17392800	0.94377300	-0.28302900
C	-1.06982700	0.55972900	-0.11206100
C	-2.31484400	0.17293900	0.03531200
H	-2.88107800	0.47932500	0.91704500
C	-3.07767200	-0.67681100	-0.95847600
H	-3.90643000	-0.08342100	-1.36279100
H	-2.42189900	-0.94038300	-1.80893000
C	3.15097200	-1.57667400	-0.50450700
H	3.93093600	-0.88863200	-0.13321200
H	2.87189200	-2.23029800	0.34052800
O	3.61367600	-2.33275500	-1.61046000
H	4.36770800	-2.87216400	-1.30773100
N	0.46243300	3.49796000	-0.23457400
C	0.50144600	2.25568400	-1.01983800
C	1.45892000	3.59040800	0.83516400
C	2.89410000	3.62724500	0.34133700
C	3.24639500	4.35903000	-0.80126300
C	4.57586900	4.43287800	-1.21732700
C	5.57822800	3.78071400	-0.49430200
C	5.23924500	3.05217300	0.64652100
C	3.90608300	2.97498700	1.05674000
C	-0.88196800	3.84395800	0.23655700
C	-1.03369900	5.31791100	0.57023200
C	-0.63638800	6.30094100	-0.34769100
C	-0.81502700	7.65411700	-0.06347100
C	-1.39685500	8.04802300	1.14530800
C	-1.79477300	7.07877900	2.06636900
C	-1.61080000	5.72367800	1.77877500
H	1.50579300	2.17086300	-1.44827200
H	-0.19658800	2.38573300	-1.85335600
H	1.25236300	4.52622800	1.36982500
H	1.34600300	2.78372700	1.58282400
H	2.46434700	4.86231300	-1.36188400
H	4.83114700	5.00255000	-2.10740400
H	6.61364800	3.83887100	-0.81945600
H	6.01003800	2.53932100	1.21627300
H	3.64825400	2.40575300	1.94768900
H	-1.58029800	3.58477500	-0.56950900

H	-1.18825400	3.23952200	1.10891800	H	5.73761500	-3.22834500	-5.45917800
H	-0.17960000	5.99182000	-1.28372900	H	3.36245400	-3.83339600	-5.71851600
H	-0.50204100	8.40393000	-0.78576000	H	1.77569400	-3.46459100	-3.86965800
H	-1.53609500	9.10296300	1.36662600	C	7.00439800	-2.21833400	-3.15397400
H	-2.24357100	7.37473400	3.01114300	C	7.81301400	-2.02500100	-4.44839100
H	-1.91943200	4.97109900	2.50144700	H	8.86774900	-1.84303700	-4.22291900
N	-3.67157400	-1.86515800	-0.33009700	H	7.43676700	-1.18785100	-5.04629700
C	-4.71226900	-2.46306800	-1.17457500	H	7.78269900	-2.92934400	-5.06269100
H	-4.32837300	-2.69979300	-2.18655900	C	7.60535100	-3.42411100	-2.37269900
C	-2.65125200	-2.84944500	0.04755200	H	8.65562700	-3.23082400	-2.12709900
H	-1.82677300	-2.29002100	0.50490400	H	7.55174400	-4.33328500	-2.98184400
H	-2.22718200	-3.35826500	-0.84050400	H	7.06342400	-3.60603900	-1.43971800
H	-4.98204000	-3.42183700	-0.71548000	C	7.06404300	-0.98326000	-2.24750000
C	-3.15342000	-3.88779500	1.03277400	C	8.08130500	-0.02506500	-2.29285600
C	-3.80064000	-3.49229900	2.21272900	C	6.07993300	-0.84967300	-1.25585300
C	-2.94803500	-5.25350700	0.80694300	C	8.13257200	1.01256000	-1.36230300
C	-4.22789000	-4.43956400	3.14218400	H	8.85355800	-0.09142900	-3.05110900
H	-3.97014900	-2.43376300	2.38887000	C	6.10391100	0.18386800	-0.29530700
C	-3.37147100	-6.20597900	1.73784000	C	7.16070200	1.10650200	-0.36946100
H	-2.45186600	-5.57427900	-0.10673200	H	8.93572800	1.74221400	-1.40640800
C	-4.01320900	-5.80124500	2.90846900	H	7.21133100	1.91642300	0.35076500
H	-4.72794100	-4.11657400	4.05188300	O	5.05360300	-1.77315800	-1.20483100
H	-3.20441900	-7.26246200	1.54394000	P	2.04458300	-2.35782500	-1.11932300
H	-4.34662500	-6.53949600	3.63308600	P	4.79323600	0.32297400	1.01144000
C	-5.95877300	-1.60682200	-1.29585200	C	2.00510500	-4.02320600	-0.31225400
C	-6.55021400	-1.37421300	-2.54281000	C	1.57948200	-5.18234500	-0.98246100
C	-6.56638000	-1.06710500	-0.15280500	C	2.47114200	-4.13581300	1.00614000
C	-7.72654200	-0.62780700	-2.65039800	C	1.60788800	-6.42061400	-0.34203600
H	-6.08564600	-1.78185100	-3.43829500	H	1.22243900	-5.12101100	-2.00629000
C	-7.73786000	-0.31814900	-0.25683500	C	2.50511800	-5.37830100	1.64535300
H	-6.10495400	-1.23563500	0.81582200	H	2.82316800	-3.24489300	1.52027500
C	-8.32376200	-0.09704900	-1.50675900	C	2.07061300	-6.52111100	0.97354000
H	-8.17064300	-0.45730300	-3.62780300	H	1.27454100	-7.30898500	-0.87161900
H	-8.19681200	0.09336200	0.63871600	H	2.87746900	-5.45075500	2.66369200
H	-9.23692400	0.48687100	-1.58706600	H	2.09716900	-7.48834600	1.46790200
H	0.99694800	-0.58705300	0.99466200	C	0.40396600	-2.21364200	-1.96363700
H	2.12052200	0.71752100	0.60777200	C	0.24822100	-1.32884100	-3.04674800
H	1.17617500	-1.45604600	-1.34097600	C	-0.74175600	-2.83562300	-1.43923000
H	2.23944400	-0.12569600	-1.78660800	C	-1.01163900	-1.09233700	-3.59910400
O	5.27439600	-4.35568300	-0.56537600	H	1.11687100	-0.83190900	-3.47058300
C	6.62916400	-4.72585500	-0.36945500	C	-2.00287400	-2.59006400	-1.98943700
H	6.71577000	-5.45290900	0.45211100	H	-0.65051200	-3.52346900	-0.60399800
H	7.04226600	-5.19113400	-1.27754200	C	-2.14341900	-1.72065100	-3.07241700
C	4.42833100	-5.44714600	-0.89261500	H	-1.10568700	-0.41952400	-4.44785500
H	3.44383400	-5.02307700	-1.09924200	H	-2.87960500	-3.08379700	-1.57928000
H	4.78946700	-5.97766900	-1.78606000	H	-3.12612100	-1.54307300	-3.49964500
H	4.36211900	-6.16065100	-0.05840800	C	5.51767800	-0.56301300	2.46283600
C	7.41475700	-3.46760300	-0.02878600	C	6.89896500	-0.72171700	2.65425800
H	7.32703100	-2.73827100	-0.85155600	C	4.63557900	-1.09170100	3.42004600
H	6.99379300	-2.99966600	0.87671000	C	7.38454000	-1.39129500	3.77903700
O	8.75731000	-3.85282900	0.17096400	H	7.59890500	-0.32911100	1.92325400
C	9.59822500	-2.76502700	0.48981200	C	5.12294900	-1.75037300	4.55001800
H	10.60654700	-3.16549900	0.62264600	H	3.56318600	-0.99154600	3.27164400
H	9.61435400	-2.01317800	-0.31551800	C	6.49924100	-1.90388100	4.72975500
H	9.28472200	-2.26748900	1.42176500	H	8.45620000	-1.51197300	3.91171300
				H	4.42777900	-2.15075500	5.28301400
				H	6.88043100	-2.42449200	5.60385700
				C	4.89115500	2.11058600	1.49923000
				C	5.17700000	2.52153900	2.80955600
				C	4.55813300	3.09124500	0.54523400
				C	5.13147300	3.87543300	3.15807000
				H	5.44332200	1.78710700	3.56276100
				C	4.52625300	4.44217400	0.89134500
<b>TS6'</b>							
C	4.60390400	-2.30610400	-2.40089500				
C	5.52729100	-2.51708800	-3.43615100				
C	5.05425700	-3.05821300	-4.63474800				
C	3.71155500	-3.40297700	-4.78454800				
C	2.81935900	-3.20105100	-3.73549000				
C	3.23746600	-2.63332900	-2.52114900				

