

Supporting Information

Mechanistic Study Reveals the Roles of Ligand and Substrate on the Pd-catalyzed C-H Bond Hydroxylation of Carboxylic Acid with Molecular Oxygen

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1. The formation of subK (energies are in kcal/mol).

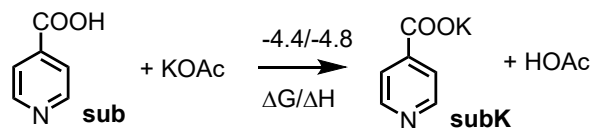


Figure S1. The formation of subK.

2. The tautomerization of the ligand (energies are in kcal/mol)

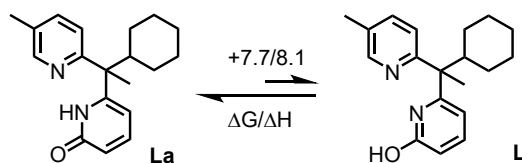


Figure S2. The tautomerization of the ligand.

3. The reaction free energy for protonation-dimerization with different possible proton forms.

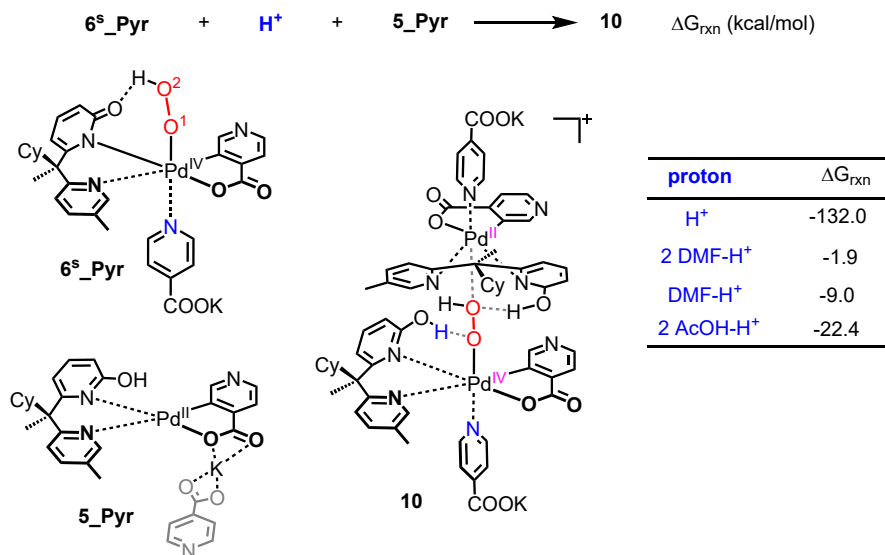


Figure S3. The reaction free energy for protonation-dimerization with different possible proton forms.

4. The dissociative mechanism for the ligand exchange process of subK + **1'** → **2** + HOAc.

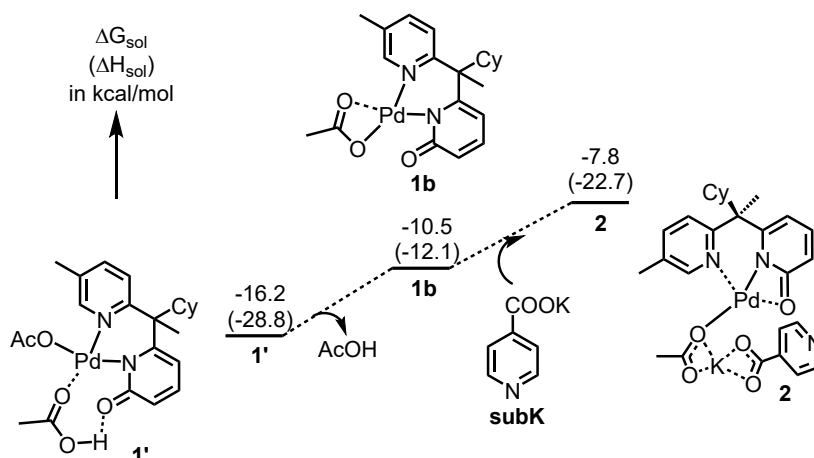


Figure S4. The dissociative mechanism for the process of subK + **1'** → **2** + HOAc.

5. The Geometry Parameters, Spin Densities, and Energies for Different Pd-O₂ Complexes.

Table S1. The Geometry Parameters, Spin Densities, and Energies for Different Pd-O₂ Complexes (Bond Distances Are Given in Å; Spin Densities Are in |e|; Energies Are in kcal/mol and Are Relative to Pd(OAc)₂; The Superscript “t” and “s” Means “Triplet” and “Singlet”, respectively).

Species	Pd-N ¹	Pd-N ²	Pd-C ¹	Pd-O ⁴	Pd-O ¹	O ¹ -O ²	O ² -H ¹ (O ¹ -H ¹)	O ³ -H ¹	Pd-O ⁵	Pd-N ³	spin Pd	spin O ¹	spin O ²	ΔG(ΔH)
6^t	2.11	2.07	2.01	2.04	3.84	1.21	3.15	0.98	-	-	0	1.00	1.00	-9.1(-16.5)
6^s	2.12	2.11	2.02	2.03	2.15	1.29	1.57	1.01	-	-	-	-	-	22.3(10.1)
6^t_AcOH	2.11	2.07	2.01	2.06	3.75	1.21	2.85	0.98	3.19	-	0	1.00	1.00	1.9(-16.9)
6^s_AcOH	2.13	2.11	2.02	2.07	2.07	1.32	1.39	1.07	2.41	-	-	-	-	21.7(-3.6)
6^t_Pyr	2.21	2.51	2.01	2.25	2.11	1.30	1.64	1.00	-	2.13	0.50	0.57	0.60	1.3(-22.5)
6^s_Pyr	2.15	2.09	2.03	2.05	2.01	1.40	1.01	1.57	-	2.16	-	-	-	6.5(-20.4)
6^t_BQ	2.12	2.07	2.01	2.05	3.52	1.21	2.70	0.98	3.95	-	0	0.99	1.00	-5.2(-24.8)
6^s_BQ	2.14	2.12	2.02	2.05	2.08	1.32	1.40	1.06	2.45	-	-	-	-	25.2(0.8)

6. The ligand exchange process between benzoquinone and pyridine of intermediate **12**.

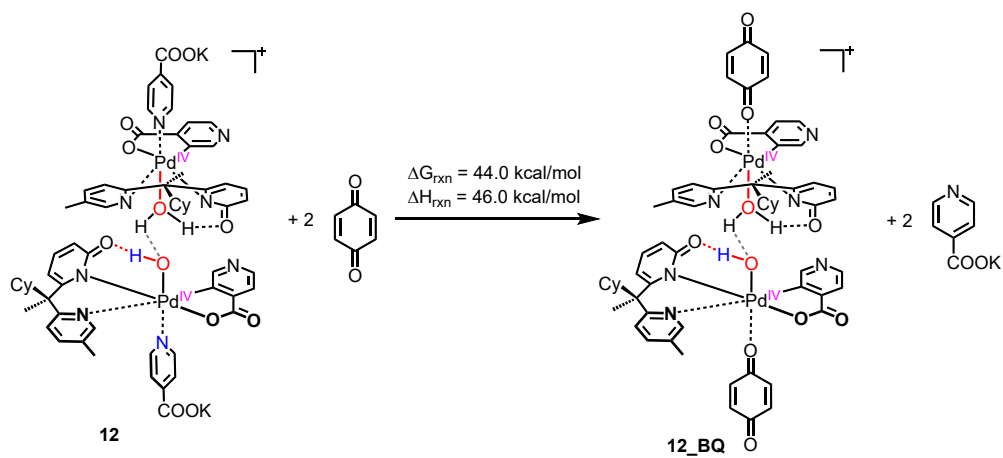


Figure S5. The ligand exchange process between benzoquinone and pyridine of intermediate **12**.

7. The reaction pathway of **5** to **6^s_Pyr**.

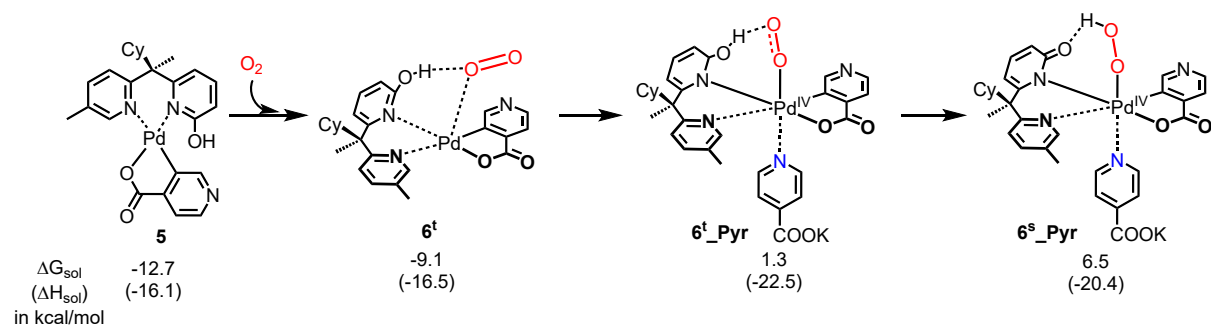


Figure S6. The reaction pathway of **5** to **6^s_Pyr**.

8. The reaction pathway from **6^s_Pyr** to **10**

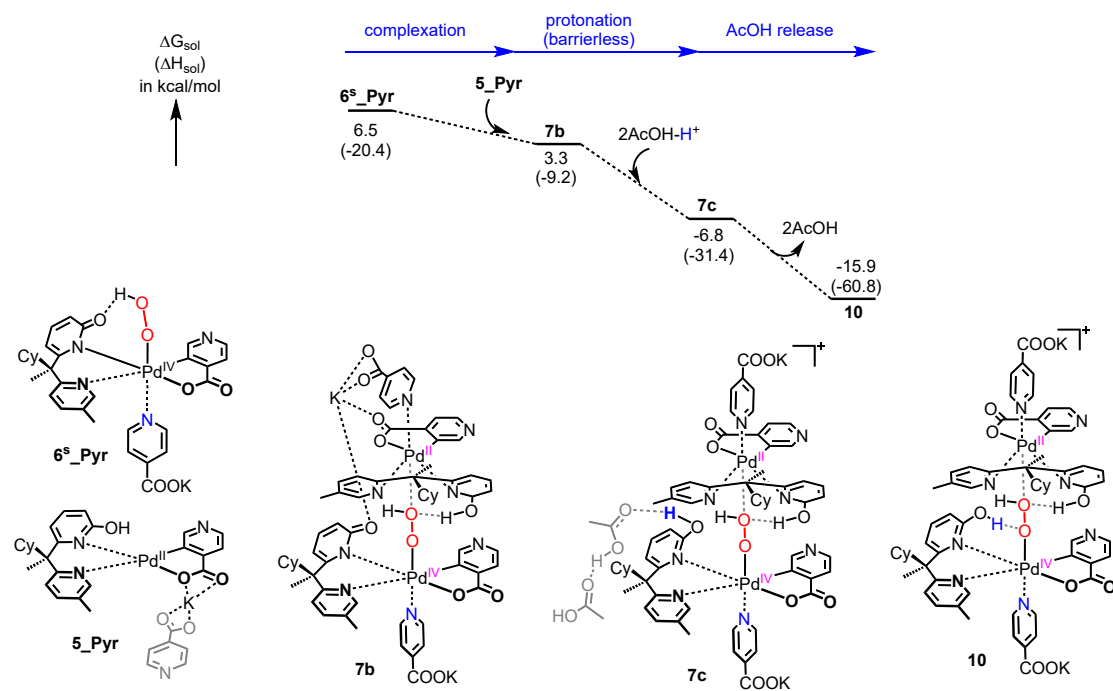


Figure S7. The reaction pathway from **6^s_Pyr** to **10**.

9. The 3D geometries for the key intermediates 6^t , 6^s , 6^t_AcOH , 6^s_AcOH , 6^t_Pyr , and 6^s_Pyr .

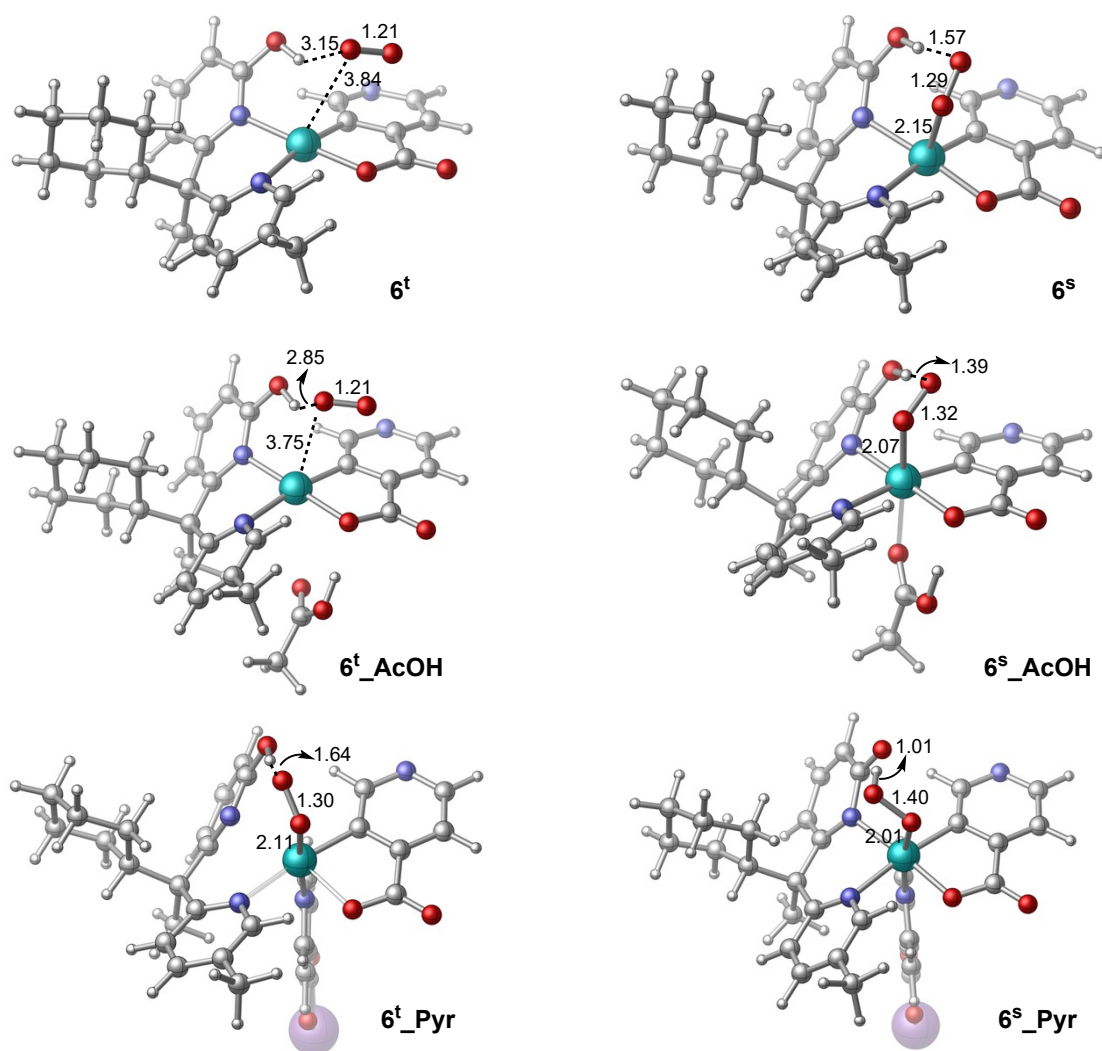


Figure S8. The 3D geometries for the key intermediates 6^t , 6^s , 6^t_AcOH , 6^s_AcOH , 6^t_Pyr , and 6^s_Pyr (bond distances are given in Å).

10. The 3D geometry of the transition state 11-ts.

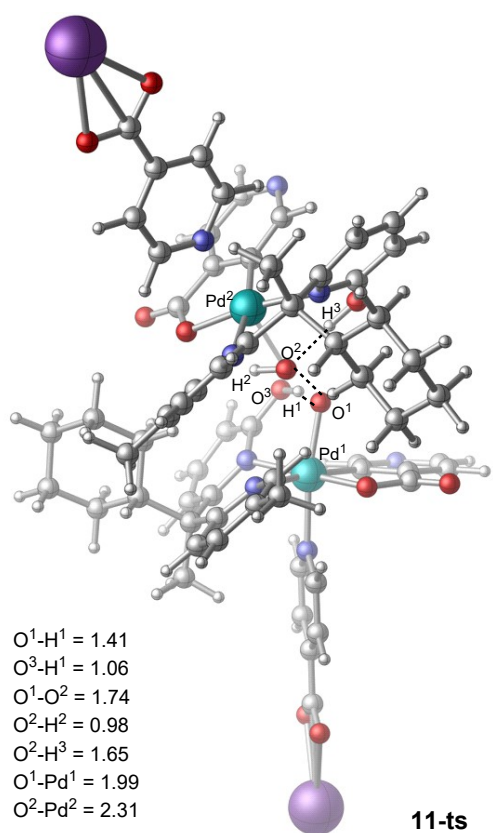


Figure S9. The 3D geometries for the transition state **11-ts** (bond distances are given in Å).

11. Energetics for all calculated species

Species	Thermal correction to enthalpy	Thermal correction to free energy	High-level Single point energy in solvent	EE + Thermal Enthalpy Correction	EE + Thermal Free Energy Correction	Imaginary Frequency (cm ⁻¹ *i)
H⁺	0.002360	-0.010000	-0.213677	-0.211317	-0.223677	
2AcOH-H⁺	0.146809	0.098579	-458.792132	-458.645323	-458.693553	
2DMF-H⁺	0.233289	0.176585	-497.691675	-497.458386	-497.515090	
DMF-H⁺	0.123530	0.087148	-249.048877	-248.925347	-248.961729	
sub	0.111935	0.071715	-437.024086	-436.912151	-436.952371	
KOAc	0.057130	0.017535	-828.595484	-828.538354	-828.577949	
subK	0.101984	0.055642	-1036.445299	-1036.343315	-1036.389657	
HOAc	0.067248	0.034521	-229.182133	-229.114885	-229.147612	
AcOOH	0.070462	0.037025	-304.334974	-304.264512	-304.297949	
O₂ triplet	0.007088	-0.016198	-150.381320	-150.374232	-150.397518	
La	0.418593	0.348685	-923.585225	-923.166632	-923.236540	
L	0.419495	0.350227	-923.599081	-923.179586	-923.248854	
PdOAc₂	0.114565	0.063633	-585.099595	-584.985030	-585.035962	
1	0.534406	0.437185	-1508.744799	-1508.210393	-1508.307614	
1'	0.535588	0.438521	-1508.746112	-1508.210524	-1508.307591	
2(subK₂DMF)	0.570837	0.462105	-2316.035193	-2315.464356	-2315.573088	
3	0.512084	0.420089	-1487.391336	-1486.879252	-1486.971247	
4-ts	0.506233	0.417811	-1487.358447	-1486.852214	-1486.940636	-1124.82
5	0.512274	0.423347	-1487.392561	-1486.880287	-1486.969214	
2	0.570894	0.463816	-2316.000103	-2315.429209	-2315.536287	
6^s	0.519824	0.424840	-1637.732725	-1637.212901	-1637.307885	
6^t	0.520890	0.418298	-1637.776129	-1637.255239	-1637.357831	
6^s_AcOH	0.587723	0.480902	-1866.937258	-1866.349535	-1866.456356	
6^t_AcOH	0.590140	0.472780	-1866.960818	-1866.370678	-1866.488038	
6^t_Pyr	0.624456	0.501547	-2674.232549	-2673.608093	-2673.731002	
6^s_Pyr	0.624815	0.506815	-2674.229577	-2673.604762	-2673.722762	
5_Pyr	0.616042	0.502377	-2523.873067	-2523.257025	-2523.370690	
8-ts	1.239857	1.031452	-5198.070641	-5196.830784	-5197.039189	-291.71
13-ts'	0.617952	0.501569	-2599.025154	-2598.407202	-2598.523585	-381.74
10	1.256240	1.048913	-5198.564513	-5197.308273	-5197.515600	
11-ts	1.253767	1.047247	-5198.548220	-5197.294453	-5197.500973	-337.24
12	1.254097	1.049456	-5198.628996	-5197.374899	-5197.579540	
7'	0.632791	0.517768	-2599.527715	-2598.894924	-2599.009947	
7	0.620651	0.505127	-2599.062485	-2598.441834	-2598.557358	
13-ts	0.513869	0.424321	-1562.563235	-1562.049366	-1562.138914	-286.56

14	0.517682	0.424245	-1562.640539	-1562.122857	-1562.216294	
1b	0.466977	0.382028	-1279.536044	-1279.069067	-1279.154016	
7b	1.244264	1.035488	-5198.120671	-5196.876407	-5197.085183	
7c	1.396296	1.161643	-5656.953427	-5655.557131	-5655.791784	
7d	0.515606	0.424562	-1562.575300	-1562.059694	-1562.150738	
12_BQ	1.233231	1.042577	-3888.861996	-3887.628765	-3887.819419	
6^t_BQ	0.615531	0.49446	-2019.390891	-2018.775360	-2018.896431	
6^s_BQ	0.613119	0.499661	-2019.34763	-2018.734511	-2018.847969	

12. Cartesian coordinates for all species

H⁺

H 0.00000000 0.00000000 0.00000000

2AcOH-H⁺

C 1.98814100 -0.02590400 -0.04817900
 O 1.11867900 0.55148600 -0.75691300
 O 3.18424700 0.48245000 0.00562700
 H 3.23782900 1.29445500 -0.54262600
 C 1.74446100 -1.25071500 0.75074200
 H 1.25346400 -2.00395600 0.12880600
 H 2.67784700 -1.64046500 1.15362600
 H 1.06833900 -0.99915400 1.57606500
 H 0.10086800 0.07988500 -0.74686100
 C -1.97602200 0.01700100 -0.06025000
 O -1.07185000 -0.48064100 -0.76103100
 O -3.16149500 -0.54650100 -0.03175800
 H -3.16025500 -1.33650600 -0.61084800
 C -1.82620600 1.24308000 0.77147700
 H -1.56332100 2.08237300 0.11952000
 H -2.74602800 1.46925900 1.30855000
 H -1.00763200 1.09899200 1.48363100

2DMF-H⁺

H -0.09706200 -0.94260100 0.02393200
 C 1.81957200 -0.04295100 0.29168800
 H 1.35793200 0.56302800 1.07842700
 O 1.14532900 -0.89331000 -0.35706900
 N 3.10369000 0.18445100 0.08645100
 C 3.86249700 -0.54400900 -0.92600100
 H 3.21138900 -1.26221400 -1.42034600
 H 4.26096500 0.16209600 -1.66055200
 H 4.69586700 -1.06708300 -0.44801400
 C 3.82983000 1.18386300 0.86364800
 H 3.15684400 1.65958500 1.57803900
 H 4.65164900 0.70425700 1.40335500
 H 4.24157100 1.94319800 0.19226400
 C -1.81678100 -0.02363800 -0.27998700
 H -1.31406100 0.61350400 -1.00971800
 O -1.16664500 -0.93500900 0.34047800

N -3.09140000 0.19485400 -0.08286500
 C -3.88077000 -0.59017300 0.86630500
 H -3.25151400 -1.34207400 1.33721600
 H -4.29314800 0.07968300 1.62556000
 H -4.70197800 -1.07388700 0.33094500
 C -3.79753600 1.25016800 -0.80930600
 H -3.11029100 1.76235400 -1.48300400
 H -4.61384200 0.80641000 -1.38510400
 H -4.21069700 1.96561100 -0.09343800

DMF-H⁺

H -2.63172200 -0.61350000 0.00061900
 C -0.74743300 -0.65760200 -0.00022400
 H -0.75448500 -1.74444500 -0.00012400
 O -1.87875900 0.00621600 0.00011600
 N 0.38128600 -0.03038900 -0.00035000
 C 0.48542800 1.43365200 0.00002800
 H -0.50319400 1.88577700 -0.00435600
 H 1.03364600 1.73765100 0.89443300
 H 1.04128100 1.73732100 -0.88971100
 C 1.64599800 -0.77533700 0.00016200
 H 1.44785000 -1.84661200 0.00018000
 H 2.21216700 -0.49879200 -0.89187600
 H 2.21157500 -0.49868000 0.89256100

sub

C 1.86260000 -1.17080800 -0.00002300
 C 0.46859900 -1.19337400 -0.00002300
 C -0.21259100 0.02706600 -0.00000300
 C 0.53026700 1.21015300 0.00002100
 C 1.92003800 1.12165700 0.00002400
 N 2.58691200 -0.04242200 0.00000100
 H 2.42047500 -2.10445300 -0.00004100
 H -0.06525100 -2.13576300 -0.00004100
 H 0.03032600 2.17158300 0.00004400
 H 2.52373600 2.02632100 0.00005100
 C -1.70141900 0.11782700 -0.00000700
 O -2.32205100 1.16357400 -0.00005300
 O -2.29819300 -1.08890600 0.00005300
 H -3.26069700 -0.93320200 0.00005300

KOAc

C 0.99491800 0.00987000 0.00011500
 O 0.41334900 1.13528700 0.00013600

O	0.41954100	-1.12000500	0.00003600	O₂_triplet			
C	2.52890700	-0.00282600	0.00001000	O	0.00000000	0.00000000	0.60697700
H	2.89473400	-0.54310300	0.88060000	O	0.00000000	0.00000000	-0.60697700
H	2.89462800	-0.54329000	-0.88050900				
H	2.94251100	1.00841300	-0.00011500	La			
K	-1.92305000	-0.00455500	-0.00011100	C	-1.35532300	-0.39046800	0.46723700
				C	-1.89883900	-1.60703200	0.03481500
subK				C	-3.24714900	-1.67192100	-0.30491800
C	-2.94057500	-1.14468100	-0.00003400	C	-4.05043200	-0.53127800	-0.20454800
C	-1.54802200	-1.19596000	-0.00006800	C	-3.42065900	0.62548100	0.26496900
C	-0.82562200	0.00000700	0.00000800	N	-2.12637200	0.70237700	0.59448800
C	-1.54803000	1.19595800	0.00011400	H	-3.67572800	-2.61060200	-0.64725100
C	-2.94059800	1.14465300	0.00013900	H	-1.28639700	-2.49753900	-0.03285300
N	-3.64253100	-0.00000900	0.00006700	H	-4.00104400	1.54035100	0.38398600
H	-3.52170200	-2.06534500	-0.00009000	C	0.09171100	-0.24388900	0.96522700
H	-1.02047300	-2.14283400	-0.00015100	C	-0.01741000	-0.42123500	2.49937500
H	-1.02051800	2.14285300	0.00017600	H	-0.42549000	-1.41183500	2.72190500
H	-3.52171900	2.06532300	0.00022100	H	0.94373000	-0.33542700	3.00887700
C	0.69763200	0.00001800	-0.00001600	H	-0.69566300	0.32688000	2.91909900
O	1.26782800	1.12877700	0.00009100	C	1.04749800	-1.34793400	0.38642200
O	1.26783000	-1.12873300	-0.00012500	C	1.10686400	-1.42987900	-1.15153100
K	3.62779700	-0.00001400	-0.00006400	C	2.48945000	-1.24412500	0.92180900
				H	0.64817200	-2.30415500	0.75254900
HOAc				C	1.92386000	-2.64600300	-1.60741500
C	-0.09038600	0.12150300	-0.00001600	H	1.57108400	-0.51787900	-1.54053000
O	-0.64511200	1.20208900	-0.00004900	H	0.10346100	-1.46952500	-1.58390300
O	-0.77732300	-1.04301000	0.00004900	C	3.33809000	-2.44259800	0.47436200
H	-1.72403700	-0.81038300	0.00005300	H	2.94624800	-0.31740700	0.55068800
C	1.39442400	-0.10951300	0.00000100	H	2.50143600	-1.18436600	2.01373100
H	1.68073100	-0.69005800	0.88263300	C	3.35083800	-2.59480900	-1.05044300
H	1.68073000	-0.69032000	-0.88245600	H	1.94431100	-2.69252900	-2.70309100
H	1.91782600	0.84619300	-0.00013300	H	1.43132700	-3.56632800	-1.26197600
				H	4.36102500	-2.33661400	0.85568400
AcOOH				H	2.92806900	-3.35748600	0.92505900
C	-0.42033900	0.17035300	0.00015300	H	3.91154700	-3.49183700	-1.34042000
O	-0.10038600	1.34541600	0.00008200	H	3.87559000	-1.73615400	-1.49265400
O	0.51952100	-0.80977400	0.00023400	C	0.61907800	1.14477200	0.59229500
C	-1.80255000	-0.40358000	-0.00015000	C	1.28713800	1.96888800	1.50033100
H	-1.94941400	-1.02915100	-0.88552400	N	0.44191000	1.51192800	-0.69226200
H	-1.94969600	-1.02936000	0.88502400	C	1.77510200	3.20223900	1.05769100
H	-2.52474100	0.41275400	-0.00017700	H	1.42817500	1.67080400	2.53033100
O	1.84906300	-0.24461000	-0.00015600	C	0.91124700	2.68386800	-1.09887400
H	1.61559900	0.71685800	-0.00062100	C	1.59100000	3.58406400	-0.26303000
				H	2.29508700	3.86203600	1.74602800

H	1.95373700	4.53566600	-0.63963300	C	0.93355700	1.04242600	0.71723500
O	0.68094600	2.95529200	-2.41008500	C	2.00772300	1.48328100	1.46019300
H	1.05597500	3.82480100	-2.61992500	N	0.63044800	1.72803900	-0.42246300
C	-5.50834300	-0.54244400	-0.57555800	C	2.73998000	2.61242500	1.01000600
H	-5.98828800	0.40702800	-0.32175500	H	2.30866200	0.98346400	2.36777300
H	-5.64118900	-0.70915900	-1.65113000	C	1.28056400	2.85797500	-0.93047000
H	-6.04383200	-1.34538500	-0.05701400	C	2.40815000	3.28282600	-0.13694300
				H	3.58867100	2.94805400	1.60090800
L				H	2.96562800	4.14737200	-0.47999600
C	-2.97139500	0.53405800	-0.92402700	O	0.86609300	3.38851700	-1.97143000
C	-1.37645500	-0.11950700	0.64354300	H	-0.22827800	1.42433700	-0.90369300
C	-2.38844000	-0.70754200	1.41876100				
C	-3.70850000	-0.65973100	0.98398100	PdOAc₂			
C	-4.03674800	-0.02529800	-0.21890200	Pd	0.00000500	0.00002500	-0.00031400
H	-3.14862000	1.04775000	-1.86690100	C	-2.45078300	-0.00002600	-0.02596500
H	-2.16456000	-1.20124000	2.35368600	O	-1.77095900	-1.08723200	-0.03255200
H	-4.48918500	-1.11682700	1.58646800	O	-1.77076100	1.08709300	-0.03242700
N	-1.69784700	0.48072800	-0.51592200	C	-3.93690100	0.00007400	0.02756300
C	0.11660800	-0.22182300	1.04171500	H	-4.24703400	-0.00358500	1.07909500
C	0.72730600	-1.46886400	0.26215000	H	-4.33275400	0.89972700	-0.44773000
C	0.71774600	-1.34096900	-1.27137300	H	-4.33314300	-0.89622300	-0.45376400
C	2.14645400	-1.84329600	0.72881900	C	2.45075700	0.00005000	0.02635100
H	0.06042900	-2.30123900	0.52911800	O	1.77097600	1.08726900	0.03250600
C	1.20008500	-2.63243600	-1.94698100	O	1.77073400	-1.08706200	0.03264900
H	1.37832500	-0.51760300	-1.57067900	C	3.93689600	-0.00016300	-0.02643400
H	-0.28198800	-1.08928400	-1.63242100	H	4.33255300	-0.89650700	0.45527900
C	2.64444200	-3.12900700	0.05290400	H	4.24754900	-0.00413800	-1.07781200
H	2.83105400	-1.01963900	0.49077300	H	4.33289000	0.89942800	0.44888400
H	2.17758800	-1.97878100	1.81285700				
C	2.60299000	-3.02241900	-1.47378900	I			
H	1.18321500	-2.50575400	-3.03612300	C	-1.19584500	1.42947100	0.61580800
H	0.49941800	-3.44648900	-1.71337400	C	-1.84630700	2.66192200	0.80527900
H	3.66208700	-3.35233800	0.39524200	C	-1.32963300	3.83591700	0.28468300
H	2.01312300	-3.96975700	0.37315900	C	-0.14149500	3.81474100	-0.45654400
H	2.91581500	-3.96796300	-1.93303500	C	0.49765800	2.58907300	-0.55166900
H	3.31998900	-2.25689900	-1.80257400	N	-0.00421300	1.45453500	-0.00972100
C	0.19969200	-0.50378600	2.55720200	H	-1.85502600	4.77281100	0.44517100
H	1.22478300	-0.50599900	2.91882700	H	-2.77235700	2.70022300	1.36247700
H	-0.35525300	0.24842100	3.12437600	H	1.44993400	2.49061600	-1.05416600
H	-0.21083100	-1.48897100	2.78749800	C	-1.91748900	0.14504100	1.08830100
C	-5.45027000	0.05211700	-0.72479300	C	-2.11043900	0.27339100	2.61659600
H	-6.09763700	0.56569100	-0.00516000	H	-2.68592700	1.16719700	2.86609700
H	-5.50214900	0.59096000	-1.67466600	H	-2.63909800	-0.58361700	3.03276800
H	-5.86816600	-0.94934400	-0.87731600	H	-1.13510900	0.34321700	3.10796400

C	-3.31391200	0.19612400	0.31136100	H	5.48297900	-1.27747200	0.07587900
C	-3.12881000	0.01065700	-1.20460500	H	5.01108700	-2.29209000	1.45179700
C	-4.44416500	-0.71756000	0.81006500	H	2.23737600	-2.43276600	-1.48328200
H	-3.68799400	1.21160900	0.46719500				
C	-4.42769900	0.32323500	-1.95909600	I'			
H	-2.82826000	-1.02469400	-1.41005300	C	-1.06007500	1.49479200	0.59091500
H	-2.32043200	0.65088200	-1.57557200	C	-1.62571500	2.77730900	0.70596500
C	-5.75288400	-0.37290900	0.08108100	C	-0.99214400	3.89008400	0.17984700
H	-4.20596500	-1.76593400	0.60916400	C	0.22788100	3.75070300	-0.49352200
H	-4.58117500	-0.61447000	1.89140600	C	0.77122400	2.47616700	-0.52289700
C	-5.59777200	-0.51904400	-1.43739300	N	0.15640700	1.40283000	0.02889100
H	-4.28524100	0.15529300	-3.03320100	H	-1.44950900	4.86972900	0.28344700
H	-4.66419400	1.38917200	-1.83433000	H	-2.57349800	2.90383400	1.21061500
H	-6.55844500	-1.02146700	0.44528100	H	1.73204700	2.27867600	-0.98269700
H	-6.04427400	0.65911600	0.32131300	C	-1.88330000	0.28464400	1.08113800
H	-6.52735500	-0.23641800	-1.94583900	C	-2.10676100	0.49224800	2.59823200
H	-5.41418600	-1.57582400	-1.67702000	H	-2.60554300	1.44457400	2.78874300
C	-1.29223900	-1.22346400	0.75226400	H	-2.72441900	-0.29019600	3.03710100
C	-1.89008200	-2.38028900	1.23189000	H	-1.14314200	0.49817500	3.11652100
N	-0.28465100	-1.32926300	-0.15505800	C	-3.25410000	0.39768100	0.26473900
C	-1.55080200	-3.61911600	0.65788500	C	-3.04347500	0.15618000	-1.24002600
H	-2.64872800	-2.33756300	1.99824600	C	-4.45270200	-0.42853200	0.75724600
C	0.01801300	-2.50312300	-0.80569200	H	-3.56576800	1.43865400	0.38422600
C	-0.65797000	-3.68392200	-0.38703600	C	-4.29931000	0.53181200	-2.03717000
H	-2.02832600	-4.52323300	1.02514600	H	-2.81093700	-0.90302800	-1.40910600
H	-0.40937300	-4.61649900	-0.88088500	H	-2.18401600	0.72859600	-1.60668100
O	0.88890500	-2.49673000	-1.74257600	C	-5.71777500	-0.02250300	-0.01632800
C	0.43350000	5.04781900	-1.09284100	H	-4.27803700	-1.49561100	0.59086500
H	1.41396100	4.84740700	-1.53198900	H	-4.61167700	-0.28654900	1.83107200
H	-0.22668300	5.41830200	-1.88504800	C	-5.53401800	-0.21942800	-1.52574100
H	0.54098400	5.85089900	-0.35629700	H	-4.14066000	0.32546000	-3.10223200
Pd	1.28230200	-0.06765400	0.16125600	H	-4.46898000	1.61371500	-1.94657100
C	3.78412200	1.31653200	-0.02196400	H	-6.57169600	-0.60905500	0.34255500
O	3.90971800	0.72229500	-1.09925700	H	-5.94891200	1.03185900	0.18936400
O	2.73753700	1.25799400	0.74937200	H	-6.43040200	0.10809400	-2.06577700
C	4.89853400	2.18870100	0.53494300	H	-5.41301900	-1.29186500	-1.73351400
H	4.49708200	3.11170400	0.96175100	C	-1.35957900	-1.14281500	0.81506600
H	5.40824300	1.64731600	1.34030800	C	-2.05954800	-2.20826500	1.36742500
H	5.62524600	2.42217400	-0.24552900	N	-0.37528600	-1.39572000	-0.10072200
C	3.54568100	-2.06494000	-0.09119100	C	-1.87707700	-3.50126200	0.86061100
O	2.69611900	-1.55648800	0.68112900	H	-2.78804700	-2.04397200	2.14538700
O	3.28546900	-2.49545500	-1.27911000	C	-0.23238600	-2.62992700	-0.64298300
C	4.96714300	-2.19984500	0.36561900	C	-1.01489900	-3.70953300	-0.19364300
H	5.46274500	-3.04412500	-0.11602900	H	-2.44105400	-4.32854000	1.27985500