H	4.33978900	2.79941500	-0.47902300	C	-1.35648800	3.57250000	4.81040700
C	4.80866600	4.83971700	2.20298600	C	-0.92266100	4.35585800	5.88136800
H	5.36397500	4.17300900	4.17709400	C	0.28458100	5.04932400	5.79608300
H	4.29316300	5.18650200	0.13385200	C	1.04215900	4.96020100	4.62741600
H	4.79058900	5.89260400	2.47115400	C	0.59669100	4.18609800	3.55437500
Pd	2.85048600	-0.65398300	0.22191700	H	-0.64990900	-0.07081300	0.58035200
C	1.02945300	2.34102900	0.50083500	H	-1.31140500	1.46015200	-0.01496500
H	1.52801100	2.92165400	1.26385500	H	1.25759400	0.32944000	2.07498900
N	0.59801300	2.98820200	-0.57485500	H	1.03136300	1.52306800	3.35469500
C	0.36553800	2.25579400	-1.85211200	H	-0.85919400	0.99105600	5.14020800
H	-0.61231200	2.55143300	-2.24107300	H	-1.70919500	-0.85365500	6.54617200
C	0.52940800	4.47362900	-0.62850500	H	-1.36735000	-3.21630300	5.85341900
H	1.14216800	4.85095900	0.19424200	H	-0.15264100	-3.71687100	3.73499500
H	1.02749200	4.76239800	-1.56013100	H	0.67324200	-1.86511600	2.31593000
H	1.40426200	1.32602600	0.34451100	H	-1.51923200	3.32701200	1.67627400
H	0.31260000	1.19323700	-1.60925200	H	-2.12548100	2.19208700	2.85832700
C	-0.86035900	5.07996600	-0.56177800	H	-2.30130300	3.04016200	4.89010500
C	-1.29308400	5.70422500	0.61634100	H	-1.52814100	4.41974800	6.78096800
C	-1.71802000	5.07662700	-1.67266000	H	0.63028000	5.65480800	6.62875900
C	-2.56249500	6.28054700	0.69563200	H	1.98348300	5.49567700	4.54281600
H	-0.63169700	5.74829800	1.47852000	H	1.20926600	4.15983500	2.66048000
C	-2.99190900	5.64056700	-1.59350500	N	-6.50160300	1.52179700	-1.49001200
H	-1.38641000	4.64961600	-2.61508200	C	-7.29557000	2.69423100	-1.11731600
C	-3.41776000	6.24025800	-0.40595100	H	-8.34830900	2.41885300	-1.26462000
H	-2.87703400	6.76458200	1.61600600	C	-7.04861800	0.26879400	-0.95888500
H	-3.65020400	5.62543900	-2.45732800	H	-8.14190000	0.35346500	-1.01530200
H	-4.40829200	6.68055600	-0.35139100	H	-6.80991600	0.12717600	0.10926700
C	1.45219200	2.50161900	-2.88220300	H	-7.20505200	2.95290000	-0.04564400
C	2.70209400	1.87734700	-2.74255800	C	-6.63069200	-0.97302000	-1.73275100
C	1.22604600	3.32478100	-3.99215100	C	-6.42548000	-0.93682200	-3.11829600
C	3.70755500	2.08838300	-3.68638000	C	-6.52289100	-2.20253000	-1.06800800
H	2.88055400	1.20424500	-1.90225300	C	-6.11312000	-2.10220400	-3.82257200
C	2.23283500	3.53804100	-4.93775300	H	-6.51640500	0.01229900	-3.63834800
H	0.25433900	3.79387700	-4.13008000	C	-6.21575400	-3.37093400	-1.77141000
C	3.47587600	2.92371800	-4.78359000	H	-6.67315000	-2.25716300	0.00773500
H	4.66648500	1.59062700	-3.57031800	C	-6.00731900	-3.32441300	-3.15194100
H	2.04230700	4.17893800	-5.79387300	H	-5.96573600	-2.05837800	-4.89901800
H	4.25823000	3.08637600	-5.51948300	H	-6.14700200	-4.31151700	-1.23023800
C	-4.40273100	-1.35763100	1.87046000	H	-5.77233900	-4.23131200	-3.70297700
C	-2.94277800	-0.90409400	1.94001800	C	-7.00730000	3.93306500	-1.94953300
C	-2.66836300	0.40105700	1.20586900	C	-6.75160400	3.84212500	-3.32456100
C	-3.64038600	1.13872500	0.70637500	C	-7.06807600	5.20247000	-1.36139900
C	-4.57224000	1.86685200	0.14598500	C	-6.55528900	4.99256000	-4.09021200
H	-5.00442900	2.69786300	0.70546000	H	-6.70855800	2.86012300	-3.78646600
C	-5.05797200	1.67548800	-1.29353400	C	-6.88746500	6.35728200	-2.12702300
H	-4.74174700	2.55237800	-1.87157800	H	-7.27287100	5.28862400	-0.29608200
H	-4.56102100	0.80137500	-1.72387400	C	-6.62445600	6.25552800	-3.49498800
C	-4.62451500	-2.77988400	2.37776300	H	-6.36097000	4.90423000	-5.15605900
H	-4.03221700	-3.48015700	1.76636700	H	-6.95683300	7.33490200	-1.65659300
H	-4.26425900	-2.87790100	3.41596400	H	-6.48500700	7.15159200	-4.09360300
O	-6.01104900	-3.07951200	2.29808600	H	-5.04247700	-0.67691400	2.44598100
H	-6.12116900	-4.01245500	2.03138900	H	-4.74934400	-1.31291300	0.83365600
N	-0.38811300	1.59060000	1.83506900	H	-2.62382400	-0.82291500	2.98544600
C	-1.23439400	0.81243200	0.85977300	H	-2.29547300	-1.67384300	1.49462600
C	0.50795900	0.79214200	2.73291700	O	-10.12498900	-5.26281800	1.46661000
C	-0.07062900	-0.30583500	3.60412100	C	-8.79701400	-4.83259300	1.26173700
C	-0.72885800	-0.03595500	4.81328200	H	-8.65528000	-4.44018500	0.24120100
C	-1.20027800	-1.07836300	5.61280900	H	-8.52170700	-4.03241000	1.96760700
C	-1.00539600	-2.40716200	5.22524000	C	-11.06976500	-4.22490100	1.30700800
C	-0.32750500	-2.68792800	4.03771900	H	-12.05638700	-4.65865400	1.48754800
C	0.13594300	-1.64346900	3.23568900	H	-10.89981700	-3.40728700	2.02542900
C	-1.20773400	2.65882000	2.48810100	H	-11.04328700	-3.80473200	0.28897600
C	-0.60640600	3.46501900	3.62778200	C	-7.91098300	-6.05246400	1.47655200