H	-0.87041700	-4.68082600	-0.65054700	H	2.63757600	1.25595600	1.52660100
O	0.62127600	-2.85575100	-1.62082500	C	5.78353100	-0.93612600	0.59164200
C	0.93503600	4.91299400	-1.13079200	H	3.98816100	-2.10689800	0.48944300
H	1.91649300	4.61871800	-1.51092000	H	4.57965700	-1.59328500	-1.09025200
H	0.34943900	5.31222000	-1.96648900	C	5.60527100	-0.48954200	2.04742200
H	1.07192000	5.72696600	-0.41113100	H	4.46522600	0.95778200	3.19979500
Pd	1.30761200	-0.23551900	0.23187200	H	5.08321900	1.57237100	1.66904400
C	3.75745600	1.31398600	0.12804200	H	6.44047900	-1.81258100	0.54041700
O	3.70444400	1.21218000	-1.10238700	H	6.27766700	-0.13668500	0.02204200
O	2.84341300	0.90650100	0.96019100	H	6.57403300	-0.22588400	2.48859300
C	4.93635300	1.98197900	0.82100900	H	5.20920700	-1.33135100	2.63269700
H	4.59070800	2.85498300	1.38450800	C	1.22976200	-1.11032500	-0.01540300
H	5.39229200	1.29131800	1.53732800	C	1.59037900	-2.44749300	0.04292700
H	5.68162800	2.29522900	0.08784800	N	0.21765400	-0.66183900	0.77154600
C	3.33577300	-2.14499100	-0.42829000	C	1.01531200	-3.26972600	1.03518300
O	2.59304400	-1.82517000	0.57339200	H	2.34742900	-2.85125800	-0.61085700
O	2.98197700	-2.05342300	-1.62723400	C	-0.31864100	-1.39665100	1.82776500
C	4.71909300	-2.64490200	-0.08170300	C	0.13139600	-2.75441300	1.94902900
H	5.15211200	-3.20371800	-0.91293400	H	1.30587400	-4.31561800	1.08763100
H	5.35333800	-1.77553800	0.12840900	H	-0.29917700	-3.35882200	2.74036800
H	4.69452700	-3.26203400	0.81964600	O	-1.17093900	-0.87036700	2.58846700
H	1.49428500	-2.31094400	-1.63015000	C	0.93834900	5.61675400	-0.68813400
				H	-0.03294100	5.80522200	-0.22364200
2(subK₂DMF)				H	1.70840400	6.10477600	-0.08022700
C	1.68457500	1.36580200	-0.88055400	H	0.94987500	6.09513800	-1.67311100
C	2.56486200	2.27169600	-1.49938200	Pd	-1.04581100	0.68870700	-0.06240700
C	2.33251600	3.63644300	-1.47077100	C	-3.19962200	2.57627600	-0.15367400
C	1.20906800	4.14380200	-0.80625800	O	-3.28928300	2.34421100	1.06705800
C	0.33495100	3.20541500	-0.28079600	O	-2.29856400	2.08956900	-0.94411300
N	0.55542300	1.87182500	-0.34645600	C	-4.21362600	3.47780000	-0.83693100
H	3.03171200	4.31264600	-1.95401700	H	-3.76806800	4.01557600	-1.67685100
H	3.44875800	1.90198200	-2.00101800	H	-5.02667600	2.85470300	-1.22870600
H	-0.59038100	3.50621400	0.19074500	H	-4.63905100	4.18384900	-0.12045700
C	2.11975000	-0.11876000	-0.79438900	C	-0.61467600	-2.69678400	-3.00728600
C	2.32835300	-0.61880800	-2.24218600	C	-1.39436600	-1.93767300	-2.13526500
H	3.11827100	-0.05646900	-2.74488500	C	-1.96497100	-2.56207500	-1.02303500
H	2.60751200	-1.67171900	-2.27067600	C	-1.72600900	-3.92695200	-0.84698500
H	1.40310300	-0.49886200	-2.81176300	C	-0.91541200	-4.59365100	-1.76239500
C	3.50395800	-0.04255500	0.00357600	N	-0.36140800	-4.00205900	-2.83274900
C	3.29499500	0.38098800	1.46817600	H	-0.16805400	-2.23025200	-3.88258400
C	4.42948000	-1.26809600	-0.05549500	H	-1.55302400	-0.88183800	-2.32119300
H	4.06906400	0.75712400	-0.48386400	H	-2.15571300	-4.44790400	0.00031400
C	4.63399000	0.69183000	2.14948200	H	-0.70053800	-5.65227000	-1.63061800
H	2.78907200	-0.42830100	2.00982800	C	-2.83734600	-1.81735900	-0.04018800

O	-3.64015800	-2.44982400	0.66167300	H	-1.21183000	-4.85726800	0.11842900
O	-2.74595900	-0.52575100	-0.00205700	O	0.28380600	-2.87883900	-1.18531100
K	-3.57846400	0.06100200	2.39509900	C	2.39941600	4.25793700	-0.05976200
3				H	2.90965100	3.95322600	-0.97701900
C	-0.64473200	1.34523100	0.94587600	H	1.98930800	5.26219600	-0.20532400
C	-0.57776300	2.57710600	1.61815600	H	3.14661900	4.32238900	0.73960500
C	0.38901300	3.52619600	1.32313100	Pd	0.56454900	-0.69207100	-0.93018200
C	1.31883600	3.28338100	0.31095000	C	4.33184100	0.27783100	1.91222000
C	1.20927500	2.06005900	-0.33230500	C	4.18951300	0.53704900	0.55057400
N	0.28757300	1.12330600	-0.01902600	C	3.58166900	-0.42592000	-0.25988200
H	0.41024000	4.46059000	1.87616200	C	3.18610000	-1.62979800	0.33549700
H	-1.29860400	2.80973300	2.38558400	C	3.39780600	-1.80137800	1.70270800
H	1.87685400	1.80308800	-1.14160600	N	3.94620600	-0.86771400	2.49545800
C	-1.87351800	0.43086700	1.25002800	H	4.77599400	1.02695500	2.56487500
C	-2.31020900	0.68002200	2.71481000	H	4.52530500	1.47946000	0.13141200
H	-2.74584000	1.67153100	2.83885500	H	2.71991900	-2.41960800	-0.24433100
H	-3.07482900	-0.02474400	3.02815200	H	3.10338400	-2.73226800	2.18354000
H	-1.46079300	0.57694700	3.39513000	C	3.36590700	-0.13268200	-1.72954000
C	-3.02834000	0.94058200	0.27558400	O	2.13879500	-0.18666500	-2.16628500
C	-2.70851900	0.78344500	-1.22049700	O	4.33056800	0.17396800	-2.42781800
C	-4.40495900	0.31859700	0.57252800	4-ts			
H	-3.10241500	2.01559900	0.48911300	C	-1.44296700	1.21371600	0.82648100
C	-3.79874900	1.41837400	-2.09502800	C	-2.19348300	2.29071500	1.33533800
H	-2.62774900	-0.28317800	-1.46514900	C	-1.92833900	3.59705200	0.96498700
H	-1.74379300	1.23625700	-1.46266300	C	-0.89917300	3.87151700	0.05702300
C	-5.49961900	0.95618000	-0.29535200	C	-0.15425300	2.78373000	-0.36854500
H	-4.36789100	-0.75822600	0.36877800	N	-0.40731800	1.51005800	0.01763800
H	-4.66749900	0.43557800	1.62746600	H	-2.52917200	4.40512800	1.37195100
C	-5.18010500	0.83297200	-1.78802400	H	-3.01261800	2.10106000	2.01429000
H	-3.54787900	1.27792800	-3.15310000	H	0.70691100	2.91413500	-1.01038000
H	-3.81628700	2.50250700	-1.91560200	C	-1.96672200	-0.20984600	1.13677900
H	-6.46464200	0.48719800	-0.06941300	C	-2.14200800	-0.31427000	2.67236900
H	-5.59554500	2.01857800	-0.03134600	H	-2.86917600	0.40744300	3.04590200
H	-5.95057300	1.33263300	-2.38733400	H	-2.48970600	-1.30049700	2.97457100
H	-5.19361600	-0.22827500	-2.07371300	H	-1.18404400	-0.12767800	3.16678300
C	-1.69498000	-1.07871400	1.05826100	C	-3.37629200	-0.22595700	0.37498300
C	-2.43651600	-2.06461300	1.71389900	C	-3.19801200	-0.25847100	-1.15253900
N	-0.85549400	-1.50955100	0.11474500	C	-4.41510500	-1.27668200	0.79851600
C	-2.25741900	-3.41464000	1.36144200	H	-3.83430500	0.73588900	0.62449400
H	-3.16278800	-1.81422900	2.47183600	C	-4.53143700	0.00537200	-1.86507200
C	-0.63010000	-2.80210900	-0.26154600	H	-2.81307600	-1.24179300	-1.45222700
C	-1.36101000	-3.81649900	0.38152500	H	-2.45467800	0.48012000	-1.47209100
H	-2.84429700	-4.16619200	1.88157400	C	-5.76008000	-0.98002900	0.11586800

H	-4.09638400	-2.27873700	0.49813400	N	-0.39772400	1.60888200	-0.11415700
H	-4.54051800	-1.28444300	1.88617800	H	-2.63192200	4.50525700	1.04416800
C	-5.61776000	-0.97669100	-1.41091000	H	-3.07130800	2.22405100	1.79520700
H	-4.39240700	-0.05415200	-2.95099600	H	0.71726400	2.99216800	-1.16304400
H	-4.85513400	1.03180500	-1.64323600	C	-1.88325100	-0.10444400	1.08237400
H	-6.50190300	-1.72497600	0.42709400	C	-1.94211300	-0.14276300	2.62959500
H	-6.13320900	-0.00228000	0.45100100	H	-2.66149300	0.58021900	3.01749100
H	-6.57593500	-0.72965700	-1.88347800	H	-2.23466700	-1.12270500	3.00505600
H	-5.35081100	-1.98862900	-1.74661900	H	-0.95655900	0.09625600	3.04033800
C	-1.19252400	-1.44988700	0.64628500	C	-3.33740000	-0.23212400	0.42631500
C	-1.69129100	-2.70820900	0.96953400	C	-3.26532100	-0.30945200	-1.10937500
N	-0.14812300	-1.37143500	-0.21439100	C	-4.28839600	-1.31728700	0.95598300
C	-1.23155400	-3.84130800	0.28395800	H	-3.82972700	0.71170000	0.67480300
H	-2.47160300	-2.81959000	1.70446800	C	-4.65698900	-0.13171200	-1.73057900
C	0.31035800	-2.45586000	-0.93892200	H	-2.85641800	-1.28406800	-1.40698500
C	-0.28083000	-3.72141000	-0.70398100	H	-2.58209900	0.45195400	-1.50202500
H	-1.64968700	-4.81458000	0.52372300	C	-5.69138800	-1.10663800	0.36396800
H	0.07726200	-4.56809900	-1.27725300	H	-3.94537900	-2.31321800	0.66171300
O	1.28905400	-2.29321800	-1.75858000	H	-4.33662100	-1.29564800	2.04956500
C	-0.59218600	5.26326200	-0.41745400	C	-5.65807700	-1.14791700	-1.16868200
H	0.27460500	5.27336900	-1.08294800	H	-4.59351300	-0.22111100	-2.82151400
H	-1.44615000	5.68439600	-0.95945800	H	-5.01364400	0.88533200	-1.51642500
H	-0.38578900	5.92617700	0.42959200	H	-6.37264200	-1.87399000	0.75006700
Pd	1.12501600	0.19584200	-0.33432200	H	-6.08599600	-0.13618500	0.69533400
C	5.37445000	-1.52623700	0.99095500	H	-6.65848400	-0.96294600	-1.57776100
C	5.22946400	-0.31442300	0.31932500	H	-5.36526900	-2.15671400	-1.49194400
C	4.00368200	-0.02497200	-0.27468000	C	-1.08988000	-1.33124100	0.58505600
C	2.96687600	-0.97902100	-0.22851500	C	-1.51593700	-2.60049300	0.97444500
C	3.23006800	-2.16029900	0.49041100	N	-0.10263700	-1.24359600	-0.34765400
N	4.39172600	-2.43596300	1.09458600	C	-1.08239500	-3.73269600	0.27878100
H	6.31265600	-1.77139300	1.48423400	H	-2.22024100	-2.71889600	1.78216100
H	6.03453400	0.41177500	0.28826600	C	0.26440300	-2.32190700	-1.06748400
H	2.46800600	-2.93316800	0.55499900	C	-0.23485900	-3.59911500	-0.80648500
C	3.72767400	1.35639000	-0.80346000	H	-1.44112800	-4.71382600	0.57228200
O	2.46697500	1.70277100	-0.73035600	H	0.08964300	-4.43812000	-1.40925600
O	4.62326100	2.09390400	-1.20345300	O	1.16212200	-2.16679200	-2.04810600
H	2.11777000	-1.34839600	-1.14336400	C	-0.66153000	5.33523100	-0.71661800
				H	0.25134000	5.34927400	-1.31765100
5				H	-1.48733900	5.69297800	-1.34198100
C	-1.44595400	1.32813600	0.67852300	H	-0.54480300	6.04885300	0.10591100
C	-2.24497400	2.39960800	1.11987500	Pd	1.26644500	0.30464900	-0.18843000
C	-2.00028100	3.69432200	0.69265400	C	5.41859500	-1.89476800	0.55794900
C	-0.94802400	3.95644100	-0.19327400	C	5.34447600	-0.52125700	0.33760400
C	-0.16312800	2.86771500	-0.54408000	C	4.08817900	0.03517100	0.10631300

C	2.94417800	-0.77803600	0.07223000	C	-2.64385100	-2.45763100	0.56256000
C	3.13697700	-2.13952900	0.33856500	N	-1.03583300	-1.28522700	-0.71073300
N	4.33986300	-2.69354500	0.57529900	C	-2.45095900	-3.58520100	-0.26868200
H	6.37789500	-2.37453300	0.74341700	H	-3.36150000	-2.50530800	1.36639400
H	6.22818700	0.10905600	0.35836300	C	-0.82378800	-2.34895300	-1.59101800
H	2.29801600	-2.82968500	0.37825300	C	-1.61611100	-3.52781700	-1.35395500
C	3.87295300	1.51167800	-0.05421200	H	-2.99700800	-4.49907700	-0.04933300
O	2.60516400	1.84973900	-0.12627900	H	-1.46248800	-4.37687600	-2.01136200
O	4.79689200	2.32120100	-0.09008600	O	0.06079800	-2.25110800	-2.47052500
H	1.52131000	-1.25624400	-1.99304500	C	0.09613200	5.07352400	-0.65846700
2				H	1.00037700	4.88586700	-1.24333900
C	-1.64639000	1.32785000	0.61215500	H	-0.61268800	5.61975100	-1.29093700
C	-2.12541200	2.54600000	1.12697300	H	0.35432200	5.72556900	0.18208100
C	-1.56259900	3.75540300	0.75494600	Pd	0.63805000	-0.22899600	-0.35557200
C	-0.51003200	3.78967100	-0.16900800	C	2.59092400	1.55662900	1.08785300
C	-0.02785800	2.56091800	-0.59042300	O	3.54332400	2.34710100	1.15134900
N	-0.56021300	1.38727900	-0.17926500	O	2.28852000	0.97235900	-0.04164900
H	-1.94991400	4.67990500	1.17270200	C	1.72394500	1.27011300	2.29664300
H	-2.95288100	2.54501200	1.82342900	H	0.84899600	1.92954600	2.26504500
H	0.83225000	2.48902300	-1.24222400	H	1.36547900	0.23861100	2.29896700
C	-2.42777000	0.03366800	0.94042000	H	2.27887300	1.47661400	3.21354500
C	-2.41231000	-0.13245200	2.47786000	C	1.31719700	-2.79532800	0.82277100
H	-2.89737600	0.71122600	2.97384000	C	2.19250100	-2.28030800	-0.14870400
H	-2.93106900	-1.03929700	2.78824100	C	3.41278200	-1.71987800	0.27866900
H	-1.37955800	-0.19424800	2.83386700	C	3.67874800	-1.70500800	1.64385200
C	-3.89494500	0.34682300	0.39373900	C	2.73247500	-2.22851200	2.52835700
C	-3.92555600	0.42878700	-1.14210800	N	1.56474200	-2.76393500	2.14422600
C	-5.05135700	-0.53636700	0.88927000	H	0.38996600	-3.27491300	0.52548900
H	-4.12934700	1.34573000	0.77217100	H	4.60479800	-1.27192500	2.00225900
C	-5.26556700	0.99098100	-1.63482700	H	2.92242500	-2.21131400	3.59976900
H	-3.77211900	-0.57388100	-1.56153500	C	4.37313800	-1.05874600	-0.70890500
H	-3.10336200	1.05258800	-1.51106900	O	5.42770000	-0.57225700	-0.21416100
C	-6.39249200	0.05722700	0.43039900	O	3.98621500	-0.97318000	-1.90462100
H	-4.96804600	-1.54573700	0.47718500	K	4.53094700	1.67899900	-1.36813900
H	-5.03519000	-0.62512800	1.98047400	H	1.97384200	-2.38299800	-1.20744300
C	-6.45000500	0.17931400	-1.09708100	6*			
H	-5.28247800	1.01052900	-2.73094900	C	1.59428000	1.41139800	-0.68227900
H	-5.35849900	2.03310800	-1.29833000	C	2.47086400	2.48396400	-0.93445400
H	-7.21553500	-0.57016100	0.79261800	C	2.17356900	3.76271000	-0.49341700
H	-6.52879700	1.04962800	0.88236500	C	0.98933900	4.00924100	0.21324100
H	-7.39708300	0.63576200	-1.40885200	C	0.14573600	2.92172900	0.38414300
H	-6.42401100	-0.82783400	-1.53629200	N	0.43929700	1.68200300	-0.05912700
C	-1.97150200	-1.28188700	0.27495300	H	2.86488700	4.57559800	-0.69649100

H	3.39117200	2.32298400	-1.47926200	N	-4.16298600	-2.84149300	-0.45796300
H	-0.81656100	3.02986500	0.87022000	H	-6.20203700	-2.59626000	-0.70341300
C	2.00834800	-0.00548600	-1.14447200	H	-6.10361600	-0.08044900	-0.73131700
C	2.10073600	0.06768800	-2.68889200	H	-2.12133000	-2.90964200	-0.21570000
H	2.81256100	0.83636300	-2.99556200	C	-3.77435000	1.41017200	-0.51668800
H	2.42638000	-0.87041400	-3.13587700	O	-2.50686300	1.77660700	-0.48461900
H	1.12126400	0.32150900	-3.10548200	O	-4.69510600	2.20870800	-0.64262600
C	3.44172000	-0.23928900	-0.47951400	H	-1.16670400	-1.36965600	2.36299100
C	3.35368100	-0.34422600	1.05337100	O	-1.37610500	0.77734900	2.05994700
C	4.30766400	-1.38375700	-1.02757000	O	-2.01212500	-0.10317100	2.75465000
H	4.00480100	0.66949900	-0.70630800				
C	4.74989100	-0.29133900	1.68650300	6'			
H	2.86926800	-1.29004700	1.32788100	C	1.61082800	1.25929600	-0.90492000
H	2.72786800	0.45888400	1.45888500	C	2.39393800	2.33136300	-1.37273800
C	5.71690700	-1.31081600	-0.41737400	C	2.06327900	3.64141500	-1.06820500
H	3.87249500	-2.35375800	-0.76890000	C	0.93800900	3.91850800	-0.28233300
H	4.37425500	-1.33571700	-2.11924900	C	0.17782100	2.82292200	0.09962100
C	5.66565500	-1.37919900	1.11358400	N	0.49731200	1.54742100	-0.21079800
H	4.67000200	-0.39354300	2.77522700	H	2.68452500	4.45286400	-1.43669300
H	5.19291800	0.69549800	1.49293400	H	3.27764500	2.14361400	-1.96746400
H	6.33156900	-2.12730400	-0.81425300	H	-0.75003500	2.95183800	0.64330700
H	6.19933100	-0.37276500	-0.72496600	C	2.14701400	-0.17483600	-1.14797500
H	6.67427200	-1.28928500	1.53429800	C	2.37272200	-0.32551000	-2.67220400
H	5.28329900	-2.36480200	1.41411800	H	3.08291300	0.41441100	-3.04329300
C	1.16345300	-1.23092900	-0.72542600	H	2.76582500	-1.30660900	-2.93564800
C	1.47963000	-2.46632800	-1.27575000	H	1.42397500	-0.18725100	-3.19943700
N	0.27948900	-1.18212700	0.32310400	C	3.52874900	-0.17349300	-0.33593200
C	1.05712800	-3.64417800	-0.64263600	C	3.29390100	-0.14140900	1.18432800
H	2.11036800	-2.53882200	-2.14771300	C	4.57684600	-1.24509600	-0.67479400
C	-0.06290200	-2.30916000	0.98680400	H	4.00140800	0.77452800	-0.60687400
C	0.34842200	-3.57635300	0.53662600	C	4.60053600	0.15052100	1.93395100
H	1.32988600	-4.60687700	-1.06285500	H	2.89702500	-1.11120100	1.51201300
H	0.04644400	-4.45466000	1.09374600	H	2.54033000	0.61049800	1.44329000
O	-0.82305800	-2.27208200	2.06751300	C	5.89730200	-0.92394000	0.04456400
C	0.63383500	5.37100900	0.73806600	H	4.24387900	-2.23260800	-0.34203500
H	-0.35892600	5.37232100	1.19513000	H	4.74280700	-1.30107300	-1.75561200
H	1.35829500	5.69785500	1.49237900	C	5.69844800	-0.85332800	1.56334300
H	0.64503600	6.11409400	-0.06643300	H	4.42121300	0.13845000	3.01554200
Pd	-1.17724200	0.30709100	-0.03134100	H	4.93636900	1.16553100	1.68024100
C	-5.25517600	-2.07332900	-0.58517000	H	6.64630400	-1.68439500	-0.20582800
C	-5.21040500	-0.68114600	-0.59159300	H	6.28744700	0.03690400	-0.31868300
C	-3.96768000	-0.07218800	-0.43145500	H	6.63960100	-0.58875800	2.05996500
C	-2.82095300	-0.85264200	-0.24610400	H	5.41453400	-1.84881400	1.93273200
C	-2.97083000	-2.23998500	-0.29344100	C	1.36498600	-1.40224800	-0.63451200

C	1.88036400	-2.67125500	-0.89572400	H	-1.41876600	0.72107100	2.94855100
N	0.30229400	-1.30217200	0.21100100	C	-3.55972800	-0.13752100	0.25895300
C	1.44478400	-3.77538000	-0.15793000	C	-3.37639900	-0.48495700	-1.22858400
H	2.65712300	-2.80843700	-1.63050000	C	-4.49554800	-1.16532600	0.91335600
C	-0.06947500	-2.34821600	0.97547900	H	-4.09677500	0.81499100	0.30688700
C	0.50600900	-3.61301300	0.84454400	C	-4.72531900	-0.49693600	-1.95893200
H	1.87237900	-4.75372100	-0.35153100	H	-2.91194700	-1.47479800	-1.31581500
H	0.17204700	-4.42460700	1.47870600	H	-2.69518200	0.22348700	-1.71211500
O	-1.04548200	-2.17481400	1.87536200	C	-5.85810600	-1.16487000	0.20158000
C	0.55365900	5.31716300	0.10879200	H	-4.06591000	-2.16954200	0.84082100
H	-0.40438600	5.33203900	0.63485900	H	-4.63550900	-0.94779600	1.97680100
H	1.31070100	5.75903000	0.76662100	C	-5.71020400	-1.46564500	-1.29433500
H	0.47387800	5.96179100	-0.77294100	H	-4.57719200	-0.76461000	-3.01179300
Pd	-1.11063600	0.17605700	-0.13274500	H	-5.14820900	0.51736200	-1.94635300
C	-5.13663000	-2.23606500	-0.91646600	H	-6.51878800	-1.90118700	0.67431100
C	-5.12489200	-0.84916600	-0.78503000	H	-6.33535400	-0.18347000	0.33064700
C	-3.90224300	-0.22774000	-0.54034600	H	-6.68659700	-1.41855300	-1.79129300
C	-2.73142600	-0.98981100	-0.40212700	H	-5.34094700	-2.49339600	-1.41825100
C	-2.85945400	-2.37218600	-0.58777000	C	-1.36210000	-1.16578700	0.87491600
N	-4.02829400	-2.98939100	-0.83812100	C	-1.73943000	-2.22690200	1.68374800
H	-6.06801600	-2.76560600	-1.10863600	N	-0.47822400	-1.39874300	-0.14941500
H	-6.03019200	-0.25835400	-0.88511700	C	-1.34942500	-3.53614000	1.35818800
H	-1.99257300	-3.02713200	-0.54672400	H	-2.39732300	-2.07505200	2.52464700
C	-3.74756200	1.26398800	-0.48065400	C	-0.19962200	-2.66681200	-0.55427200
O	-2.49602300	1.65496000	-0.39809200	C	-0.64150600	-3.77303900	0.20448900
O	-4.70111000	2.03689900	-0.53759600	H	-1.65546100	-4.36082000	1.99421600
H	-1.45625800	-1.30049100	1.71086800	H	-0.36921900	-4.76783800	-0.12664500
O	-2.23064500	1.26289500	3.37290200	O	0.50133400	-2.91564800	-1.63082200
O	-3.39742400	1.30418700	3.04127500	C	-0.56602100	4.99226700	-1.89584200
				H	0.38523500	4.83409600	-2.41028600
6^s_AcOH				H	-1.32577300	5.23650600	-2.64653800
C	-1.65647700	1.43756800	0.29682700	H	-0.46381100	5.86425700	-1.24099800
C	-2.45672900	2.59286500	0.37763400	Pd	1.02846200	0.06745200	-0.29731900
C	-2.11687300	3.74582500	-0.30962000	C	5.06780800	-2.38371000	0.18795700
C	-0.96709200	3.77771200	-1.10856200	C	5.07054700	-1.04738300	-0.20098900
C	-0.20272600	2.62087400	-1.11957600	C	3.84053100	-0.39664700	-0.29506200
N	-0.53322400	1.50744700	-0.43140000	C	2.65967700	-1.09747800	-0.03596300
H	-2.75118800	4.62427000	-0.23231300	C	2.76770900	-2.41800200	0.39986400
H	-3.35982800	2.59014500	0.97193200	N	3.94837300	-3.05172100	0.50531800
H	0.72445000	2.56864500	-1.67732900	H	6.00070700	-2.93683300	0.27168400
C	-2.16273900	0.15224100	0.98801000	H	5.99244100	-0.51294800	-0.40665100
C	-2.38005600	0.50770600	2.47921900	H	1.89865700	-2.99678100	0.69154900
H	-3.01988500	1.38460700	2.58252700	C	3.73451700	1.06523000	-0.57283300
H	-2.85922800	-0.29576700	3.03502000	O	2.48548900	1.53045700	-0.46180100

O	4.68085000	1.79175500	-0.82473700	H	-5.70868400	-2.41940600	-1.21134300
H	0.90997200	-2.11342700	-2.20031000	C	-1.46614300	-1.35513500	0.80693800
O	0.94827400	-0.06560800	-2.36496400	C	-2.00131900	-2.44865700	1.48562400
O	1.60407400	-1.10252100	-2.86113300	N	-0.45858500	-1.58438600	-0.08125100
C	1.29282500	1.58905600	2.54873800	C	-1.65641700	-3.74962300	1.10689700
O	1.00479100	0.48256700	2.07483200	H	-2.72562300	-2.30441600	2.27142100
O	1.90478100	2.54121500	1.87199200	C	-0.17435500	-2.83275800	-0.49768800
H	2.14070000	2.22066400	0.94902700	C	-0.78800900	-3.96015100	0.05047300
C	0.94628100	1.97332000	3.95591000	H	-2.10183700	-4.59465400	1.62157800
H	1.78836200	2.48355800	4.42978900	H	-0.52995900	-4.94636500	-0.31443800
H	0.10322400	2.67292900	3.92814000	O	0.75477600	-2.99444800	-1.44838100
H	0.66190400	1.09174200	4.52945600	C	-0.44952900	4.65987600	-2.17617800
				H	0.38205600	4.39075900	-2.83256700
				H	-1.27671800	5.02073100	-2.79661700
6^t_AcOH				H	-0.12817000	5.49520300	-1.54374900
C	-1.61030500	1.24714600	0.19303600	H	-0.12817000	5.49520300	-1.54374900
C	-2.32468900	2.45426600	0.29742800	Pd	1.02831900	-0.15578300	-0.21314300
C	-1.96278900	3.56273100	-0.45155500	C	4.96063300	-2.44268000	1.19544600
C	-0.87792700	3.49293700	-1.33332700	C	5.00497200	-1.13608900	0.71670900
C	-0.18228000	2.29299000	-1.34714600	C	3.80647600	-0.54706300	0.31647900
N	-0.52608700	1.22276700	-0.59976700	C	2.60192100	-1.26705400	0.37335800
H	-2.52886700	4.48485700	-0.35502600	C	2.67542400	-2.55824900	0.91248200
H	-3.17583500	2.52850100	0.96028500	N	3.81979900	-3.14021900	1.31214400
H	0.71299400	2.17731300	-1.94678500	H	5.87067100	-2.94616300	1.51579200
C	-2.17539400	0.00993600	0.93358100	H	5.93395500	-0.57668100	0.66928400
C	-2.30065300	0.38782600	2.42976100	H	1.78266700	-3.16211100	1.04910500
H	-2.99310000	1.22093800	2.56462000	C	3.73040700	0.88783700	-0.09968400
H	-2.67537900	-0.44048700	3.03043700	O	2.49385400	1.29088100	-0.36133500
H	-1.32108000	0.68345200	2.81408200	O	4.70110700	1.63182000	-0.15594600
C	-3.61073900	-0.18789600	0.24962200	H	1.18791200	-2.12802000	-1.59336000
C	-3.48870500	-0.67029000	-1.20589500	O	2.07069600	-0.55406200	-3.79363900
C	-4.65894100	-1.03413600	0.98888100	O	3.26291800	-0.37574200	-3.65207800
H	-4.03634700	0.81897300	0.21934900	C	0.88998500	2.73702300	2.17075100
C	-4.83920600	-0.57801200	-1.92882000	O	0.93341700	1.55311200	2.47623800
H	-3.14124400	-1.71171500	-1.21508600	O	1.54266900	3.25624200	1.13068900
H	-2.73718300	-0.08325900	-1.74527400	H	1.96899700	2.52192600	0.59878600
C	-6.01992300	-0.89905600	0.28727300	C	0.08429300	3.76944200	2.91506100
H	-4.37963200	-2.09160100	0.98102700	H	0.69729800	4.64822600	3.13430400
H	-4.74399900	-0.72386200	2.03534200	H	-0.74760800	4.09668700	2.28305000
C	-5.93463500	-1.34431500	-1.17779900	H	-0.30802000	3.34579900	3.83963100
H	-4.74161700	-0.95680300	-2.95308900				
H	-5.12700500	0.47960300	-2.00881800	6^t_Pyr			
H	-6.77003900	-1.49354600	0.82205600	C	-1.70169900	-1.16703300	1.49665500
H	-6.35303600	0.14701900	0.33333400	C	-2.22800100	-1.80796500	2.63545500
H	-6.90252900	-1.20953000	-1.67527800	C	-2.51006800	-1.10315900	3.79181500

C	-2.26536000	0.27365400	3.84247300	C	1.74090600	4.94371600	-0.84710400
C	-1.71829900	0.83899900	2.69985600	C	1.04719700	3.91925300	-0.20228400
N	-1.43751900	0.14904500	1.56977300	C	0.44387300	2.92137200	-0.97204900
H	-2.92024700	-1.61973300	4.65512100	C	0.57699600	2.97790600	-2.35835900
H	-2.42185900	-2.87170000	2.61444200	N	1.24947100	3.96084900	-2.98638900
H	-1.46279900	1.89096800	2.68019100	H	2.34572100	5.70189600	-2.77557900
C	-1.42985700	-2.04893700	0.25711400	H	2.21423200	5.72571600	-0.26207000
C	-0.31197800	-3.03294200	0.68884700	H	0.13902800	2.22260900	-3.00020200
H	-0.57551100	-3.51956900	1.62925900	C	0.95989300	3.85218000	1.30207100
H	-0.14888600	-3.82324200	-0.04363100	O	0.33856800	2.80758800	1.76508600
H	0.63075000	-2.49861200	0.83487500	O	1.46029300	4.73050000	2.00866500
C	-2.77262500	-2.85536600	-0.03972200	H	-2.53018900	1.87511300	-2.01510100
C	-4.00073200	-1.94554800	-0.21920300	O	-2.19759000	2.75369400	0.24860200
C	-2.69827700	-3.84587300	-1.21465900	O	-3.06001900	2.73139400	-0.72433600
H	-2.94588700	-3.46708700	0.85212000	C	1.93642300	0.02720600	-1.02085700
C	-5.29203300	-2.77004100	-0.30445000	C	3.09295400	-0.74017300	-1.00304300
H	-3.88402300	-1.35458700	-1.13486500	C	3.64233700	-1.12372800	0.22219200
H	-4.07528000	-1.23042000	0.60644300	C	3.00143700	-0.70902500	1.39275900
C	-3.97842900	-4.69137200	-1.28739500	C	1.84805100	0.05778700	1.30332000
H	-2.58336200	-3.30051500	-2.15774800	N	1.32602500	0.40712600	0.11382000
H	-1.82802700	-4.50263100	-1.11930100	H	1.47482300	0.34500300	-1.94653000
C	-5.22290400	-3.80802700	-1.43010900	H	3.56807300	-1.04309000	-1.92795100
H	-6.14979200	-2.10301500	-0.45193300	H	3.40592200	-0.98761500	2.35806300
H	-5.45335600	-3.28437100	0.65342700	H	1.31995900	0.40781700	2.18149900
H	-3.91022800	-5.39252700	-2.12773300	C	4.90856400	-1.97134200	0.28276600
H	-4.06547200	-5.29865800	-0.37559100	O	5.33100300	-2.27287100	1.43415500
H	-6.13045100	-4.42364500	-1.44026100	O	5.42420200	-2.29702700	-0.82314600
H	-5.18235300	-3.28658000	-2.39683100	K	7.38756200	-3.53012400	0.40253700
C	-1.05719000	-1.35761400	-1.05693200				
C	-0.29930000	-2.02885800	-2.01645000	6^s_Pyr			
N	-1.63051400	-0.16423500	-1.34777000	C	-1.28559300	-1.36562800	1.38015000
C	-0.20514400	-1.50223800	-3.30996100	C	-1.38331900	-2.21506400	2.49805100
H	0.18811800	-2.96524200	-1.79154400	C	-1.66639300	-1.70520600	3.75467600
C	-1.55665500	0.32113800	-2.59748300	C	-1.88085900	-0.33161400	3.92779400
C	-0.85848000	-0.32562100	-3.62943400	C	-1.72829200	0.45569200	2.79554500
H	0.37352800	-2.02679000	-4.06410300	N	-1.42104800	-0.04879000	1.58408500
H	-0.83393400	0.10817900	-4.62205700	H	-1.73334300	-2.37782300	4.60517700
O	-2.16500600	1.47910400	-2.86104000	H	-1.24693000	-3.28212200	2.38518400
C	-2.56290100	1.10129000	5.06088800	H	-1.83195200	1.53313300	2.83406000
H	-2.25711000	2.14100500	4.91780300	C	-1.11846700	-2.00779300	-0.01368600
H	-3.63482900	1.08879000	5.28815300	C	0.11648200	-2.93982900	0.06710100
H	-2.04083700	0.70660600	5.93935700	H	-0.05226500	-3.74931500	0.77939600
Pd	-0.49207800	1.52185700	0.12150400	H	0.34937600	-3.40493800	-0.88849500
C	1.81169100	4.92107800	-2.23755500	H	0.99552800	-2.38058100	0.39289900

C	-2.46178900	-2.86168500	-0.18138600	H	-3.18490700	2.11211200	-1.00687600
C	-3.70170800	-1.96727200	-0.34643600	O	-2.24875400	2.62394500	0.51421200
C	-2.47044300	-3.95837000	-1.25780900	O	-3.42408500	2.08236600	-0.02427600
H	-2.57166400	-3.39167500	0.77037700	C	1.80924500	0.06966100	-1.06199800
C	-4.99152000	-2.79189800	-0.24473900	C	3.02945200	-0.58869400	-1.11526600
H	-3.66351700	-1.47311800	-1.32527500	C	3.67667600	-0.93220200	0.07379800
H	-3.70651200	-1.17053900	0.40441400	C	3.06375100	-0.59348700	1.28265600
C	-3.74635800	-4.80614400	-1.13413900	C	1.84105100	0.06376000	1.26581200
H	-2.44790500	-3.51068600	-2.25599700	N	1.22964000	0.37813800	0.11055800
H	-1.58835000	-4.60068500	-1.16915900	H	1.27538500	0.35531100	-1.95889400
C	-5.00500600	-3.93989900	-1.26059000	H	3.48119200	-0.83517700	-2.06818800
H	-5.86236500	-2.14198400	-0.39150200	H	3.54147500	-0.84553300	2.22139500
H	-5.07279900	-3.20470800	0.77054200	H	1.32929400	0.34865200	2.17657500
H	-3.74416300	-5.58852600	-1.90231000	C	5.01587600	-1.66214800	0.05291400
H	-3.75164300	-5.31748500	-0.16144600	O	5.52808400	-1.93261300	1.17485100
H	-5.90544600	-4.55254400	-1.13227100	O	5.49321600	-1.93194000	-1.08444200
H	-5.04943000	-3.52039300	-2.27550800	K	7.61219500	-3.02206500	0.01316800
C	-1.03169900	-1.10865300	-1.27238700				
C	-0.74217500	-1.72074400	-2.48001800	5_Pyr			
N	-1.43030600	0.20228200	-1.27719300	C	1.98815700	1.20377300	-0.53855900
C	-0.96590900	-1.03543500	-3.69258700	C	2.63306600	2.21957700	-1.27070500
H	-0.40297100	-2.74351800	-2.51546800	C	2.51670000	3.54870600	-0.89926100
C	-1.85786400	0.83894100	-2.43828800	C	1.77862300	3.90018300	0.24148800
C	-1.55966000	0.19766300	-3.68589700	C	1.14514400	2.85589700	0.90087900
H	-0.70927100	-1.51822600	-4.63146100	N	1.22348100	1.56477800	0.50322500
H	-1.80619700	0.73513500	-4.59478100	H	3.01065500	4.31789000	-1.48618200
O	-2.43945500	1.95818700	-2.38400500	H	3.23452900	1.97144800	-2.13421400
C	-2.23330500	0.26645800	5.26014100	H	0.50469600	3.04542600	1.75441500
H	-2.29962300	1.35576200	5.19936000	C	2.29340800	-0.26235700	-0.92262300
H	-3.19656000	-0.11539000	5.61658800	C	2.07152600	-0.38617700	-2.45267100
H	-1.48248600	0.00824000	6.01470600	H	2.82668600	0.17749200	-3.00343000
Pd	-0.65654400	1.43363800	0.22925000	H	2.13736700	-1.41756900	-2.79624100
C	1.54359300	5.00781300	-1.98638500	H	1.08333100	0.00863100	-2.70041900
C	1.44037100	4.95944300	-0.59957200	C	3.84466100	-0.40545500	-0.54869900
C	0.77551900	3.87060400	-0.03552500	C	4.08210700	-0.38907400	0.97153500
C	0.22730700	2.89392600	-0.86445100	C	4.62774300	-1.56590200	-1.18223400
C	0.40519300	3.01280700	-2.24039700	H	4.30085200	0.50245300	-0.95684400
N	1.05327200	4.05358100	-2.79256600	C	5.57665000	-0.25212900	1.29142000
H	2.05157200	5.83703000	-2.47404200	H	3.70193700	-1.32190100	1.40879800
H	1.87017600	5.72716300	0.03573400	H	3.52463400	0.42856400	1.44125400
H	0.04383500	2.26279500	-2.93195900	C	6.12847200	-1.39837600	-0.89595600
C	0.68223600	3.66217800	1.44295700	H	4.30768500	-2.52245100	-0.75872000
O	0.11865300	2.51973600	1.78202600	H	4.45419500	-1.61050600	-2.26212700
O	1.11515500	4.45806900	2.26752300	C	6.40163300	-1.35149800	0.61217100