H	-8.04385900	-6.43599600	2.49884000
H	-8.19783500	-6.84859700	0.77482900
O	-6.55127000	-5.67710600	1.25910000
C	-5.65210400	-6.76139000	1.43576200
H	-4.64559200	-6.38191200	1.24359200
H	-5.70145100	-7.16058500	2.45935600
H	-5.87261700	-7.57386300	0.72914900

**INT5'**

C	-1.52781200	-3.00471400	-0.19148200
H	-1.80982100	-3.78078400	0.52372600
H	-2.40670800	-2.73128600	-0.77001100
N	-0.45138900	-3.36361100	-1.05875000
C	0.35332000	-4.53632400	-0.64095600
H	0.48481500	-4.48334700	0.44318600
H	-0.19269200	-5.47301200	-0.84514100
C	-0.85114300	-3.48583600	-2.49276300
H	-1.64951000	-4.23901700	-2.59521600
H	0.02631000	-3.88044500	-3.01020400
C	1.71824100	-4.59462200	-1.30069900
C	2.63416800	-3.54108100	-1.15707000
C	2.09788300	-5.72184100	-2.03810200
C	3.90052000	-3.61496000	-1.73659800
H	2.35790900	-2.65697400	-0.58675500
C	3.36615800	-5.80049100	-2.61930900
H	1.39848700	-6.54630500	-2.15763300
C	4.26823700	-4.74744800	-2.46988100
H	4.60448800	-2.79611500	-1.61360600
H	3.64488000	-6.68277600	-3.18831300
H	5.25477400	-4.80639000	-2.92053800
C	-1.27608300	-2.19111000	-3.14699000
C	-0.31135800	-1.26281500	-3.56685300
C	-2.63028200	-1.89575400	-3.35460100
C	-0.69327200	-0.05723000	-4.15419600
H	0.74315300	-1.49259900	-3.43153800
C	-3.01704000	-0.68610800	-3.94084800
C	-2.04852400	0.23801700	-4.33513800
H	0.06446400	0.64967700	-4.48045400
H	-2.34624300	1.17731300	-4.79152600
H	-3.38840200	-2.62528600	-3.07543600
H	-4.07014700	-0.47271300	-4.10065600
C	-2.02384300	2.23429100	-0.46929800
C	-1.19426600	1.78345000	0.74555800
C	-0.21136100	0.65422300	0.44112900
C	1.08740600	0.82464600	0.59840100
C	2.38219200	0.96379400	0.71945400
H	2.86896800	0.69622800	1.65907200
C	3.31975200	1.42393800	-0.38053600
H	3.81889600	0.53484200	-0.78409600
H	2.74174400	1.87298200	-1.20982200
C	-2.90699500	3.44338000	-0.16632800
H	-3.53987500	3.22790000	0.71373100
H	-2.27019200	4.30301800	0.10357300
O	-3.68285600	3.70570200	-1.31606500
H	-4.17614600	4.54025700	-1.17043000
N	-1.26531500	-1.73557400	0.70844200
C	-0.65795100	-0.64388100	-0.20692100
C	-2.61310000	-1.20870000	1.28703400
C	-3.80403000	-2.14338400	1.33558600
C	-4.71721700	-2.13307600	0.26743500
C	-5.86469800	-2.92458400	0.29921300
C	-6.12410500	-3.72979600	1.41032700
C	-5.23684200	-3.72919000	2.48808700