H	5.72908700	-0.27557900	2.37691100	C	-2.16733400	0.65732300	-2.17290400
H	5.92625800	0.73018400	0.94431700	O	-3.17054800	1.42098800	-2.13422900
H	6.68537200	-2.22189200	-1.35821600	O	-0.95474500	1.02205300	-2.23205800
H	6.48842700	-0.47081500	-1.36229100	K	-1.65609500	3.37902500	-1.17206800
H	7.47050200	-1.19851700	0.80308900				
H	6.13655300	-2.32309000	1.05223900	8-ts			
C	1.57834500	-1.42181200	-0.19423200	O	1.37111900	-1.80178200	-2.51833900
C	1.85540100	-2.72716400	-0.59865900	H	0.68101500	-1.32831000	-1.22122100
N	0.83610800	-1.24654500	0.93537100	O	-0.87742800	-0.18308300	-0.08598300
C	1.53308400	-3.80749800	0.22722500	O	0.64666200	-1.03087000	-0.24638700
H	2.36145800	-2.91537300	-1.53172500	H	-0.97842900	0.12509000	-1.05659600
C	0.60917400	-2.27298400	1.77755600	C	-2.89325800	3.17223500	1.66058000
C	0.96242500	-3.58686700	1.46794100	C	-2.23972800	4.20217000	2.34212100
H	1.76811500	-4.81731600	-0.09262800	C	-1.15101300	3.91181000	3.15934100
H	0.74611100	-4.38350500	2.16860900	C	-0.69726700	2.59836500	3.29935900
O	0.00130200	-2.02237100	2.94415300	C	-1.37796600	1.63041300	2.56681900
C	1.64764700	5.32284900	0.71011900	N	-2.42025300	1.91735300	1.77620000
H	0.94529000	5.40171000	1.54406000	H	-0.64304000	4.71806400	3.68147800
H	2.61605000	5.71384300	1.04168300	H	-2.56377900	5.22805000	2.23321600
H	1.29766700	5.97010400	-0.10135800	H	-1.07888900	0.58976200	2.57841500
Pd	-0.44581300	0.37242500	1.04062600	C	-4.06968400	3.38011300	0.67869400
C	-4.81067900	-1.49671300	1.49966000	C	-3.40504800	3.23364700	-0.71679800
C	-4.60063500	-0.12152100	1.46298500	C	-3.26341300	4.30507600	-1.58283100
C	-3.28747100	0.33566800	1.36292800	N	-2.88657500	2.01067100	-1.04399500
C	-2.21589000	-0.57156800	1.30133400	C	-2.64993300	4.10683300	-2.83487600
C	-2.55435700	-1.93175800	1.30948400	H	-3.63145000	5.28456800	-1.32131800
N	-3.81303900	-2.39097300	1.41454600	C	-2.12959600	1.82369800	-2.19428200
H	-5.81727600	-1.90116000	1.58493600	C	-2.11865300	2.88525300	-3.15511300
H	-5.42635100	0.58225600	1.49791100	H	-2.58534900	4.93480500	-3.53594800
H	-1.79576500	-2.70084400	1.20626700	H	-1.60441900	2.70200900	-4.09072700
C	-2.95598000	1.78669200	1.22690300	O	-1.46854900	0.75998500	-2.37770800
O	-1.66456500	2.02117300	1.11500000	Pd	-2.94915600	0.41958600	0.30749500
O	-3.79575500	2.68575300	1.18216000	C	-4.08647600	-3.26658400	-2.41385700
H	-0.30197000	-1.08965500	2.93664800	C	-3.63968300	-3.43641600	-1.10606000
C	-1.70745600	-3.12643900	-1.97751900	C	-3.34219600	-2.29338100	-0.36369000
C	-1.40256100	-1.77232700	-2.08736800	C	-3.47818800	-1.03418600	-0.95392000
C	-2.44193900	-0.83933300	-2.10726500	C	-3.94965200	-0.96925200	-2.26504400
C	-3.74847300	-1.32485700	-2.02377800	N	-4.25569300	-2.06216600	-2.98621600
C	-3.95441600	-2.69926500	-1.91976500	H	-4.33802500	-4.12947900	-3.02675900
N	-2.96075700	-3.60160500	-1.89339700	H	-3.55385900	-4.42122200	-0.65954200
H	-0.90757800	-3.86435000	-1.94857200	H	-4.09270600	-0.01362200	-2.76120600
H	-0.37626100	-1.44098800	-2.14375600	C	-2.94305100	-2.32537100	1.08401300
H	-4.58013000	-0.63040900	-2.02557100	O	-2.89766500	-1.14466200	1.64804100
H	-4.96565500	-3.09504200	-1.84535900	O	-2.70779700	-3.37667300	1.68439100

C	-6.80618500	-0.78211600	0.00321800	O	1.69130000	1.45066000	0.79385700
C	-7.04413300	-1.95919500	-0.70281100	O	0.60545300	3.37614300	0.46634400
C	-6.74463800	-3.18099200	-0.09681300	C	5.14659800	0.58091100	-1.40607200
C	-6.25365900	-3.16083600	1.21056600	C	6.31693900	1.29348600	-1.61761300
C	-6.05544600	-1.93397800	1.83782800	C	6.61968900	2.37951000	-0.79302000
N	-6.31272200	-0.75603600	1.25002700	C	5.71988300	2.70996100	0.22281500
H	-6.98965300	0.18469400	-0.46089800	C	4.56404000	1.96021300	0.38428000
H	-7.41309900	-1.94100200	-1.72137600	N	4.29882200	0.91335000	-0.41668400
H	-5.99693400	-4.09142400	1.70182300	H	4.87282100	-0.27076100	-2.01498500
H	-5.63800600	-1.89073200	2.84060700	H	6.99371100	1.01310500	-2.41518300
C	-6.86188500	-4.48473200	-0.86972600	H	5.92624400	3.54666700	0.87868200
O	-6.47772800	-5.53617600	-0.27993600	H	3.83491500	2.17288500	1.15551700
O	-7.31534200	-4.41236900	-2.04875900	C	7.90023200	3.18353500	-0.99675100
K	-6.74331300	-6.91081400	-2.48204000	O	8.08920600	4.14970000	-0.20686200
C	3.24951100	-2.52561800	1.71781000	O	8.65522400	2.80989800	-1.93673000
C	2.66660900	-3.64656600	2.31333700	K	10.35358500	4.74019500	-1.40045900
C	1.48364300	-3.50903300	3.03328200	C	-5.17537700	2.31871900	0.87460100
C	0.87187700	-2.25714400	3.16162100	H	-5.88637100	2.36376100	0.04816500
C	1.45875500	-1.21228200	2.45037200	H	-4.82476300	1.28691400	0.93165000
N	2.59212200	-1.35222700	1.74211400	H	-5.71101000	2.49745800	1.80867400
H	1.03763700	-4.37963100	3.50626400	C	-4.74221600	4.78010300	0.87522400
H	3.13542700	-4.61802300	2.22721500	C	-5.93129400	5.04608000	-0.07729800
H	0.99642000	-0.23398200	2.40093300	C	-5.26351700	5.04403300	2.30790400
C	4.59280600	-2.55382100	0.96346200	H	-3.98072300	5.54194500	0.67042400
C	4.17366200	-2.72611800	-0.53192400	C	-6.37135700	6.51307800	0.01312300
C	4.66230400	-3.77395900	-1.29107800	H	-6.77313800	4.40772900	0.21579200
N	3.17886500	-1.93256300	-1.07336900	H	-5.69167900	4.78744600	-1.11041000
C	4.15782300	-4.02658200	-2.58254100	C	-5.69005600	6.51170000	2.45524200
H	5.41234200	-4.43780000	-0.89821300	H	-6.13192700	4.40405000	2.50335100
C	2.48477900	-2.32037000	-2.21930600	H	-4.52099500	4.79682400	3.06893800
C	3.08615900	-3.31875400	-3.04792700	C	-6.78109400	6.88433800	1.44363700
H	4.59512800	-4.82285800	-3.17818000	H	-7.20246500	6.69793800	-0.67800100
H	2.60722200	-3.52880900	-3.99737000	H	-5.54238500	7.15825600	-0.31045100
Pd	2.47064600	-0.14996400	-0.19699100	H	-6.04328100	6.69636400	3.47680400
C	1.39572600	2.79290900	-3.73041600	H	-4.81294900	7.15632200	2.30310000
C	1.03690700	3.07619200	-2.41720200	H	-7.01581200	7.95365000	1.50990000
C	1.37456100	2.14245900	-1.43771000	H	-7.70203900	6.34237600	1.70045100
C	2.03420200	0.98549900	-1.82285700	C	0.52025700	2.24196300	4.10338300
C	2.38585200	0.78397000	-3.15001700	H	0.48863300	1.20158600	4.43854600
N	2.06152700	1.68464100	-4.09226800	H	1.41538500	2.36094900	3.48191300
H	1.15318300	3.48928100	-4.52967300	H	0.62617600	2.88783200	4.97986000
H	0.52318700	3.99054500	-2.14362100	C	5.38500300	-1.26175300	1.27274400
H	2.93958000	-0.08615300	-3.47841400	H	5.89046200	-1.37217600	2.23328100
C	1.15573000	2.38052300	0.02044100	H	6.13910400	-1.06958300	0.50966300

H	4.74113400	-0.39922300	1.35824300	H	-3.82218500	-0.87373200	0.50099400
C	5.50177100	-3.74482900	1.44530100	C	-4.26111000	-4.44664500	-1.12045600
C	6.94369100	-3.69306700	0.87648800	H	-2.95926800	-3.21208900	-2.30443100
C	5.66319600	-3.86254100	2.98175000	H	-2.10180000	-4.39986000	-1.32291900
H	5.03757700	-4.67785700	1.10671000	C	-5.45522300	-3.48508200	-1.12568400
C	7.68615500	-5.00207600	1.17428600	H	-6.10011500	-1.65371600	-0.14967800
H	7.48204600	-2.86900600	1.35807800	H	-5.31226000	-2.80836000	0.92165800
H	6.96395000	-3.48119700	-0.19406100	H	-4.37787500	-5.20274400	-1.90611900
C	6.38310700	-5.17135400	3.33882200	H	-4.23133700	-4.98691100	-0.16389500
H	6.25595900	-3.01898900	3.35572600	H	-6.38787700	-4.03198700	-0.94183700
H	4.70860300	-3.82345300	3.50678600	H	-5.54478900	-3.03278600	-2.12340600
C	7.76590700	-5.25873300	2.68405000	C	-1.26185500	-0.95458800	-1.36265300
H	8.69347600	-4.96597100	0.74262400	C	-1.11405500	-1.55027200	-2.60452000
H	7.16204800	-5.83520300	0.68533800	N	-1.54135200	0.39050600	-1.31099500
H	6.47497100	-5.25643200	4.42817200	C	-1.35838300	-0.81787600	-3.78475800
H	5.76644000	-6.01859800	3.00776300	H	-0.88158900	-2.59905100	-2.69034900
H	8.22370100	-6.23485500	2.88480000	C	-1.99619300	1.08249500	-2.42854700
H	8.42192200	-4.50233300	3.13699900	C	-1.83841300	0.46010800	-3.70923800
C	-0.39415700	-2.06183500	3.94804100	H	-1.20992600	-1.29659600	-4.74869700
H	-1.25859900	-2.42376400	3.37820600	H	-2.09917200	1.04406100	-4.58469500
H	-0.35264800	-2.61333700	4.89303300	O	-2.49609500	2.23904200	-2.31541000
H	-0.55932700	-1.00526000	4.17320800	C	-1.83793900	0.16229600	5.31413100
				H	-2.02802100	1.23859900	5.29068900
				H	-2.67898400	-0.32249900	5.82235600
				H	-0.94528400	-0.01478600	5.92422400
13-ts'				Pd	-0.59961200	1.53953400	0.16384400
C	-1.35427400	-1.32180700	1.29900800	C	1.93062000	5.04003000	-1.79403300
C	-1.23011900	-2.20373200	2.38898700	C	1.90031500	4.82932300	-0.41852200
C	-1.37194900	-1.73839200	3.68764300	C	0.97069100	3.92860800	0.09763600
C	-1.65740800	-0.38799300	3.92745000	C	0.08775600	3.29237800	-0.78328300
C	-1.74723900	0.42273300	2.80216700	C	0.18808900	3.55596900	-2.15657800
N	-1.59445200	-0.02797000	1.54320200	N	1.10253900	4.40746200	-2.64167400
H	-1.26822600	-2.42820600	4.52084400	H	2.64404800	5.73064900	-2.23678800
H	-1.03554700	-3.25534400	2.22851400	H	2.59353500	5.32448700	0.25418400
H	-1.92551500	1.48857400	2.90283400	H	-0.48519400	3.09720600	-2.86851800
C	-1.33969000	-1.90116400	-0.13129300	C	0.93887200	3.54548200	1.53857600
C	-0.19179000	-2.94144400	-0.19387900	O	0.23953200	2.45739900	1.78152500
H	-0.41184600	-3.80620000	0.43361300	O	1.52608400	4.17055300	2.41558700
H	-0.02584300	-3.32158800	-1.19844700	O	-1.70251900	3.23701300	-0.10515400
H	0.74382800	-2.50060400	0.15488800	C	1.69832000	0.02139300	-1.04662700
C	-2.75937600	-2.63677300	-0.21912800	C	2.87661700	-0.70796500	-1.11285700
C	-3.93484800	-1.64605400	-0.26630900	C	3.45548800	-1.18443600	0.06594700
C	-2.93712900	-3.69246700	-1.32132900	C	2.82194400	-0.89889800	1.27807100
H	-2.83171900	-3.18452900	0.72838900	C	1.64689500	-0.16014000	1.27677300
C	-5.27447600	-2.37265200	-0.08663800				
H	-3.92981200	-1.12850900	-1.23420300				

N	1.09833300	0.27694000	0.12999100	C	-5.23506100	3.50403900	-0.19472500
H	1.21278100	0.41234600	-1.93261900	N	-3.19481100	2.36321900	-0.54473200
H	3.34768300	-0.90873300	-2.06712500	C	-4.82814000	4.49973000	-1.08984900
H	3.24815000	-1.25423900	2.20809700	H	-6.20803900	3.57786200	0.26456400
H	1.12570800	0.09451300	2.19098000	C	-2.75535200	3.36468100	-1.33539600
C	4.74514300	-1.99833900	0.03050200	C	-3.55125700	4.47941300	-1.61929100
O	5.19168200	-2.39548700	1.14277400	H	-5.50520300	5.31253400	-1.33184000
O	5.25117800	-2.20338600	-1.10790900	H	-3.16897400	5.26092500	-2.26433000
K	7.24890000	-3.52176500	-0.03049400	O	-1.54272600	3.29483100	-1.88531800
H	-2.16192400	2.95792700	-0.96233000	C	-1.17734400	-2.70949100	3.26282500
				H	-0.30777500	-2.82598800	2.61631000
10				H	-0.82374800	-2.49257700	4.27642100
C	-3.74005800	0.43565000	1.78761600	H	-1.71025900	-3.66572200	3.30315600
C	-4.09295800	-0.28995000	2.94100600	Pd	-2.42252800	0.48105100	-0.92546400
C	-3.28426200	-1.30518700	3.42177700	C	-2.74118700	0.19820100	-5.63959900
C	-2.08619200	-1.62034100	2.76918500	C	-1.91833300	-0.66795000	-4.92352100
C	-1.80323700	-0.88379800	1.62730800	C	-1.82552900	-0.49234900	-3.54327300
N	-2.60588600	0.09471300	1.15082700	C	-2.53444900	0.54383600	-2.91673100
H	-3.58090800	-1.85450100	4.31081400	C	-3.35043600	1.33786400	-3.73038800
H	-5.00200600	-0.05454500	3.47698800	N	-3.45491200	1.17817700	-5.06189000
H	-0.91729400	-1.08712500	1.03923000	H	-2.84275700	0.09822200	-6.71846400
C	-4.64769400	1.63809200	1.40867500	H	-1.37140600	-1.46842300	-5.41185900
C	-6.10208000	1.11269500	1.33207500	H	-3.95828000	2.13381500	-3.30734600
H	-6.42075000	0.66132600	2.27203500	C	-1.01272100	-1.40024700	-2.66897800
H	-6.81203800	1.90688100	1.10615900	O	-1.03043000	-1.05230300	-1.39231200
H	-6.17619500	0.35944800	0.54595400	O	-0.39129500	-2.36408200	-3.10639400
C	-4.43216900	2.63862900	2.63844800	H	-1.06331900	2.47958800	-1.60974100
C	-3.03167200	3.27438800	2.61077200	O	0.34605300	1.25620900	-1.12397600
C	-5.48724300	3.72835200	2.87973400	O	1.54436200	1.31569900	-1.88422200
H	-4.47695200	1.99751900	3.52428200	C	-5.48326400	-1.24239700	-1.81217500
C	-2.72965900	3.98462000	3.93533600	C	-6.77869400	-1.48491100	-1.36065900
H	-2.98062700	4.00276100	1.79096900	C	-6.96018600	-2.19214500	-0.16865300
H	-2.26864600	2.51774600	2.40519100	C	-5.82068900	-2.63157800	0.51002700
C	-5.20879400	4.42537600	4.22197500	C	-4.56586800	-2.35211300	-0.02546500
H	-5.45188800	4.48143900	2.08661000	N	-4.38605000	-1.66449500	-1.16401800
H	-6.49616200	3.30335900	2.88319900	H	-5.30938100	-0.68054700	-2.72731400
C	-3.80099200	5.03390900	4.25881400	H	-7.64174500	-1.12691600	-1.90998600
H	-1.73854300	4.45167700	3.89396000	H	-5.92462700	-3.17590400	1.44132700
H	-2.69450000	3.23841100	4.74135700	H	-3.66308800	-2.67953700	0.48332400
H	-5.96226100	5.20251200	4.39657000	C	-8.35409800	-2.44864600	0.38750500
H	-5.31218800	3.69565000	5.03702600	O	-8.42347900	-3.05531700	1.49499800
H	-3.60827000	5.48782100	5.23824500	O	-9.32821600	-2.02923400	-0.30122600
H	-3.74243500	5.84338500	3.51773000	K	-11.03839200	-2.94224000	1.44773900
C	-4.36193300	2.47204600	0.14362300	C	2.50794000	-1.31598500	1.46530300

C	2.21467500	-1.55584800	2.81843400	Pd	3.13676400	0.72443200	-0.77026900
C	1.48806100	-0.64138900	3.56377800	C	5.59945400	3.31049000	-3.87945000
C	1.01171600	0.53163200	2.96866500	C	4.96805300	3.89769900	-2.78476000
C	1.37814400	0.73645100	1.64580500	C	4.27479700	3.05862200	-1.91470900
N	2.10804400	-0.14799400	0.93381100	C	4.22999300	1.69495400	-2.18288100
H	1.27377100	-0.84789800	4.60798000	C	4.90876100	1.18556900	-3.28227700
H	2.54011000	-2.47305400	3.28943000	N	5.58356000	1.99157300	-4.12026000
H	1.09684100	1.63940400	1.12253000	H	6.15238700	3.92192100	-4.58846700
C	3.20276300	-2.44392000	0.67291200	H	5.01746900	4.96530800	-2.59786100
C	4.45924300	-2.86310000	1.47682900	H	4.94311800	0.12554400	-3.50712800
H	4.17400100	-3.31886000	2.42571400	C	3.61836500	3.53650900	-0.66143100
H	5.06561100	-3.59395700	0.94536400	O	3.11037200	2.55984100	0.07720200
H	5.08535900	-1.99708100	1.69422900	O	3.56955700	4.70486400	-0.31134500
C	2.11171700	-3.62492100	0.67254400	H	1.83306800	0.24463300	-2.99231400
C	0.93376500	-3.29996800	-0.25166200	H	0.01385500	0.32252600	-1.23301300
C	2.61699200	-5.04921500	0.39903300	C	5.98630300	-0.25521300	-0.36974700
H	1.73675700	-3.64238800	1.70089400	C	7.19578700	-0.43821000	0.28276500
C	-0.20886000	-4.30884900	-0.09996400	C	7.35012200	0.02875600	1.58976100
H	1.26071700	-3.31054400	-1.29608600	C	6.26830900	0.67179200	2.19574400
H	0.55675100	-2.29087300	-0.07892900	C	5.08320300	0.82793700	1.49256900
C	1.47368700	-6.05604100	0.60886500	N	4.95410600	0.35996100	0.23724900
H	2.96161900	-5.14168400	-0.63527800	H	5.82920000	-0.60015100	-1.38248600
H	3.46037700	-5.30079000	1.04993600	H	8.01617900	-0.93898300	-0.21585900
C	0.28349500	-5.74543900	-0.30688500	H	6.35609300	1.04437700	3.20870200
H	-0.99641700	-4.05850400	-0.81821500	H	4.22372900	1.32648800	1.92036000
H	-0.64712600	-4.22217300	0.90241600	C	8.66491100	-0.16543300	2.34032400
H	1.84307500	-7.07195400	0.42539500	O	8.70750800	0.27945600	3.52038600
H	1.14588000	-6.02296200	1.65737200	O	9.58724100	-0.75583200	1.71352000
H	-0.52979300	-6.46001300	-0.13070600	K	11.18049800	-0.56622000	3.79828000
H	0.59590000	-5.87326000	-1.35304600				
C	3.56178700	-2.22999900	-0.81278200	11-ts			
C	4.26903200	-3.22778200	-1.46967500	C	-2.08651000	0.58948200	2.17278200
N	3.03443900	-1.21501500	-1.56929200	C	-2.14936000	0.38150900	3.56335000
C	4.28621300	-3.28441600	-2.87035500	C	-1.22554500	-0.42327900	4.20966700
H	4.75992000	-4.00853600	-0.91162700	C	-0.19647200	-1.03172600	3.48372500
C	2.93512200	-1.32628400	-2.91771300	C	-0.19081000	-0.79171800	2.11677000
C	3.55648400	-2.37684300	-3.60692300	N	-1.10571800	-0.02329600	1.48792000
H	4.83384200	-4.07823500	-3.36746300	H	-1.29760000	-0.57130900	5.28335800
H	3.47341500	-2.41798500	-4.68581800	H	-2.91988700	0.86066100	4.15069800
O	2.28186600	-0.40971600	-3.60965400	H	0.55164900	-1.25164800	1.47778600
C	0.14588900	1.51498300	3.70210800	C	-3.12514300	1.56236900	1.56009100
H	-0.85388600	1.09557500	3.86011700	C	-4.51539700	1.10654200	2.07507100
H	0.56293000	1.74958300	4.68645600	H	-4.60854500	1.26600900	3.14967600
H	0.03851500	2.44390700	3.13773100	H	-5.33159500	1.65244800	1.60763000