C	-4.08611000	-2.93973200	2.45500900
C	-0.23668400	-2.04424300	1.81058400
C	-0.70260300	-2.80114500	3.03162600
C	-0.79876400	-4.20081400	3.07268200
C	-1.18424500	-4.85547100	4.24279100
C	-1.46930200	-4.12272900	5.39726200
C	-1.35438900	-2.73126800	5.37968800
C	-0.96897400	-2.07973600	4.20743200
H	-1.41573400	-0.46824700	-0.97211400
H	0.18552200	-1.13682500	-0.68303200
H	-2.37625900	-0.82536300	2.27866300
H	-2.87034000	-0.36352000	0.65092500
H	-4.53616700	-1.48868400	-0.59060800
H	-6.56095000	-2.90136000	-0.53400800
H	-7.02024800	-4.34257100	1.44199000
H	-5.44403700	-4.33704100	3.36395600
H	-3.41959000	-2.93388600	3.30985700
H	0.58063500	-2.55231600	1.29638100
H	0.13595800	-1.06773400	2.11839700
H	-0.56190500	-4.79538400	2.19640100
H	-1.25070800	-5.93931900	4.25510900
H	-1.76260500	-4.63444900	6.30911300
H	-1.55182400	-2.15437700	6.27829100
H	-0.85704800	-0.99774100	4.21099200
N	4.36239600	2.30842700	0.13227700
C	5.51942100	2.36852300	-0.77582400
H	5.22285400	2.70412800	-1.78806900
C	3.83895000	3.64507100	0.44966100
H	2.90182200	3.49499200	1.00112800
H	3.57385600	4.20257500	-0.46950400
H	6.19192500	3.13600100	-0.37752500
C	4.78613600	4.47757400	1.29114500
C	5.28651700	3.97839600	2.50265400
C	5.15109000	5.76858200	0.89379600
C	6.12957200	4.75430300	3.29688800
H	5.01509800	2.97290800	2.81340600
C	5.99293600	6.55054000	1.68911300
H	4.77381100	6.16636400	-0.04589300
C	6.48435300	6.04482200	2.89265600
H	6.51002600	4.35446800	4.23318100
H	6.26701800	7.55063500	1.36455100
H	7.14118700	6.64942400	3.51185000
C	6.25791900	1.04804600	-0.87383200
C	6.49223300	0.44354000	-2.11425900
C	6.73637700	0.41681600	0.28442800
C	7.19447600	-0.76250600	-2.20213300
H	6.13012700	0.92422200	-3.02063600
C	7.43402000	-0.78718700	0.20141200
H	6.55526500	0.87986600	1.25042100
C	7.66584800	-1.38167300	-1.04346600
H	7.37721600	-1.21140500	-3.17498100
H	7.80583700	-1.26020300	1.10655700
H	8.21817200	-2.31527800	-1.10806600
H	-0.61467100	2.63225800	1.12451800
H	-1.87139500	1.49607300	1.56287400
H	-1.35947300	2.48188500	-1.30574700
H	-2.68081900	1.42956300	-0.82635600
O	-5.21558500	6.01007500	-0.81116800
C	-6.60001700	5.76413500	-1.04213200
H	-7.20438300	6.58274800	-0.62635700
H	-6.80827600	5.70026000	-2.12035300
C	-4.77463600	7.24703300	-1.35399900
H	-3.70886700	7.33479400	-1.13110400

H	-4.92284200	7.28316500	-2.44281600	C	5.08722600	0.77616600	-3.21999300
H	-5.31118300	8.08829200	-0.89412700	C	5.96295900	1.54309900	-4.00195900
C	-6.96530900	4.45035500	-0.36435800	C	5.41019600	2.35441500	-4.99739400
H	-6.32126200	3.64225900	-0.74866700	C	4.03422500	2.37617600	-5.22222000
H	-6.79001600	4.53142200	0.72176200	C	3.18837300	1.58162600	-4.45195800
O	-8.32524900	4.20606500	-0.64551800	C	3.69272500	0.76609300	-3.42634100
C	-8.81167500	3.02986400	-0.03682000	H	6.05539300	2.96958600	-5.61463500
H	-9.86333500	2.93338000	-0.31750500	H	3.62213200	3.00718900	-6.00420100
H	-8.26505300	2.13698900	-0.38206400	H	2.11974400	1.60636000	-4.63769500
H	-8.73738200	3.07909300	1.06154700	C	7.46778800	1.37598300	-3.76184100
				C	8.27755100	2.55773100	-4.32212500
4'				H	9.34897000	2.40134200	-4.16719800
C	-5.45699700	1.06490700	-0.65778200	H	7.99493800	3.50726400	-3.85494700
C	-4.45517000	1.11754700	0.51205800	H	8.13363000	2.64740600	-5.40275200
C	-3.81189100	-0.24676000	0.69800000	C	7.93473200	0.07470300	-4.47854200
C	-2.52216500	-0.44311400	0.81046400	H	9.00327800	-0.09154600	-4.30156400
C	-1.23382200	-0.65733200	0.92590900	H	7.76973300	0.15752200	-5.55865200
H	-0.77036500	-0.65548800	1.91440900	H	7.38775900	-0.80057000	-4.11540800
C	-0.29735900	-0.94408400	-0.22779400	C	7.67620000	1.19699700	-2.25337700
H	0.08821800	-1.96462900	-0.11746400	C	8.79105000	1.66977700	-1.55529700
H	-0.85426400	-0.90917100	-1.18226400	C	6.72146500	0.45446800	-1.54187800
C	-6.39522500	-0.13450100	-0.49990800	C	8.95942600	1.39021200	-0.19964400
H	-7.02438300	-0.00534300	0.39987200	H	9.54504900	2.25363200	-2.07132700
H	-7.05942000	-0.23700800	-1.36362000	C	6.85522500	0.15951100	-0.16954000
O	-5.67387000	-1.35635200	-0.41455800	C	8.00490000	0.63872000	0.48062400
C	-4.81138900	-1.39350600	0.71665000	H	9.83645800	1.75664600	0.32566700
H	-5.41627200	-1.33478500	1.64092200	H	8.14270400	0.43322700	1.53683100
H	-4.30777500	-2.36214000	0.69476000	O	5.60754800	-0.01652900	-2.21322600
N	0.86538500	-0.04609200	-0.23139700	P	2.58497400	-0.30543700	-2.39055400
C	1.94627800	-0.56096800	-1.08044200	P	5.56355900	-0.79878000	0.76174600
H	1.59385800	-0.75789300	-2.11215900	C	2.53785700	-1.88453200	-3.35154000
C	0.49462700	1.32466000	-0.60044400	C	2.45796000	-1.91596800	-4.75367700
H	-0.42843700	1.55932000	-0.05719900	C	2.60510100	-3.09745400	-2.64962400
H	0.25054000	1.40471100	-1.67816500	C	2.43122600	-3.13384100	-5.43352100
H	2.69618400	0.23546600	-1.15760800	H	2.42615600	-0.98868900	-5.31829000
C	1.55396900	2.35062700	-0.24515900	C	2.57859600	-4.31642000	-3.33101200
C	2.08516000	2.40255900	1.05202300	H	2.70345500	-3.07524700	-1.56699200
C	1.99263300	3.28814700	-1.18692300	C	2.48952300	-4.33620300	-4.72339600
C	3.02854000	3.36953500	1.39659300	H	2.37126600	-3.14422600	-6.51839800
H	1.75412000	1.67188200	1.78468300	H	2.64082900	-5.24815000	-2.77526700
C	2.93523800	4.26138800	-0.84442000	H	2.47505300	-5.28322600	-5.25578400
H	1.59238200	3.25608600	-2.19818200	C	0.91327300	0.44648700	-2.67294600
C	3.45620700	4.30434000	0.44891800	C	0.67440500	1.74286900	-2.17667600
H	3.43049300	3.39649900	2.40633500	C	-0.15433200	-0.25252400	-3.25673700
H	3.26473700	4.98039000	-1.59009800	C	-0.58824000	2.32734900	-2.28045900
H	4.19163600	5.05802600	0.71780400	H	1.48527200	2.30455300	-1.71942500
C	2.60733800	-1.80901300	-0.52648800	C	-1.42320300	0.32996100	-3.34772500
C	2.84210500	-2.91969800	-1.34502100	H	0.00204500	-1.25124800	-3.65133000
C	3.03391100	-1.85598300	0.80877800	C	-1.64460000	1.61999200	-2.86497800
C	3.49561400	-4.05067200	-0.84871900	H	-0.74547600	3.33758500	-1.91103800
H	2.51072600	-2.89883800	-2.38117300	H	-2.23480600	-0.22638800	-3.80916200
C	3.68255300	-2.98450100	1.30855700	H	-2.62890200	2.07310200	-2.94310000
H	2.84444300	-1.00068600	1.45077700	C	6.17358100	-2.54250900	0.69356000
C	3.91757900	-4.08616700	0.48053800	C	7.51193100	-2.88015500	0.44147300
H	3.66840300	-4.90388800	-1.49967200	C	5.24672100	-3.57417600	0.91705700
H	4.00757800	-3.00529200	2.34580800	C	7.91203200	-4.21800000	0.41720100
H	4.42338800	-4.96545100	0.87076500	H	8.24468900	-2.10028600	0.25957500
H	-3.69570600	1.88916000	0.35308000	C	5.64980200	-4.90980800	0.90554600
H	-4.99950900	1.38140500	1.43275400	H	4.20328100	-3.32147100	1.09102000
H	-6.04191000	1.99247800	-0.70623000	C	6.98443700	-5.23455700	0.65210900
H	-4.91182100	0.96418400	-1.60420800	H	8.95080600	-4.46451900	0.21518600
				H	4.92181500	-5.69676200	1.08437000
				H	7.29879300	-6.27436000	0.63302700

TS8'

C	5.89504400	-0.29067100	2.51340100	C	-8.86028600	6.17282300	-1.22563000
C	6.39474400	-1.16772700	3.48645700	C	-8.54765100	6.72452500	-2.47205200
C	5.56893900	1.02424700	2.89418700	C	-7.65614300	6.06290700	-3.31575600
C	6.56352000	-0.74102300	4.80789800	C	-7.08050600	4.85482700	-2.91294000
H	6.66018000	-2.18488700	3.21694600	C	-4.79472500	3.70857400	-0.06349500
C	5.75255100	1.45194400	4.20835200	C	-4.88681300	5.17826400	0.31780500
H	5.17716900	1.71959500	2.15545800	C	-5.58494200	5.57666000	1.46519800
C	6.24681500	0.56716200	5.17228600	C	-5.59736400	6.91308100	1.86188600
H	6.95278600	-1.43431400	5.54868900	C	-4.90762600	7.87428700	1.11710100
H	5.50940300	2.47561800	4.48117800	C	-4.21064500	7.48777200	-0.02781300
H	6.38488200	0.89810600	6.19777900	C	-4.20247300	6.14744300	-0.42208900
Pd	3.52043400	-0.52504400	-0.29242400	H	-6.97663900	1.26582000	0.76470300
C	0.76507600	-0.08608000	1.40419900	H	-5.59089400	1.84748300	1.68383100
H	1.42573500	-0.94518900	1.44865200	H	-6.18751600	2.57333400	-2.09755600
N	0.90664900	0.85413500	2.32689000	H	-7.63190400	2.23928800	-1.13487700
C	0.35877400	2.20704300	2.10107200	H	-8.52209300	4.54329600	0.14279700
H	-0.21721100	2.49764500	2.98429500	H	-9.55485100	6.68376800	-0.56416700
C	1.81639000	0.67045800	3.49729900	H	-8.99781300	7.66394700	-2.78108700
H	2.19507500	-0.35197100	3.44359400	H	-7.40708400	6.48425600	-4.28608600
H	2.66920700	1.33651300	3.33444900	H	-6.38799300	4.33984800	-3.57601500
H	0.41718200	0.21677000	0.42547800	H	-4.09534200	3.22191400	0.62767000
H	-0.34850100	2.12923300	1.27072700	H	-4.33270100	3.61995400	-1.06227100
C	1.19948700	0.94353100	4.85562200	H	-6.13468300	4.83202200	2.03448900
C	0.77584600	-0.11083700	5.67647700	H	-6.14793600	7.20745700	2.75177800
C	1.10175100	2.25494800	5.34590100	H	-4.92080600	8.91662600	1.42394500
C	0.23277600	0.13751300	6.93858000	H	-3.68121300	8.22891900	-0.62090800
H	0.89535800	-1.13880900	5.34436800	H	-3.66544400	5.85422900	-1.32216700
C	0.55342300	2.50686000	6.60436800	N	-0.93077000	-1.37932100	1.59953400
H	1.47401000	3.08269600	4.74774200	C	-0.55216100	-2.22101700	2.78139600
C	0.11139400	1.44890100	7.40132900	H	0.19192100	-2.93911500	2.42256300
H	-0.08202500	-0.69419700	7.56233800	C	-0.89495900	-2.07408200	0.27925300
H	0.48525400	3.52833500	6.96777500	H	0.16097900	-2.29781700	0.08483700
H	-0.30821800	1.64421400	8.38397000	H	-1.20187300	-1.33184000	-0.46325400
C	1.41092700	3.26222300	1.79522200	H	-0.04856100	-1.53789700	3.47068800
C	2.52822000	2.98312300	0.99531600	C	-1.69770200	-3.34750200	0.09178700
C	1.22285200	4.56632300	2.27092200	C	-1.02863100	-4.56028900	-0.12233800
C	3.43751100	3.99546600	0.67971500	C	-3.09965700	-3.34053300	0.06229300
H	2.70670300	1.97406000	0.62007000	C	-1.74222700	-5.74185100	-0.33814700
C	2.12882100	5.57910300	1.94841900	H	0.05948300	-4.57997500	-0.12954000
H	0.35793200	4.79544600	2.88986700	C	-3.81976900	-4.51762100	-0.14626800
C	3.23977900	5.29517700	1.15277100	H	-3.63276200	-2.40509400	0.19665800
H	4.29960500	3.76432000	0.05969800	C	-3.13798400	-5.72251900	-0.34287300
H	1.96706500	6.58585900	2.32286500	H	-1.20772500	-6.67301200	-0.50572400
H	3.94796200	6.08036100	0.90414100	H	-4.90735600	-4.49128800	-0.16440100
C	-6.45776400	-1.50355700	-0.37756000	H	-3.69446000	-6.64076400	-0.50920100
C	-5.68796200	-0.34045100	-1.03218400	C	-1.63894400	-2.93900800	3.57016400
C	-5.07505900	0.59708900	0.00174900	C	-1.98365300	-4.27293200	3.31317800
C	-3.81871400	0.46543100	0.35420800	C	-2.26395800	-2.28168400	4.64223700
C	-2.56293600	0.34104300	0.72223400	C	-2.94230600	-4.92334800	4.09113300
H	-1.80757200	0.93326400	0.20417800	H	-1.50397300	-4.80863500	2.50106100
C	-2.12177900	-0.53334500	1.87497700	C	-3.22796300	-2.92767000	5.41696500
H	-1.84026200	0.09119100	2.73571000	H	-1.98311100	-1.25943200	4.88491100
H	-2.96074700	-1.15529900	2.20184500	C	-3.57192300	-4.25203900	5.14062300
C	-6.92005900	-2.55456300	-1.38523100	H	-3.19514300	-5.95756700	3.87573900
H	-7.74737300	-2.15841200	-1.99659400	H	-3.70101800	-2.40026900	6.24071300
H	-6.09017000	-2.78724800	-2.07571700	H	-4.31830800	-4.76005600	5.74472900
O	-7.31451100	-3.70663300	-0.66019500	H	-4.89136400	-0.75043200	-1.66463500
H	-7.77830400	-4.31432500	-1.27314500	H	-6.35758100	0.22385600	-1.69233400
N	-6.06039500	2.96730400	0.00009500	H	-5.80828100	-2.00368700	0.34992400
C	-5.96131400	1.66894800	0.66964100	H	-7.32329900	-1.13498900	0.18683600
C	-6.80681200	2.95221000	-1.26276200	O	-8.90460000	-5.29415300	-2.37291300
C	-7.38629500	4.29536900	-1.66861700	C	-10.28732500	-4.97959900	-2.23280000
C	-8.28517000	4.96745200	-0.82923300	H	-10.53327400	-4.05914400	-2.78356500