H	-4.66238500	0.04431600	1.87444800	O	0.72601400	-3.74957400	-1.87830500
C	-2.71877800	2.98442900	2.18141600	H	-0.18962200	1.45070900	-2.14369000
C	-1.43341400	3.54706700	1.55049700	O	0.80577500	0.61699000	-1.11870500
C	-3.80421800	4.07147400	2.19912900	O	2.16402500	1.40518000	-1.86428800
H	-2.49873100	2.77068300	3.23260000	C	-4.52486800	-1.21695000	-0.70197000
C	-0.93054200	4.77017700	2.32690800	C	-5.76140300	-1.71707200	-0.30511300
H	-1.63730200	3.84845200	0.51588900	C	-5.82957800	-2.55249300	0.81283400
H	-0.65581000	2.77803800	1.50358300	C	-4.64100200	-2.85046200	1.48543300
C	-3.31240700	5.29652700	2.98807300	C	-3.44695800	-2.30500200	1.02313600
H	-4.04102200	4.38965600	1.17886800	N	-3.38858800	-1.50069900	-0.04897700
H	-4.72900500	3.69137200	2.64459000	H	-4.43379600	-0.56149500	-1.56261900
C	-2.00984000	5.85573700	2.40423400	H	-6.66589300	-1.46668100	-0.84681700
H	-0.02246600	5.16361500	1.85421500	H	-4.66196000	-3.49510200	2.35617700
H	-0.65136000	4.46448000	3.34384200	H	-2.50577100	-2.50239200	1.52831500
H	-4.09140600	6.06800900	2.99015800	C	-7.16243100	-3.11775900	1.28929600
H	-3.14722700	5.01075100	4.03621400	O	-7.13094300	-3.86106400	2.31088100
H	-1.65717100	6.70364900	3.00351700	O	-8.18647500	-2.79555000	0.62248000
H	-2.20545400	6.24136700	1.39386000	K	-9.71550100	-4.26384200	2.15664000
C	-3.18164900	1.80723900	0.03798600	C	4.12229400	-0.22688900	1.66359400
C	-4.23257300	2.55909800	-0.47997100	C	4.07682200	-0.26222000	3.06428900
N	-2.12232300	1.52987300	-0.77368800	C	3.17519500	0.52724000	3.76469400
C	-4.11754400	3.15310600	-1.74312500	C	2.26905500	1.34227600	3.08155800
H	-5.11914600	2.74897000	0.10388900	C	2.37906800	1.35045900	1.69472300
C	-1.95148200	2.19169000	-1.93925700	N	3.28853100	0.61591300	1.02703600
C	-2.94415600	3.03354000	-2.45925100	H	3.16310800	0.49528000	4.84981300
H	-4.93653000	3.75017400	-2.13121400	H	4.73963700	-0.91561000	3.61484500
H	-2.77651000	3.53027800	-3.40700800	H	1.74270500	1.97678300	1.08250500
O	-0.83377700	2.02793500	-2.63516500	C	5.05104200	-1.22678900	0.94192000
C	0.83676400	-1.90822300	4.13204000	C	6.44752200	-1.13013800	1.60783100
H	1.68025200	-2.08524100	3.46313500	H	6.41829200	-1.53140900	2.62188200
H	1.21492000	-1.45142600	5.05141100	H	7.20416900	-1.69391800	1.06609000
H	0.40601600	-2.87950100	4.40274900	H	6.77846800	-0.09310300	1.66735400
Pd	-1.22389800	-0.36875100	-0.61746200	C	4.37610700	-2.64337400	1.27349800
C	-1.80059900	-2.15174800	-4.97880400	C	3.03889700	-2.83484000	0.54480100
C	-0.92595200	-2.74028600	-4.06987600	C	5.24269300	-3.90112600	1.10324400
C	-0.78727100	-2.14293300	-2.81701600	H	4.16101700	-2.58557300	2.34585400
C	-1.49545000	-0.97477300	-2.51558700	C	2.28681800	-4.05670800	1.08393400
C	-2.37247700	-0.48645900	-3.48800000	H	3.21813700	-2.97834500	-0.52770100
N	-2.52405900	-1.05650200	-4.69568700	H	2.41285900	-1.94292500	0.63046900
H	-1.94085500	-2.58058900	-5.96889400	C	4.50532900	-5.12092400	1.68020900
H	-0.37669500	-3.64552600	-4.30874100	H	5.43651600	-4.09273700	0.04351100
H	-2.99366000	0.38438500	-3.30361100	H	6.21182900	-3.78244200	1.59821600
C	0.04917600	-2.73602900	-1.72591300	C	3.14737700	-5.32192700	0.99791200
O	-0.03158400	-2.07671800	-0.58732900	H	1.36368300	-4.17650600	0.51272500

H	2.01231300	-3.87861500	2.13259500	C	9.64574300	2.76411600	1.66841300
H	5.12941600	-6.01495400	1.56383700	O	9.64222600	3.36074400	2.78048500
H	4.35443800	-4.97811900	2.75937700	O	10.65378400	2.40222300	1.00082400
H	2.62013300	-6.17464600	1.44305200	K	12.27281600	3.39712800	2.81196400
H	3.31255400	-5.57058700	-0.06006800				
C	5.18140700	-1.18024500	-0.59636100	12			
C	6.07278100	-2.05082200	-1.20733200	C	3.71354800	1.50756900	-1.89542300
N	4.32198400	-0.47697600	-1.39875700	C	3.91982900	1.50692600	-3.28675900
C	5.97621200	-2.31985300	-2.58075600	C	2.97165800	0.97829800	-4.14453300
H	6.81092200	-2.57741100	-0.62423200	C	1.77790500	0.44871400	-3.63922000
C	4.12558800	-0.81754000	-2.70320400	C	1.64857300	0.44235900	-2.25680900
C	4.96114400	-1.76211400	-3.32516500	N	2.59295600	0.93770200	-1.42747000
H	6.67668300	-3.00925300	-3.04086800	H	3.15140100	0.98562500	-5.21574700
H	4.80095500	-1.98909200	-4.37197300	H	4.81886300	1.93831700	-3.70405300
O	3.17184500	-0.24019400	-3.39403800	H	0.78083300	0.00771500	-1.77886100
C	1.24952600	2.19079300	3.78628400	C	4.73268500	2.26904700	-1.02197300
H	0.24858100	2.00898500	3.39105700	C	6.14135300	1.74681000	-1.39745600
H	1.24015700	1.97877800	4.85806400	H	6.38214700	1.97523200	-2.43634300
H	1.46925500	3.25491600	3.64994700	H	6.92439400	2.19371800	-0.78874200
Pd	3.88171200	1.49271300	-0.86206400	H	6.18947400	0.66341500	-1.26663600
C	5.21149300	4.18958700	-4.51575100	C	4.53159600	3.78519600	-1.49993000
C	4.51771700	4.72699300	-3.43306300	C	3.16437100	4.35254500	-1.08213200
C	4.16985800	3.86312000	-2.39663300	C	5.63685300	4.78828700	-1.14083900
C	4.51272900	2.51896200	-2.49359400	H	4.53720500	3.72772600	-2.59348200
C	5.22748500	2.06889400	-3.59622400	C	2.89239900	5.68848100	-1.78502100
N	5.56975500	2.89960500	-4.59619000	H	3.15179500	4.50608400	0.00422400
H	5.50356700	4.82243400	-5.35042300	H	2.36258100	3.64244000	-1.30703600
H	4.26219700	5.78027600	-3.38131700	C	5.38646800	6.11953800	-1.86736300
H	5.55469900	1.03959800	-3.69369800	H	5.64439300	4.97719700	-0.06294400
C	3.49395800	4.30992400	-1.14121700	H	6.62272700	4.39643900	-1.41095500
O	3.36255200	3.34971700	-0.24032100	C	4.01174700	6.70107900	-1.51321200
O	3.12194700	5.45499800	-0.93258800	H	1.92551500	6.09084200	-1.46019700
H	2.64924100	0.46137800	-2.79444100	H	2.81440500	5.51312500	-2.86714700
H	1.14679300	-0.29132900	-1.21725400	H	6.17827300	6.83316000	-1.61079300
C	6.92552200	1.47493800	-0.66917500	H	5.44532200	5.95799100	-2.95265500
C	8.17928700	1.76348800	-0.15165500	H	3.83329900	7.62696600	-2.07293300
C	8.28142200	2.44193700	1.06518800	H	4.00106000	6.96836600	-0.44721800
C	7.10318800	2.80931400	1.71996300	C	4.56927700	2.29475800	0.51330300
C	5.87806900	2.49808900	1.14852500	C	5.56336800	2.88296300	1.27339300
N	5.80285500	1.83535300	-0.01983900	N	3.38534200	1.98508100	1.12848500
H	6.80430800	0.94430500	-1.60431900	C	5.30165000	3.27051900	2.60597300
H	9.07411200	1.46457400	-0.68323300	H	6.51855500	3.13135100	0.83897300
H	7.14991200	3.33370700	2.66628000	C	3.01243200	2.52725600	2.35502200
H	4.94039000	2.77131400	1.61476700	C	4.04112600	3.15589300	3.12651800

H	6.09906300	3.71460600	3.19453100	H	-2.98708500	-0.01702000	-4.13001200
H	3.78130100	3.50065400	4.12079600	H	-1.20568800	2.08322600	-0.12176400
O	1.82297400	2.41752200	2.76735600	C	-3.31675400	-1.58748100	-1.95299400
C	0.71295800	-0.09498600	-4.54657600	C	-4.66877400	-1.51027600	-2.70631300
H	-0.10538500	-0.53907800	-3.98163800	H	-4.51399500	-1.28726400	-3.76305100
H	0.30054200	0.70053200	-5.17662300	H	-5.22300200	-2.44498500	-2.65802700
H	1.12946300	-0.85494200	-5.21589900	H	-5.29700100	-0.72364100	-2.28367600
Pd	2.43463400	0.22414300	0.61179600	C	-2.25596700	-2.47040900	-2.77005300
C	1.84613000	-2.21319500	4.64190100	C	-0.96459200	-2.68231600	-1.96853500
C	1.36815600	-2.69493400	3.42680400	C	-2.74904600	-3.81195800	-3.33275000
C	1.60409400	-1.92308900	2.28979800	H	-2.00866800	-1.86176900	-3.64653500
C	2.27363200	-0.71089500	2.41911400	C	0.12850600	-3.36302800	-2.79853300
C	2.75611700	-0.32383000	3.66418700	H	-1.17088700	-3.30675000	-1.09420600
N	2.53852800	-1.06981700	4.76057300	H	-0.59194200	-1.73438500	-1.57229100
H	1.68145200	-2.77250900	5.55985900	C	-1.66042000	-4.44783800	-4.21207400
H	0.82719000	-3.63046800	3.34630700	H	-2.97510200	-4.50652000	-2.51841800
H	3.33847300	0.57723900	3.80796100	H	-3.66784200	-3.67833100	-3.91315700
C	1.22086400	-2.36423900	0.91583700	C	-0.36989600	-4.67411800	-3.41580000
O	1.47558500	-1.45923400	-0.01751100	H	0.99573300	-3.53963700	-2.15451000
O	0.76013100	-3.46481100	0.65564800	H	0.45474900	-2.69267800	-3.60331700
H	0.97942200	1.76363700	1.69963100	H	-2.02831900	-5.39562200	-4.62303400
O	0.67058400	1.17647700	0.91435300	H	-1.45037000	-3.79192000	-5.06884200
O	-1.13679700	-0.04220200	1.97094900	H	0.40320700	-5.11574900	-4.05651600
C	5.23487100	-0.63501800	1.23345400	H	-0.56931500	-5.39911800	-2.61377400
C	6.43790900	-1.29532200	1.04044900	C	-3.50431500	-2.31034200	-0.59571600
C	6.59851500	-2.12536400	-0.07106300	C	-4.16686700	-3.52371000	-0.59603700
C	5.52608300	-2.26791100	-0.95472800	N	-2.85506700	-1.92651400	0.55035800
C	4.34370000	-1.58685500	-0.71147200	C	-4.04446800	-4.40042300	0.50545200
N	4.21967000	-0.78282000	0.36147000	H	-4.71467800	-3.85376400	-1.46401000
H	5.06720800	0.01991500	2.07704600	C	-2.54965000	-2.81867400	1.58216400
H	7.24981100	-1.16838700	1.74554900	C	-3.20960500	-4.09391000	1.54335200
H	5.62032800	-2.90554900	-1.82473500	H	-4.58181000	-5.34446400	0.49312000
H	3.48163300	-1.67107200	-1.35958600	H	-3.04367900	-4.76231200	2.38062200
C	7.91635800	-2.85494700	-0.31832800	O	-1.78473000	-2.48533500	2.52039900
O	7.97690000	-3.56539700	-1.35935400	C	-0.54177100	3.54375100	-2.34705900
O	8.82447800	-2.67886400	0.53967800	H	0.38834800	3.36209600	-2.89725600
K	10.44435200	-4.27029900	-0.78598500	H	-1.08859600	4.32817200	-2.88046600
C	-2.70331400	-0.17167700	-1.99377700	H	-0.28053900	3.91688600	-1.35369200
C	-2.58382800	0.45665500	-3.24567700	Pd	-2.93165200	0.06005100	1.08927800
C	-1.92309900	1.66810200	-3.37681000	C	-4.71308600	0.13849600	5.47261500
C	-1.35101100	2.28075300	-2.25723800	C	-4.19332000	1.28511600	4.87786300
C	-1.56220300	1.64492400	-1.04161300	C	-3.70055800	1.17454900	3.57784100
N	-2.21457800	0.47100000	-0.92092600	C	-3.72961600	-0.06424600	2.94703800
H	-1.83427300	2.12886700	-4.35615400	C	-4.29021700	-1.15375400	3.60306900

N	-4.77661100	-1.04947800	4.85199200	H	-3.94819400	-0.95964800	-1.13257000
H	-5.10774200	0.17382600	6.48546200	H	-3.78302700	-0.80857800	0.61197600
H	-4.17752200	2.24132400	5.39051800	C	-4.36636600	-4.27117900	-1.19410600
H	-4.37445800	-2.12831300	3.13727100	H	-3.06589400	-3.01283200	-2.34906300
C	-3.19682500	2.34461700	2.79346500	H	-2.21143200	-4.27244200	-1.45594100
O	-2.91664300	2.05713500	1.53678900	C	-5.53122600	-3.27709600	-1.11122700
O	-3.09060900	3.47313400	3.25499600	H	-6.09697100	-1.48814800	-0.01509300
H	-1.13820000	-1.00031400	2.24627000	H	-5.31126400	-2.72248100	0.96612400
H	-0.09554700	0.53269500	1.31952600	H	-4.52614600	-4.97752500	-2.01712900
C	-5.82474900	-0.66394300	0.57286600	H	-4.32519600	-4.86470300	-0.27039900
C	-7.11590500	-0.50651700	0.09275900	H	-6.47376700	-3.80776800	-0.93169200
C	-7.44842500	0.64458100	-0.62458800	H	-5.63415200	-2.76633900	-2.07890200
C	-6.45649800	1.60664000	-0.82945700	C	-1.28632900	-0.89295900	-1.33402000
C	-5.18326600	1.39476200	-0.32232800	C	-1.21169700	-1.41433100	-2.61770700
N	-4.88246400	0.27266800	0.35694600	N	-1.52861400	0.44848300	-1.20771900
H	-5.52671300	-1.54310600	1.12702200	C	-1.54412900	-0.62073800	-3.72618500
H	-7.86252600	-1.27069500	0.26943300	H	-0.95937200	-2.45109100	-2.77447200
H	-6.68318700	2.50997900	-1.38194800	C	-2.00010500	1.19024600	-2.24480300
H	-4.38510600	2.11428900	-0.44912400	C	-2.01445700	0.66209100	-3.54625600
C	-8.85682600	0.84357900	-1.17690900	H	-1.48393600	-1.04447900	-4.72326000
O	-9.06437700	1.91276500	-1.81480300	H	-2.36028700	1.28618900	-4.36105100
O	-9.68597600	-0.07990500	-0.94777600	O	-2.40883500	2.42120800	-2.03033200
K	-11.56508400	1.22942500	-2.23581300	C	-1.90054900	0.09195700	5.34134300
				H	-1.88827100	1.18458100	5.36101100
7'				H	-2.86550100	-0.24719900	5.73409000
C	-1.33786400	-1.31243800	1.30160900	H	-1.12484000	-0.27566600	6.02131500
C	-1.40835000	-2.23134900	2.36304000	Pd	-0.54829800	1.49715900	0.29592700
C	-1.56645400	-1.79642900	3.66903700	C	1.93077900	4.93084500	-1.85256700
C	-1.68085000	-0.42914900	3.95035300	C	1.88874300	4.82695500	-0.46466700
C	-1.55802100	0.42790300	2.86611200	C	1.12817400	3.79387300	0.08089100
N	-1.37236000	-0.00552000	1.60305400	C	0.43945500	2.93317700	-0.76760100
H	-1.61635100	-2.52294200	4.47494100	C	0.55896500	3.09158200	-2.14378700
H	-1.35901000	-3.29360800	2.16608800	N	1.29433900	4.08326500	-2.67398400
H	-1.58033100	1.50219200	2.99837700	H	2.50851000	5.71939000	-2.32855500
C	-1.34920800	-1.86551100	-0.13884200	H	2.43326200	5.50932300	0.17948500
C	-0.22605800	-2.92476700	-0.24492900	H	0.08560300	2.42079900	-2.85031200
H	-0.43389500	-3.77497800	0.40580500	C	1.04422100	3.52867400	1.54618500
H	-0.12426500	-3.31711200	-1.25468200	O	0.30069100	2.46960200	1.84978800
H	0.73387200	-2.49715400	0.05022800	O	1.59862800	4.19371300	2.40478100
C	-2.79379500	-2.55885100	-0.23874300	H	-2.39607200	2.63021800	-1.01608400
C	-3.93775900	-1.53163400	-0.19585200	O	-2.18767600	2.66435900	0.45495700
C	-3.02623600	-3.54444500	-1.39341100	C	1.68969100	0.03564600	-1.09054700
H	-2.86024300	-3.15996000	0.67349800	C	2.84221800	-0.72584800	-1.19768900
C	-5.29125000	-2.23150000	-0.01665800	C	3.48467300	-1.17127400	-0.04036500