H	-10.90296900	-5.79333600	-2.64190100
C	-8.53592300	-5.59973100	-3.70815600
H	-7.46619600	-5.82228900	-3.70477000
H	-9.08577900	-6.47730200	-4.07613800
H	-8.72969900	-4.75328900	-4.38370700
C	-10.58810900	-4.79388400	-0.75128000
H	-10.39736200	-5.73644900	-0.21163600
H	-9.91976400	-4.02819200	-0.32575300
O	-11.94276600	-4.41271100	-0.65522500
C	-12.37072500	-4.23814600	0.67938500
H	-13.42246600	-3.94357700	0.64361500
H	-12.27862400	-5.16932000	1.26075300
H	-11.79416500	-3.45115700	1.19134900

C	-3.48214800	3.68128300	-0.14299800
C	-3.92265600	5.11454900	0.10246300
C	-3.85990000	5.66534400	1.39047100
C	-4.29990300	6.96642000	1.62782900
C	-4.81065800	7.73753400	0.57907500
C	-4.87554100	7.19964100	-0.70620900
C	-4.43138800	5.89549400	-0.94078100
C	-1.08514300	4.05916400	-0.44480900
C	0.24977200	4.19399800	0.26585900
C	0.31997800	4.56610700	1.61531500
C	1.55465300	4.74359100	2.24126700
C	2.74078800	4.55981600	1.52568300
C	2.68278700	4.19527600	0.17908600
C	1.44452400	4.00766300	-0.44052800

**INT6'**

C	3.49724200	-1.39241000	-1.34455200
H	3.95045600	-2.24226500	-1.86013800
N	4.39261800	-0.78184300	-0.43578200
C	4.46687300	0.71002400	-0.48192600
H	5.04584400	1.01287200	0.39344900
C	5.71231700	-1.44552500	-0.32792600
H	5.53665300	-2.52719700	-0.37817300
H	6.34003800	-1.19800800	-1.19685600
H	3.10702500	-0.70357000	-2.09509600
H	3.45791200	1.10443000	-0.33662900
C	6.47968100	-1.13004900	0.94343600
C	7.88043300	-1.13069400	0.90483800
C	5.84111700	-0.89756000	2.16795900
C	8.62685100	-0.91983300	2.06527900
H	8.39196800	-1.30535200	-0.03936200
C	6.58497100	-0.67608300	3.32816800
H	4.75611900	-0.86875200	2.20735700
C	7.98032200	-0.69132600	3.28124000
H	9.71196800	-0.92678600	2.01687800
H	6.07427200	-0.49101200	4.26912800
H	8.55906100	-0.51997900	4.18412500
C	5.08426200	1.29221800	-1.74121200
C	4.28521200	1.67107100	-2.83126100
C	6.47383200	1.46606800	-1.84177800
C	4.85607100	2.18169200	-3.99877200
H	3.20134900	1.59637500	-2.76144400
C	7.04794000	1.97599500	-3.00720900
H	7.10797600	1.21851500	-0.99387400
C	6.24100200	2.32900700	-4.09107500
H	4.21967000	2.47664400	-4.82840900
H	8.12465000	2.10849900	-3.06457100
H	6.68748900	2.73127800	-4.99576200
C	-3.60688300	-0.56708500	-0.32393900
C	-2.78722400	0.44473200	-1.14896400
C	-1.61009300	1.00032200	-0.35918000
C	-0.39376400	0.56248200	-0.56953900
C	0.84682900	0.15209600	-0.72546100
H	1.51180000	0.72100500	-1.37388400
C	1.42890500	-0.97040800	0.09636500
H	2.15866000	-0.59839300	0.82132900
H	0.64249900	-1.48719000	0.64336100
C	-4.62433400	-1.34327700	-1.15978300
H	-5.47316900	-0.69756000	-1.43200500
H	-4.15181500	-1.66910100	-2.10339400
O	-5.04802400	-2.45952400	-0.39494800
H	-5.88808100	-2.79422400	-0.77568800
N	-2.12743500	3.41026200	0.35121700
C	-1.84285700	2.03959900	0.75984600

H	-2.67905100	1.69770700	1.38128500
H	-0.95243900	2.05719000	1.39425100
H	-3.59308500	3.45824800	-1.21950400
H	-4.15927200	2.99982900	0.38827200
H	-3.45973000	5.06633500	2.20421300
H	-4.24795000	7.38046400	2.63128400
H	-5.15383800	8.75149400	0.76476800
H	-5.26682300	7.79349900	-1.52770800
H	-4.48278100	5.48060900	-1.94541800
H	-0.92836300	3.54984300	-1.41361700
H	-1.45987100	5.06231700	-0.68222200
H	-0.60284500	4.71758700	2.16781600
H	1.59096400	5.03581900	3.28747500
H	3.70121400	4.70910800	2.01163800
H	3.59820000	4.06369800	-0.39259100
H	1.40395300	3.73416100	-1.49341600
N	2.18977900	-2.03257400	-0.69073500
C	2.66741700	-3.17037200	0.25461300
H	2.78876000	-4.04338900	-0.38963900
C	1.38820300	-2.54966500	-1.89998300
H	2.13550100	-2.98447500	-2.56846300
H	0.99220600	-1.64886200	-2.37346600
H	3.64900200	-2.83835800	0.58792100
C	0.29321300	-3.55822200	-1.66823200
C	0.50703200	-4.89657400	-2.03137600
C	-0.97175000	-3.17831100	-1.19650900
C	-0.51297700	-5.84042300	-1.89771000
H	1.47016600	-5.20192000	-2.43520900
C	-1.99515800	-4.11736600	-1.05965500
H	-1.16237100	-2.13986600	-0.94571900
C	-1.76116300	-5.45174200	-1.40633500
H	-0.33512000	-6.87208600	-2.18704100
H	-2.97435700	-3.80484700	-0.70213300
H	-2.55702600	-6.18449600	-1.30803100
C	1.84478900	-3.49707800	1.48271200
C	0.88009100	-4.51481300	1.48696100
C	2.12881200	-2.83567800	2.68955900
C	0.19840100	-4.83937200	2.66058200
H	0.66591400	-5.06543400	0.57860300
C	1.44396000	-3.15492100	3.86064600
H	2.90662200	-2.07698400	2.71799000
C	0.47116100	-4.15675500	3.84686700
H	-0.54306500	-5.63264800	2.64604100
H	1.67935100	-2.63303000	4.78350900
H	-0.06030100	-4.41314300	4.75869700
H	-2.41194200	-0.04959100	-2.05320500
H	-3.43077800	1.26491500	-1.48625500
H	-2.92796200	-1.29823600	0.13136900
H	-4.12262900	-0.07304400	0.50807500

O	-7.57915600	-3.17487000	-1.36149300	H	-5.03225300	-3.90747600	0.38764500
C	-8.55683700	-3.16995300	-0.32278200	C	3.68974300	0.01236400	0.23663200
H	-9.56645600	-3.14679600	-0.75643200	H	4.59982700	0.49996800	-0.13238700
H	-8.47114500	-4.07729800	0.29306700	N	2.51614100	0.49980900	-0.56582300
C	-7.75297500	-4.24445900	-2.27938800	C	2.53377700	-0.02855400	-1.95726600
H	-6.95760200	-4.16345600	-3.02406200	H	3.16216400	0.61592200	-2.58775400
H	-7.68398900	-5.22015400	-1.77674600	C	2.41218500	1.98245300	-0.48512300
H	-8.72714300	-4.17341500	-2.78232200	H	2.27760000	2.22365800	0.57587500
C	-8.33223800	-1.93483700	0.53932700	H	1.48535700	2.26379600	-0.99090500
H	-7.30076200	-1.93239100	0.92744700	H	3.51041700	0.38614300	1.25676200
H	-8.46157500	-1.02594600	-0.07274400	N	3.90556300	-1.40738800	0.17752200
O	-9.27868100	-1.98737100	1.58251400	C	5.29824700	-1.86319000	-0.01815000
C	-9.19436300	-0.88312900	2.45887300	H	5.79234900	-1.10913800	-0.64058500
H	-9.96287400	-1.02036100	3.22333000	H	5.85888500	-1.90518900	0.92889600
H	-8.20826100	-0.82679800	2.94717900	C	3.05189400	-2.26917000	0.98934500
H	-9.37756200	0.06759000	1.93320100	H	3.37686300	-3.29839000	0.79959400