C	2.93775700	-0.82598500	1.19744500	H	-5.49234300	-2.95583600	-2.15272400
C	1.78179200	-0.06203900	1.24551900	C	-1.21671300	-0.93955100	-1.31903300
N	1.17545300	0.34676000	0.11489900	C	-1.05600200	-1.50314100	-2.57197500
H	1.16409900	0.39995700	-1.96263700	N	-1.50736900	0.39796200	-1.23747900
H	3.24383300	-0.97482700	-2.17189500	C	-1.31472800	-0.73880000	-3.73178900
H	3.41327800	-1.15559900	2.11271900	H	-0.80790800	-2.54667300	-2.68135200
H	1.32483900	0.23315700	2.18073000	C	-1.97182200	1.13846800	-2.33159400
C	4.75215500	-2.01756400	-0.12741300	C	-1.81076500	0.53056400	-3.62618400
O	5.26245500	-2.37743500	0.96881300	H	-1.16195200	-1.18962200	-4.70858500
O	5.17163600	-2.27976000	-1.28804500	H	-2.07344200	1.13022900	-4.49066900
K	7.21223900	-3.60948800	-0.29374400	O	-2.44573900	2.28693600	-2.17768000
H	-1.85416200	3.52864300	0.74743400	C	-2.00142600	0.15230100	5.32690300
				H	-2.01418000	1.24523700	5.32121200
7				H	-2.96342700	-0.19879000	5.71679100
C	-1.34363700	-1.32520100	1.32842800	H	-1.22672000	-0.18010700	6.02626300
C	-1.42407400	-2.22555100	2.40698500	Pd	-0.61898100	1.48699600	0.26778900
C	-1.61545100	-1.76639900	3.70024100	C	1.66683900	5.03831900	-1.87768500
C	-1.75087500	-0.39469900	3.95032300	C	1.56796600	4.96635600	-0.49121700
C	-1.61975900	0.44091500	2.85004900	C	0.87764800	3.88496900	0.05623500
N	-1.40354200	-0.01564800	1.60108000	C	0.30141900	2.94211100	-0.79154400
H	-1.67302300	-2.47678900	4.52021700	C	0.47589900	3.07969500	-2.16571200
H	-1.35314200	-3.29098500	2.23405200	N	1.14952000	4.11302800	-2.70074800
H	-1.65580000	1.51834000	2.95184600	H	2.19423800	5.86350800	-2.35140000
C	-1.30247300	-1.89813700	-0.10378900	H	2.02045100	5.71068900	0.15606000
C	-0.14120300	-2.92173400	-0.14841500	H	0.09166100	2.35064400	-2.86845500
H	-0.33156500	-3.75791200	0.52627500	C	0.78552800	3.64445900	1.53088400
H	0.00212300	-3.34270500	-1.14124400	O	0.22327800	2.49685100	1.84430300
H	0.79487400	-2.44891900	0.15525400	O	1.22744900	4.42347900	2.36808200
C	-2.71603800	-2.63977500	-0.22696800	O	-2.20567500	2.63739100	0.49297000
C	-3.89361700	-1.65010200	-0.22940300	C	1.72202200	0.03472600	-1.07648100
C	-2.88844000	-3.64693700	-1.37378900	C	2.90132500	-0.68972300	-1.16837800
H	-2.79262600	-3.23190000	0.69108800	C	3.55076000	-1.09562500	-0.00035400
C	-5.23157400	-2.38788300	-0.08704300	C	2.98213800	-0.74804500	1.22748800
H	-3.88847300	-1.08451100	-1.16972300	C	1.80059100	-0.02043700	1.25042000
H	-3.78578100	-0.91724200	0.57717200	N	1.18470000	0.35240900	0.11456800
C	-4.21119200	-4.41203400	-1.20852600	H	1.18659100	0.36648000	-1.95625100
H	-2.91021300	-3.12587300	-2.33550800	H	3.31889900	-0.94134000	-2.13538500
H	-2.05086400	-4.35143300	-1.40278800	H	3.46281100	-1.04699200	2.15078300
C	-5.40647200	-3.45225000	-1.17588200	H	1.32671500	0.27770200	2.17702300
H	-6.05887200	-1.66896400	-0.11957500	C	4.84572900	-1.89923200	-0.06422300
H	-5.27047800	-2.86936600	0.90011900	O	5.36463900	-2.22111200	1.04090200
H	-4.32395400	-5.13315900	-2.02687300	O	5.28358800	-2.17112600	-1.21680200
H	-4.18348200	-4.99336300	-0.27631400	K	7.36933900	-3.38521400	-0.18647100
H	-6.33929300	-4.00750800	-1.02045700	H	-2.49823700	2.67508500	-0.44619600

				H	-2.17803800	1.43580200	5.37102400
13-ts				H	-2.82025100	-0.17710500	5.73214900
C	-1.42877600	-0.76541400	1.16814600	H	-1.09409400	0.13964200	5.91615700
C	-1.19324000	-1.69583100	2.19777600	Pd	-1.69974400	2.11096500	0.26140700
C	-1.34398200	-1.34995600	3.52846900	C	2.69728900	2.59896000	-1.30529000
C	-1.74428000	-0.05388100	3.87668900	C	2.30956500	3.09115900	-0.06037700
C	-1.89734800	0.83855400	2.82916700	C	0.95269400	3.07550800	0.26147900
N	-1.72304500	0.49228700	1.53051200	C	0.08473100	2.55628700	-0.68786200
H	-1.15941800	-2.08991200	4.30161400	C	0.52023700	2.09180900	-1.92003900
H	-0.90121600	-2.70741200	1.95194500	N	1.83157500	2.11270500	-2.20740700
H	-2.13124600	1.87765900	3.01672200	H	3.74480100	2.59783000	-1.59559100
C	-1.39528500	-1.27527400	-0.28436200	H	3.02753700	3.47502800	0.65718100
C	0.02410600	-1.86158200	-0.49809100	H	-0.15258500	1.70784100	-2.67680100
H	0.23705700	-2.65152000	0.22367200	C	0.40089100	3.54616100	1.57792600
H	0.15145800	-2.29093100	-1.48981600	O	-0.86428600	3.25133800	1.76712100
H	0.77048300	-1.07124200	-0.37392500	O	1.09004800	4.14529700	2.39439900
C	-2.52409300	-2.40806500	-0.30184800	O	-1.57203600	3.80442900	-0.80746700
C	-3.93209900	-1.80615400	-0.15048000	H	-2.25285100	3.56164500	-1.49131400
C	-2.51546400	-3.41376800	-1.46324100				
H	-2.33388100	-3.00876200	0.59187600	14			
C	-4.97397000	-2.90303100	0.10115300	C	-1.38056100	1.26716100	1.07899600
H	-4.19220000	-1.25934600	-1.06566900	C	-1.50102300	2.57602400	1.57942000
H	-3.95508700	-1.07692000	0.66731500	C	-0.44405900	3.47038300	1.56708900
C	-3.53084700	-4.53442900	-1.18792400	C	0.78698000	3.08524400	1.03073600
H	-2.79454200	-2.92073100	-2.39915500	C	0.86198000	1.79057600	0.54176300
H	-1.51671900	-3.84027200	-1.60283000	N	-0.17129500	0.91504100	0.57167600
C	-4.94429300	-3.97009000	-0.99981200	H	-0.58148300	4.47125100	1.96592400
H	-5.97362600	-2.45868100	0.17501800	H	-2.44842600	2.91047100	1.97336500
H	-4.76638900	-3.37669500	1.07082300	H	1.76977500	1.41906200	0.08633900
H	-3.51618200	-5.25426600	-2.01476900	C	-2.70003300	0.42942100	1.03896200
H	-3.23345300	-5.08426500	-0.28418000	C	-3.46561500	0.69635500	2.36199200
H	-5.65025300	-4.77662500	-0.76837200	H	-3.85197600	1.71442900	2.41000100
H	-5.27693600	-3.51920500	-1.94534100	H	-4.32575000	0.03966900	2.46549000
C	-1.72832000	-0.31455000	-1.44656800	H	-2.80989300	0.52859400	3.22062900
C	-1.54718800	-0.79966000	-2.73087800	C	-3.51374200	1.02784700	-0.19129400
N	-2.35432200	0.89037700	-1.27357900	C	-2.82842900	0.77796000	-1.54507000
C	-2.11984800	-0.13173500	-3.83173900	C	-4.98444100	0.58553200	-0.26267900
H	-1.03490900	-1.73267800	-2.89900000	H	-3.51813100	2.11123100	-0.01510600
C	-2.96028900	1.57780600	-2.33075200	C	-3.56119100	1.50186100	-2.68292900
C	-2.86443300	0.99895200	-3.63766900	H	-2.81637100	-0.29993700	-1.75152800
H	-1.98175400	-0.53703200	-4.83017200	H	-1.78397300	1.10364300	-1.51613400
H	-3.33283600	1.53863700	-4.45274500	C	-5.72009700	1.32625300	-1.38891300
O	-3.51115900	2.69273800	-2.12901600	H	-5.03700500	-0.49204000	-0.45436300
C	-1.97135800	0.36503400	5.30089200	H	-5.49139600	0.76949000	0.68921900

C	-5.03969000	1.10366100	-2.74342000	H	-0.96351300	4.81485500	0.71045200
H	-3.06583900	1.28667200	-3.63707500	H	-2.09198300	2.78244000	1.46122700
H	-3.48482500	2.58673500	-2.52465000	H	2.15468400	2.33440300	-0.87457000
H	-6.76438800	0.99423200	-1.42583600	C	-1.44364400	0.18496000	1.09567100
H	-5.73773800	2.40171700	-1.16365500	C	-1.68120500	0.32054900	2.61962100
H	-5.55591700	1.66862100	-3.52877900	H	-2.21456900	1.24299800	2.85673800
H	-5.11629800	0.04118700	-3.01408900	H	-2.27315200	-0.50327100	3.01445000
C	-2.59859500	-1.08775400	0.85638800	H	-0.72221900	0.33208400	3.14635100
C	-3.62751100	-1.98704900	1.15100500	C	-2.80807200	0.33848800	0.28372400
N	-1.51771100	-1.60560500	0.27293500	C	-2.59530200	0.20495000	-1.23400900
C	-3.47187600	-3.34644900	0.82691200	C	-3.98179500	-0.55143700	0.72159700
H	-4.55051700	-1.65711600	1.60229000	H	-3.13844200	1.36496200	0.47403400
C	-1.30006300	-2.91631000	-0.04446700	C	-3.86543300	0.58565400	-2.00578800
C	-2.32120700	-3.84322400	0.23089600	H	-2.32125600	-0.83041000	-1.47122800
H	-4.28471900	-4.02886600	1.05818000	H	-1.75914500	0.83250200	-1.56234400
H	-2.19283600	-4.89348600	-0.00408700	C	-5.26078200	-0.14869500	-0.02922500
O	-0.11761500	-3.09277300	-0.55426900	H	-3.76242000	-1.60047800	0.50064500
C	1.97334200	4.00537800	0.97302700	H	-4.14691900	-0.47503700	1.80118600
H	2.83038600	3.51463400	0.50616400	C	-5.07022600	-0.24403600	-1.54745100
H	1.73707800	4.90919300	0.40106600	H	-3.70024600	0.45741300	-3.08217500
H	2.26500900	4.32408300	1.97970100	H	-4.07670800	1.65192200	-1.84335700
Pd	0.27084900	-0.95401100	-0.12350000	H	-6.09208000	-0.78805200	0.29094400
C	6.88176700	-1.03846000	-0.11591500	H	-5.53284400	0.88155500	0.23979300
C	5.56567200	-1.35806800	0.20113400	H	-5.97865500	0.08164300	-2.06833200
C	4.52643000	-0.48925500	-0.14433700	H	-4.90713000	-1.29570900	-1.82197400
C	4.88255900	0.70904700	-0.78553000	C	-0.89008200	-1.21871200	0.78073500
C	6.23933800	0.95026900	-1.05028100	C	-1.51343000	-2.32935100	1.32365700
N	7.22072600	0.10293800	-0.73532600	N	0.06073600	-1.39432700	-0.17673500
H	7.69269300	-1.71674800	0.13783600	C	-1.21437700	-3.61477600	0.81286300
H	5.32829300	-2.28112200	0.71832200	H	-2.27295100	-2.22682900	2.08312500
H	6.52475000	1.88073900	-1.54286600	C	0.33110200	-2.62805500	-0.79432000
C	3.11175700	-0.87630900	0.21774100	C	-0.35193800	-3.77064100	-0.23738500
O	2.21726000	-0.52194700	-0.65193200	H	-1.70432300	-4.48117000	1.25029900
O	2.90385100	-1.49414900	1.26643200	H	-0.12302200	-4.74327300	-0.66019400
O	3.93289400	1.62464200	-1.11419800	O	1.14479600	-2.68128700	-1.73414800
H	4.36712600	2.40478400	-1.49599600	C	1.41308800	4.97865200	-0.70514500
				H	2.36635600	4.71072100	-1.16727300
				H	0.80605200	5.50487900	-1.45004300
1b				H	1.60902300	5.68201400	0.11103100
C	-0.61659200	1.41834900	0.67332500	Pd	1.72286400	-0.26996200	-0.10863500
C	-1.15664300	2.69366100	0.92644000	C	4.19130800	-0.62466600	0.07348000
C	-0.51992400	3.84575500	0.50178800	O	3.40732200	-1.62445700	0.00889000
C	0.69156300	3.76333200	-0.19744000	O	3.67374800	0.55051500	0.05442200
C	1.20146200	2.48965200	-0.38387500	C	5.67695900	-0.79549900	0.13960800
N	0.57162500	1.36926900	0.04679600				

H	6.10406700	-0.57289600	-0.84484800	H	5.06710900	0.78181600	4.28801400
H	6.10464800	-0.09112800	0.85784200	O	3.14371800	-0.04805000	2.73087000
H	5.93534400	-1.81946700	0.41445500	C	1.25547100	0.92065200	-4.89870500
7b				H	0.42874800	0.35563700	-4.46561900
C	4.039563	2.10611200	-1.81952200	H	0.84571200	1.76990300	-5.45129100
C	3.93222000	2.85607200	-3.00330800	H	1.76519400	0.27104300	-5.62051300
C	3.04285600	2.49509500	-4.00341000	Pd	3.78744800	-0.55717800	-0.37058600
C	2.21631600	1.37943800	-3.83926400	C	5.57209200	-4.59541100	1.43630000
C	2.35966000	0.68685600	-2.64585600	C	4.93620600	-4.56103800	0.19792200
N	3.24328700	1.02731600	-1.68055300	C	4.42149600	-3.34006200	-0.23644300
H	2.98716000	3.08575200	-4.91295700	C	4.53316400	-2.18717300	0.56377400
H	4.54641600	3.73352800	-3.14973600	C	5.21637100	-2.34053800	1.77761200
H	1.78172200	-0.20750500	-2.45502400	N	5.72062800	-3.50972300	2.21194600
C	5.04186700	2.60758700	-0.74948000	H	5.98595000	-5.52532100	1.82078100
C	6.40634500	2.76644300	-1.46568800	H	4.84132900	-5.44776000	-0.42088800
H	6.34454700	3.48249100	-2.28537900	H	5.38383500	-1.49823700	2.43980500
H	7.18712900	3.12214300	-0.79654200	C	3.71115100	-3.18950700	-1.55056800
H	6.72219000	1.80150200	-1.87382500	O	3.21908200	-1.97846400	-1.73551300
C	4.44646600	4.02448000	-0.29913200	O	3.58250300	-4.10165700	-2.36152700
C	3.13918300	3.86767400	0.49650900	H	2.41133800	0.14868600	2.09597800
C	5.39809300	4.97390300	0.44354700	O	1.29701800	0.99629900	1.06487000
H	4.19831200	4.53082700	-1.23781900	O	0.29287800	-0.02772600	1.14882400
C	2.46006800	5.21933900	0.74786100	C	-2.34161100	-7.52848700	2.39933000
H	3.35359400	3.39696900	1.46303400	C	-1.26840300	-6.74401300	1.97937200
H	2.45078400	3.19964600	-0.03028200	C	-1.35203300	-6.07971600	0.75374000
C	4.72404300	6.33877900	0.65783600	C	-2.51978200	-6.24628600	0.00429600
H	5.65932400	4.56183100	1.42341600	C	-3.53673800	-7.05566100	0.50493900
H	6.33092300	5.10390100	-0.11430300	N	-3.46719100	-7.69268700	1.68570900
C	3.41342300	6.19896800	1.44108300	H	-2.29757100	-8.04924200	3.35454800
H	1.55785800	5.06499100	1.35100800	H	-0.37838300	-6.63518700	2.58876200
H	2.13740800	5.64704300	-0.21082000	H	-2.62316000	-5.73338300	-0.94439700
H	5.41366300	7.00899900	1.18441800	H	-4.45483800	-7.19579700	-0.06349400
H	4.51771000	6.80032800	-0.31794000	C	-0.23099500	-5.16575100	0.26725200
H	2.93406300	7.17782400	1.56162400	O	-0.44937300	-4.53756700	-0.80775400
H	3.63772900	5.82933100	2.45157800	O	0.79951700	-5.08625000	0.99006300
C	5.24533700	1.81870800	0.55909600	K	0.91400100	-2.46902100	0.20814200
C	6.28076100	2.17714300	1.42066500	C	-2.04604000	0.90050800	-2.16368400
N	4.31107900	0.93366400	1.00620900	C	-2.00807700	1.63764600	-3.36104500
C	6.25877200	1.75871100	2.75629000	C	-1.18388700	2.74269500	-3.49742600
H	7.07991600	2.82197000	1.09018500	C	-0.34403300	3.12410400	-2.44758700
C	4.20686800	0.64925000	2.32105200	C	-0.41686500	2.35083500	-1.29746900
C	5.17757200	1.04570100	3.24336100	N	-1.24793000	1.29546600	-1.15894300
H	7.06343500	2.05221300	3.42256600	H	-1.18306300	3.30243100	-4.42780300
				H	-2.61879800	1.34261200	-4.20224100

H	0.17129100	2.60401700	-0.42594700	H	-2.06619800	0.63909100	6.73832000
C	-2.93878500	-0.35726400	-2.12101700	H	-0.88461700	2.50861200	5.52999500
C	-4.33402600	0.09107800	-2.63195800	H	-3.06904900	-1.22997200	3.20096500
H	-4.27504300	0.50929700	-3.63616300	C	-0.73173400	2.74878400	2.77540300
H	-5.04544100	-0.72885900	-2.68398500	O	-0.96354700	2.60227400	1.48688500
H	-4.74440000	0.85468400	-1.96524000	O	-0.17115100	3.73247500	3.24199600
C	-2.22550200	-1.34627400	-3.15429400	H	1.62606400	0.92789400	0.14732300
C	-0.84866300	-1.80030000	-2.64294700	C	-4.59610300	0.73532100	1.10543900
C	-3.03209700	-2.57345200	-3.60392400	C	-5.88696000	1.20750800	0.92298500
H	-2.06745000	-0.74253100	-4.05569000	C	-6.08551400	2.47155400	0.36412000
C	-0.06947800	-2.57870200	-3.70902000	C	-4.96204300	3.22578500	0.01685300
H	-1.00017700	-2.46198000	-1.78566700	C	-3.69543700	2.70172400	0.22661900
H	-0.26646400	-0.93647500	-2.30454300	N	-3.52867800	1.47441500	0.75255300
C	-2.26600100	-3.35100100	-4.68671900	H	-4.39926600	-0.24052600	1.52754200
H	-3.20401600	-3.23988900	-2.75289300	H	-6.73715100	0.59937500	1.20575200
H	-4.01416700	-2.27406500	-3.98520200	H	-5.08258800	4.21088200	-0.41651000
C	-0.87978900	-3.78526200	-4.19413200	H	-2.79708400	3.25071800	-0.02319200
H	0.89449300	-2.90013900	-3.29842000	C	-7.49355500	3.01171100	0.13177900
H	0.15086100	-1.91800000	-4.55871500	O	-7.57699500	4.16107700	-0.38318200
H	-2.85376700	-4.22503000	-4.99229200	O	-8.44752300	2.25896700	0.47283200
H	-2.15468700	-2.71835000	-5.57887000	K	-10.20220900	4.04602200	-0.31958800
H	-0.34215500	-4.31390900	-4.99115400				
H	-0.99119100	-4.48308000	-3.35474500	7c			
C	-3.12087500	-1.14954000	-0.80144000	C	4.629475	-2.11765300	-0.02334200
C	-4.14310200	-2.07944400	-0.74854900	C	4.89691000	-3.26816800	0.74860700
N	-2.20451200	-1.12541000	0.22199800	C	4.17066100	-3.54681000	1.89974900
C	-4.22165100	-3.00814500	0.31465000	C	3.15418100	-2.67707200	2.31345500
H	-4.86390800	-2.15530000	-1.54553400	C	2.93123000	-1.56954500	1.50518400
C	-2.11567900	-2.16196200	1.17064400	N	3.63987300	-1.30220900	0.38547100
C	-3.22619300	-3.07317800	1.24435100	H	4.39762000	-4.43950200	2.47674000
H	-5.05999300	-3.69793000	0.35435400	H	5.67987700	-3.95427000	0.45335600
H	-3.21683600	-3.80172000	2.04651500	H	2.17269500	-0.83940500	1.75940000
O	-1.12514100	-2.23752100	1.92491500	C	5.51792600	-1.89285700	-1.27791000
C	0.56309100	4.31890900	-2.52562700	C	6.97728600	-1.81783200	-0.75969600
H	1.44529700	4.18622500	-1.89790400	H	7.26021000	-2.74041200	-0.24802500
H	0.88967900	4.49673400	-3.55300800	H	7.69550000	-1.67840400	-1.56635700
H	0.04009900	5.21962500	-2.18217200	H	7.06446500	-0.97013100	-0.07394500
Pd	-1.57147200	0.73038500	0.92056800	C	5.26467200	-3.18711300	-2.18178900
C	-2.00034100	0.64988300	5.65278000	C	3.87986600	-3.15583000	-2.85117500
C	-1.33546100	1.67933400	4.99469300	C	6.33317500	-3.54902900	-3.22362300
C	-1.28668100	1.63290400	3.60084500	H	5.25909200	-4.02541900	-1.48025900
C	-1.86212200	0.55577500	2.93208400	C	3.54127600	-4.52095400	-3.46036300
C	-2.54593100	-0.40685900	3.66862100	H	3.87612200	-2.40159200	-3.64799700
N	-2.61295200	-0.35638000	5.00984500	H	3.11213300	-2.85571700	-2.13160600