### TS9'

C	-3.06056400	3.53926000	-1.39150700	C	5.39931000	-3.21500800	-0.69988300
C	-3.42777700	2.07443700	-1.13264600	C	5.07778700	-3.35736000	-2.05780800
C	-2.69692500	1.38942800	0.01031100	C	5.83062300	-4.34199800	0.00989800
C	-1.44167800	1.50120100	0.34933700	C	5.18039200	-4.59643900	-2.68792400
C	-0.29150800	1.20181900	1.05627000	H	4.76035300	-2.48774000	-2.62856100
H	0.00106900	1.85459600	1.87768900	C	5.93376000	-5.58675700	-0.61738800
C	0.46015500	0.07835300	0.77715400	H	6.09307800	-4.24428300	1.06118200
H	0.15598800	-0.60779500	-0.00181100	C	5.60751900	-5.71602000	-1.96724600
H	1.19766400	-0.26060800	1.49334500	H	4.93635200	-4.68931200	-3.74270100
C	-1.61245800	3.71891700	-1.82962500	H	6.27197000	-6.45047500	-0.05182300
H	-1.42003800	3.16917700	-2.75573000	H	5.69102500	-6.68105000	-2.45908000
H	-1.37986300	4.77720500	-1.99755600	C	3.00743100	-2.03676500	2.50084700
O	-0.70156900	3.18365800	-0.85686100	C	4.03125900	-1.39707800	3.21234900
H	-0.53299500	3.88346800	-0.17584800	C	1.90700600	-2.52918000	3.21992500
N	-4.25538300	-0.53820300	0.06260500	C	3.95925600	-1.25657300	4.60094900
C	-3.56958600	0.43967200	0.88090400	H	4.89633200	-1.00599300	2.68615600
C	-5.66219900	-0.77180600	0.42124300	C	1.83580900	-2.39749900	4.60705900
C	-6.47778800	-1.39964300	-0.69658800	C	2.86305800	-1.75700500	5.30389300
C	-6.33106300	-0.98558500	-2.02747400	H	4.76582500	-0.75910400	5.13274100
C	-7.12877500	-1.53084500	-3.03378800	H	2.80997500	-1.65168100	6.38365200
C	-8.09073000	-2.49579300	-2.72374300	H	3.02634900	-1.00061400	-1.89013500
C	-8.24629300	-2.91352300	-1.40150200	C	3.57449400	2.80707300	-1.02267800
C	-7.44113400	-2.37086100	-0.39716700	C	4.65579000	3.14925100	-0.19413300
C	-3.46771300	-1.75793300	-0.21971800	C	3.57485900	3.29070700	-2.33999800
C	-3.30879700	-2.73506700	0.93628100	C	5.71525600	3.92119700	-0.67302200
C	-2.26166000	-2.61464400	1.86323500	H	4.66315100	2.81862100	0.84236300
C	-2.14767200	-3.49787000	2.93882800	C	4.63226300	4.06368900	-2.82475700
C	-3.07466000	-4.52912300	3.09987200	H	2.73158000	3.07612100	-2.99125300
C	-4.11205900	-4.67229300	2.17660800	C	5.70907200	4.37590100	-1.99347000
C	-4.22608000	-3.78312700	1.10653800	H	6.54080900	4.17371800	-0.01342700
H	-2.96914500	0.00397200	1.68948500	H	4.61096400	4.42616800	-3.84874200
H	-4.31497600	1.08957600	1.35544500	H	6.53203200	4.97773100	-2.36796400
H	-5.76235800	-1.38706500	1.33050000	C	1.17562100	-0.22050000	-2.60425700
H	-6.09352400	0.20831400	0.66371800	C	0.61429100	0.74609500	-3.44890100
H	-5.58079800	-0.23790800	-2.26947500	C	0.48308600	-1.42989300	-2.42903400
H	-7.00305400	-1.20062000	-4.06164200	C	-0.61128300	0.52399700	-4.08339500
H	-8.71252900	-2.91901800	-3.50753100	H	1.15224500	1.67054500	-3.63976600
H	-8.99008300	-3.66455600	-1.15019100	C	-0.74462900	-1.65492200	-3.05384700
H	-7.56632500	-2.70161200	0.63164900	H	0.92843000	-2.21525900	-1.82152700
H	-3.95462800	-2.26342100	-1.05919900	C	-1.29854500	-0.67432600	-3.88178400
H	-2.48564600	-1.42779200	-0.57693900	H	-1.01472300	1.27645300	-4.75628600
H	-1.51678100	-1.83193500	1.73801500	H	-1.25445200	-2.60467800	-2.91776000
H	-1.33251400	-3.38297700	3.64863900	H	-2.24259600	-0.85657300	-4.38758200
H	-2.98455600	-5.22025800	3.93310000	H	1.10452500	-3.03651600	2.68651100
H	-4.83031900	-5.48020800	2.28590600	H	0.97969900	-2.79553600	5.14577300
				H	-4.49904400	1.99296200	-0.92564100

H	-3.25315100	1.48026700	-2.03932800	H	-2.07402300	5.82047900	1.01895900
H	-3.71343700	3.92849100	-2.18256700	H	-0.83216300	5.48551300	-1.11150500
H	-3.25580000	4.14210300	-0.49515500	H	-0.30131400	3.19597100	-1.89115800
O	-2.21372700	5.61555600	3.58570400	H	2.70791700	2.07010400	-0.39724800
C	-1.91424900	5.31191600	2.24694400	H	1.66462900	1.26292700	-1.53975700
H	-2.04704400	4.23381300	2.04071300	H	3.44776400	-0.08153900	-2.44831700
H	-2.56762100	5.86456600	1.55047300	H	4.16008300	1.52534700	-2.25103100
C	-3.56529200	5.37193200	3.92571800				
H	-3.68366800	5.64321100	4.97680200				
H	-4.25132700	5.98079400	3.31707300				
H	-3.82942900	4.31005400	3.79696500				
C	-0.46246200	5.71147600	2.01972100				
H	-0.35176400	6.79628400	2.14720300				
H	0.18342100	5.21408600	2.75757700				
O	-0.08586900	5.33754500	0.69462200				
C	1.21177300	5.80612900	0.33048900				
H	1.42055500	5.43358800	-0.67420900				
H	1.23842400	6.90314500	0.32907000				
H	1.97826600	5.42873800	1.02079100				

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C	3.73689000	0.67293000	-1.70629500
C	2.51993100	1.09555800	-0.87595500
C	2.16228300	0.07901600	0.19342300
C	3.02630600	-0.92475000	0.50261300
C	2.80568900	-1.97671000	1.50047100
H	1.85227900	-1.96542200	2.01702800
C	3.69229200	-2.93655000	1.79918000
H	3.46349900	-3.69233900	2.54459500
H	4.65822900	-2.99256700	1.30983600
C	4.77824000	0.06602000	-0.77843100
H	5.65938000	-0.29360300	-1.31696600
H	5.10451700	0.80482400	-0.03032600
O	4.25209500	-1.07708600	-0.10712300
N	-0.41958600	-0.09043300	0.29081100
C	0.85189200	0.30531300	0.93593600
C	-0.46487400	-1.49193700	-0.12633700
C	-1.87839700	-2.03745700	-0.24239300
C	-2.79349900	-1.87309700	0.80764600
C	-4.07656800	-2.41231100	0.72518200
C	-4.46658100	-3.12872100	-0.41038600
C	-3.56479500	-3.29772100	-1.46125100
C	-2.28089900	-2.75247200	-1.37580600
C	-0.96253900	0.81288500	-0.72609900
C	-1.23785200	2.21560800	-0.21790900
C	-1.93728800	2.41690000	0.98130400
C	-2.23493300	3.70498300	1.42427900
C	-1.84111000	4.81668000	0.67347300
C	-1.14572900	4.62836700	-0.52104200
C	-0.84480400	3.33592700	-0.95903800
H	0.87903600	-0.19827600	1.90680300
H	0.76192200	1.37551100	1.15682200
H	0.07221800	-1.66789800	-1.07667200
H	0.07339800	-2.07346300	0.63112300
H	-2.48921300	-1.31071000	1.68619400
H	-4.77399800	-2.27612200	1.54796700
H	-5.46674400	-3.54918900	-0.47459900
H	-3.85966400	-3.84897200	-2.35051400
H	-1.58192300	-2.88410700	-2.19918000
H	-0.33816500	0.86906600	-1.63651900
H	-1.91261200	0.36869700	-1.04994700
H	-2.23864800	1.55151000	1.56444400
H	-2.77797800	3.84322000	2.35589600