C	6.01558600	-4.92548400	-3.83202600	C	3.91164400	4.32418300	2.99425100
H	6.35212000	-2.80814900	-4.02904600	N	4.45903600	5.17619000	2.11384700
H	7.33034700	-3.56629100	-2.77239500	H	5.82644800	5.38148500	0.57453100
C	4.61762100	-4.95726700	-4.46266000	H	6.59336400	3.00127500	0.63924600
H	2.56016300	-4.48112300	-3.94821400	H	3.81311100	2.33096600	3.82917000
H	3.46537500	-5.26653200	-2.65659400	H	3.13995100	4.73176300	3.64376800
H	6.77488900	-5.18110500	-4.58046700	C	5.73182000	1.04088800	2.36104900
H	6.07711000	-5.69060000	-3.04558800	O	5.23174000	0.34474500	3.28989200
H	4.39738100	-5.95984300	-4.84830800	O	6.61834600	0.65989300	1.53864700
H	4.59888600	-4.27543500	-5.32439600	K	6.96815700	-1.54688400	2.92381200
C	5.25226000	-0.70476400	-2.22115400	C	-1.42036600	-1.79412900	1.80462500
C	6.14180500	-0.44809000	-3.26097800	C	-1.02474800	-3.04991100	2.29637600
N	4.05128500	-0.06455800	-2.22135100	C	-0.18894800	-3.87406300	1.56060800
C	5.71653000	0.29382000	-4.37067400	C	0.30068400	-3.44822000	0.32285200
H	7.13517000	-0.86927400	-3.25883900	C	-0.13757600	-2.20536700	-0.11352300
C	3.59526600	0.55296400	-3.33002100	N	-0.97642400	-1.41801400	0.59420400
C	4.40964100	0.73710000	-4.45361300	H	0.09112800	-4.84668700	1.95383200
H	6.40400000	0.47168800	-5.19132700	H	-1.36428100	-3.38496300	3.26604200
H	4.01560600	1.24593900	-5.32462700	H	0.16113000	-1.81673100	-1.07595900
O	2.34710900	1.01842500	-3.36538600	C	-2.26364900	-0.90284500	2.73769600
C	2.36907900	-2.90245700	3.57405100	C	-3.40521000	-1.80008000	3.29184400
H	1.46783500	-2.28863000	3.59469700	H	-3.01021300	-2.55112600	3.97620600
H	2.07735700	-3.95212000	3.67291400	H	-4.15352900	-1.23592600	3.84284800
H	2.97432700	-2.64579200	4.45185200	H	-3.91147900	-2.31748300	2.47449800
Pd	3.32876700	0.64504700	-0.40203000	C	-1.21933700	-0.51187300	3.89174900
C	2.97691500	5.29626500	-1.25954200	C	-0.18562200	0.50303800	3.38843100
C	2.23378700	4.69393000	-0.24766700	C	-1.78647400	-0.05347100	5.24370900
C	2.37746300	3.32072700	-0.06042100	H	-0.69358300	-1.44924400	4.10340100
C	3.22456200	2.58045000	-0.89653500	C	0.94718500	0.71370100	4.39775300
C	3.95285500	3.29426900	-1.85472300	H	-0.67030300	1.46801200	3.20667300
N	3.83765500	4.62106200	-2.03928800	H	0.23472900	0.20098900	2.42715400
H	2.89718000	6.36608500	-1.44203300	C	-0.64348900	0.08617100	6.26268400
H	1.57944600	5.26916400	0.39922700	H	-2.27011800	0.92315000	5.14667700
H	4.66724200	2.79276400	-2.50293300	H	-2.53843400	-0.75782600	5.61477300
C	1.70944500	2.58136700	1.05718600	C	0.40643700	1.09496500	5.78030900
O	2.01859200	1.29369000	1.08720800	H	1.61530100	1.48850500	4.01094700
O	0.95673200	3.11986500	1.86215700	H	1.53755800	-0.20811700	4.48437700
H	1.85270800	0.82090400	-2.53517500	H	-1.05218400	0.39340900	7.23271100
O	0.53787600	0.42778700	-1.24348300	H	-0.16780900	-0.89286900	6.41502700
O	-0.68405300	1.14070200	-1.27801400	H	1.22581100	1.16969300	6.50585700
C	5.40056900	4.68350800	1.29264800	H	-0.05751400	2.09006600	5.72414300
C	5.82930500	3.35839200	1.31967200	C	-2.85819000	0.43550900	2.23840300
C	5.26353800	2.48225600	2.24999600	C	-3.68360100	1.11723300	3.12856300
C	4.27767800	2.98412900	3.10087100	N	-2.50743500	1.06575200	1.07399600

C	-4.02012600	2.45618000	2.91760300	H	-6.05895800	6.45800900	-2.09445200
H	-4.03361600	0.63487000	4.02564500	H	-4.56446800	6.22894300	-3.05040400
C	-2.75191600	2.39035900	0.90192000	H	-5.83689200	4.97366000	-3.03053300
C	-3.50316000	3.12518600	1.83141200	H	-6.37724400	4.32724200	-0.73882700
H	-4.65381100	2.97220600	3.63148600	C	-7.96931500	2.67312600	-1.59069000
H	-3.69272900	4.17388000	1.64611100	O	-7.76690200	3.87784200	-1.45409700
O	-2.28020400	2.94114400	-0.19882300	O	-8.64994000	2.20428700	-2.63689300
C	1.24682200	-4.27224600	-0.50225400	H	-8.87891900	2.96389100	-3.20570700
H	2.28286200	-4.07962100	-0.20555100	C	-7.57958000	1.60321900	-0.61891200
H	1.05647900	-5.34051500	-0.36496200	H	-6.85676000	1.98552100	0.10042800
H	1.15339500	-4.03455900	-1.56433100	H	-8.48022400	1.28332500	-0.08222200
Pd	-2.16720300	-0.07254200	-0.66041200	H	-7.17429400	0.73688200	-1.14289500
C	-4.95985700	1.78759700	-4.01166900				
C	-4.00647500	0.82021900	-4.31741200	7d			
C	-3.22346300	0.32821900	-3.27254400	C	-0.60952600	1.39232100	0.61076800
C	-3.40127600	0.83768600	-1.99146300	C	-0.88275000	2.64680700	1.18711400
C	-4.39874100	1.77649200	-1.76944900	C	-0.27871300	3.80083100	0.72094000
N	-5.16530700	2.24587400	-2.76767400	C	0.61491700	3.73909800	-0.35510500
H	-5.59856700	2.20128600	-4.78803100	C	0.89711500	2.47291300	-0.84047200
H	-3.88085900	0.43679000	-5.32472400	N	0.32476800	1.34609300	-0.35358300
H	-4.62029300	2.16803300	-0.78678700	H	-0.51108200	4.75527000	1.18413400
C	-2.25808200	-0.79952700	-3.42980100	H	-1.58990900	2.72289600	2.00113800
O	-1.76840800	-1.23135900	-2.27958900	H	1.62854100	2.33133100	-1.62457500
O	-1.97344400	-1.31873900	-4.49893000	C	-1.46447200	0.19460700	1.06885700
H	0.89827700	0.64990300	-0.35313700	C	-1.29001900	0.09608500	2.60592500
C	-4.99173500	-0.79785000	0.29821100	H	-1.63947200	1.00449900	3.09888300
C	-6.08880700	-1.60085000	0.57051700	H	-1.84920600	-0.73324400	3.03433300
C	-6.01026700	-2.97459200	0.33142800	H	-0.23488200	-0.04506900	2.85350100
C	-4.81764900	-3.48946700	-0.18233200	C	-2.95304200	0.63405000	0.67825600
C	-3.75720000	-2.63188800	-0.43945900	C	-3.15474400	0.69443300	-0.84557200
N	-3.84953800	-1.31346000	-0.19104200	C	-4.10985200	-0.14527600	1.32286400
H	-5.01555700	0.26832600	0.47587800	H	-3.05159600	1.65548200	1.05750500
H	-6.99980300	-1.16924800	0.96557200	C	-4.49457300	1.35472100	-1.19681300
H	-4.72542700	-4.55040900	-0.37925800	H	-3.13317000	-0.32336200	-1.25478500
H	-2.81916600	-2.98484800	-0.84871200	H	-2.33422900	1.24154900	-1.32329700
C	-7.19660900	-3.88745900	0.62666400	C	-5.44676500	0.54109600	1.00075200
O	-7.03437500	-5.11605300	0.38792500	H	-4.14507900	-1.16716300	0.93367900
O	-8.23329700	-3.33051700	1.08330800	H	-3.97792300	-0.21272700	2.40760300
K	-9.49730500	-5.63284500	1.14750400	C	-5.66802500	0.64361900	-0.51286500
C	-4.66106800	5.06456400	-1.26406800	H	-4.63307900	1.36068300	-2.28442600
O	-5.44540000	4.44377600	-0.39303500	H	-4.47008100	2.40526100	-0.87526200
O	-3.44378200	5.08425400	-1.07886400	H	-6.26723500	-0.01555700	1.46878600
H	-2.72262900	3.82049300	-0.39616200	H	-5.45600000	1.54808500	1.44050400
C	-5.31621700	5.73172200	-2.43865300	H	-6.60789300	1.16610100	-0.72754700

H	-5.76615800	-0.36901700	-0.92865000	H	7.23346700	0.78915000	-0.05163100
C	-1.24762100	-1.19063600	0.42403600	H	6.13322600	1.03103800	-1.40839300
C	-1.92517300	-2.26678500	0.96772000	C	5.42815200	2.13549700	1.88099200
N	-0.58001900	-1.36091300	-0.75966300	C	4.24289300	2.04517900	2.85746500
C	-2.01032600	-3.48689100	0.26100400	C	6.73822800	1.86620000	2.63484300
H	-2.45216700	-2.17028900	1.90287600	H	5.49386500	3.17506500	1.54359900
C	-0.74065800	-2.50328400	-1.55807100	C	4.39657900	3.06099900	3.99627400
C	-1.47622500	-3.59768400	-0.99166100	H	4.19721700	1.03405000	3.28089600
H	-2.53483100	-4.32419400	0.71270900	H	3.29427900	2.20997400	2.33746700
H	-1.54561600	-4.50585600	-1.57973900	C	6.91193500	2.89924800	3.76055700
O	-0.21469200	-2.54826400	-2.69586500	H	6.72250400	0.86693800	3.08098700
C	1.25666500	4.96283400	-0.94305700	H	7.59623400	1.90783500	1.95622800
H	1.98437300	4.69769400	-1.71388800	C	5.72737000	2.87277400	4.73424400
H	0.50144300	5.61578400	-1.39449300	H	3.55549200	2.96880800	4.69358900
H	1.76802800	5.54330800	-0.16809100	H	4.35117900	4.07640000	3.57838700
Pd	1.22363300	-0.41010300	-1.05461000	H	7.84834100	2.70385500	4.29619200
C	3.35477300	-1.26303400	3.01624600	H	7.00170000	3.90270900	3.32204700
C	3.90428700	-0.36537200	2.10271500	H	5.84986800	3.64369800	5.50431300
C	3.23642700	-0.17929700	0.89362200	H	5.71394000	1.90471900	5.25434700
C	2.05303600	-0.87437300	0.69884900	C	4.93779900	-0.15115100	0.98925100
C	1.58143000	-1.79334000	1.61969000	C	6.01292000	-0.87648400	1.47047000
N	2.23919400	-1.96695800	2.78046800	N	3.68248900	-0.66293400	1.18695700
H	3.84050000	-1.44061200	3.97265400	C	5.79728000	-2.02817600	2.25839400
H	4.82917900	0.16699800	2.29989800	H	7.02269600	-0.52534700	1.32889300
H	0.69090600	-2.38715700	1.46061200	C	3.41474700	-1.65847600	2.11326300
C	3.74419700	0.67903400	-0.22610400	C	4.52889600	-2.38745100	2.63033000
O	2.99276600	0.62064100	-1.30265100	H	6.65286300	-2.59423400	2.61389400
O	4.76741100	1.34452700	-0.14541600	H	4.32206900	-3.22440500	3.28710300
O	2.20054500	-1.97793700	-1.74783600	O	2.21474300	-1.92311200	2.43268700
H	1.47150500	-2.41411200	-2.23620800	C	0.78688700	4.66290500	-1.36228800
				H	-0.14513700	4.10268200	-1.43003800
				H	0.64882000	5.46307700	-0.62677200
				H	0.98189100	5.13986600	-2.32823000
				Pd	2.30325400	-0.46616800	-0.33863100
				C	0.84058700	-4.81606600	-1.60370100
				C	0.43893300	-3.67881400	-2.29744900
				C	0.90703300	-2.44691500	-1.84318900
				C	1.74666700	-2.40599600	-0.73466500
				C	2.09735200	-3.59082000	-0.09491900
				N	1.64799500	-4.77844800	-0.53390700
				H	0.49913700	-5.80069200	-1.91403000
				H	-0.22783300	-3.72631300	-3.15019700
				H	2.74419100	-3.61687600	0.77118700
				C	0.52882900	-1.15379900	-2.48774800
12_BQ							
C	4.02169100	2.09445300	-0.12642200				
C	4.28118800	3.41669600	-0.52791600				
C	3.25363000	4.24391100	-0.94724900				
C	1.93319500	3.77760500	-0.96716600				
C	1.74915100	2.44833700	-0.61082000				
N	2.76214700	1.64558400	-0.22307700				
H	3.47305400	5.26410200	-1.24865500				
H	5.28797200	3.80866400	-0.48828900				
H	0.76929600	1.99173300	-0.64741500				
C	5.17033900	1.30490300	0.53331400				
C	6.39572500	1.38456600	-0.40840900				
H	6.75412600	2.41094100	-0.49836500				

O	0.98100900	-0.09418200	-1.83861900	H	-4.16854900	-2.76290500	-3.30670100
O	-0.12250200	-1.06640700	-3.51718000	O	-2.35815200	-2.48284600	-1.45085800
H	1.33494400	-1.03496900	1.75055500	C	0.44529200	3.42733200	2.80638600
O	0.88379300	-0.37409300	1.05454200	H	1.31913700	3.78888300	2.25230300
O	-1.19456600	-1.53660100	0.60476800	H	0.16831000	4.20553600	3.52459300
C	-2.65491900	2.44313600	-0.02302700	H	0.74329100	2.53285600	3.35929100
C	-2.35430500	3.78935200	0.24905200	Pd	-2.84265300	-0.50337900	0.94098800
C	-1.38576200	4.13087000	1.18000500	C	-4.57578900	-4.62248200	2.55553200
C	-0.68442700	3.13061900	1.86112800	C	-3.88092100	-3.74452800	3.38206900
C	-1.08327200	1.82621500	1.60412000	C	-3.40599700	-2.56117600	2.81790800
N	-2.02737800	1.50118400	0.69868800	C	-3.64324700	-2.30634200	1.47093200
H	-1.16124900	5.17737000	1.36341700	C	-4.34027800	-3.24280800	0.71396600
H	-2.86219200	4.57711300	-0.28996100	N	-4.80491100	-4.38109900	1.25682300
H	-0.63945900	1.00318800	2.14346400	H	-4.96515800	-5.55906800	2.94768900
C	-3.62088600	2.14322000	-1.18719000	H	-3.70424900	-3.95776200	4.43113800
C	-4.89744900	2.98742300	-0.94297000	H	-4.54789500	-3.10307500	-0.33859800
H	-4.68752800	4.05234500	-1.05364900	C	-2.65600700	-1.53809300	3.60930400
H	-5.69461600	2.74766500	-1.64329500	O	-2.34463300	-0.45989000	2.91994700
H	-5.27880900	2.82607900	0.06762500	O	-2.36952100	-1.67488500	4.79111900
C	-2.82709900	2.67559900	-2.47609100	H	-1.45839700	-1.99219700	-0.25840300
C	-1.64092300	1.76768200	-2.82935700	H	-0.02856100	-0.84719200	0.73748900
C	-3.65664600	2.96117500	-3.73716200	C	-6.34374200	-0.55139800	0.34322500
H	-2.42388100	3.64592600	-2.16653100	C	-5.81815200	0.41379000	1.31106200
C	-0.76158500	2.37562800	-3.92711400	C	-6.74717700	1.28983200	2.03830900
H	-2.01009700	0.79927700	-3.18111400	C	-8.07153900	1.19392900	1.83850900
H	-1.03501500	1.55233000	-1.94547400	C	-8.62917100	0.20913500	0.87811000
C	-2.77456000	3.62216300	-4.80839200	C	-7.66899000	-0.65273300	0.14580900
H	-4.05193500	2.02894600	-4.15139700	H	-5.64216200	-1.16960800	-0.19394900
H	-4.51133200	3.60546100	-3.50694800	H	-6.30671500	1.99551700	2.73453500
C	-1.58266900	2.72868600	-5.17213900	H	-8.78243100	1.82247000	2.36480700
H	0.03241700	1.66371300	-4.17346700	H	-8.08748600	-1.35948900	-0.56326200
H	-0.27703800	3.28469400	-3.54999400	O	-4.59942700	0.54932300	1.56097200
H	-3.37773900	3.83710600	-5.69855600	O	-9.83708400	0.11506500	0.69271300
H	-2.40640900	4.58810600	-4.43498400	C	6.39254900	-1.83562400	-3.78953500
H	-0.95074100	3.22041900	-5.92180900	C	6.77980800	-3.01037800	-2.96912800
H	-1.95827600	1.80362600	-5.63218400	C	6.02886800	-3.24533300	-1.71057800
C	-3.99754200	0.67845500	-1.51290100	C	5.03352100	-2.42870300	-1.32496500
C	-4.95567600	0.45589700	-2.48473100	C	4.65650400	-1.29260500	-2.16465300
N	-3.26000000	-0.39354300	-1.07572800	C	5.39350700	-1.02466200	-3.40524400
C	-5.05714500	-0.80750500	-3.10895300	H	6.95065300	-1.66965700	-4.70513400
H	-5.57697500	1.26158800	-2.84129800	H	6.32927100	-4.09930000	-1.11229400
C	-3.19313600	-1.59748900	-1.77443100	H	4.49404900	-2.59248300	-0.40522400
C	-4.16155600	-1.79761500	-2.81369500	H	5.08292100	-0.15992600	-3.98167800
H	-5.82300800	-0.96597800	-3.86247400	O	7.69007400	-3.75457800	-3.31330500

O	3.72044900	-0.50139300	-1.89130400	C	0.67046400	3.90249700	2.94413200
				H	-0.22486500	3.62519600	3.50650200
6 ^t _BQ				H	1.48366900	4.08131600	3.65603400
C	1.64241800	0.81897700	0.08925000	H	0.47577400	4.84733800	2.42474900
C	2.43498200	1.97780300	0.17898900	Pd	-1.09005100	-0.46998400	0.31520500
C	2.14220100	2.97390000	1.09498900	C	-5.17550900	-2.03734700	-1.53930700
C	1.04443000	2.83869900	1.95321700	C	-5.14324400	-0.97379700	-0.64007300
C	0.27931000	1.69279500	1.78874000	C	-3.90570300	-0.59197300	-0.12611600
N	0.56103200	0.72984500	0.88569900	C	-2.74167900	-1.28593400	-0.48985500
H	2.76529600	3.86186200	1.14156700	C	-2.89046600	-2.31684900	-1.42574400
H	3.29837500	2.09954500	-0.46010400	N	-4.07432800	-2.69106100	-1.94265000
H	-0.62892600	1.54462800	2.35989300	H	-6.11892800	-2.37098100	-1.96733400
C	2.16095900	-0.32471900	-0.82142300	H	-6.04450200	-0.44015100	-0.35449000
C	2.42935900	0.27148300	-2.22540200	H	-2.02928600	-2.86931500	-1.79401700
H	3.09829000	1.13081400	-2.17728900	C	-3.72892600	0.60028300	0.76730600
H	2.89486700	-0.45167700	-2.89291100	O	-2.46758000	0.88973500	1.00392600
H	1.48795100	0.58768100	-2.67835500	O	-4.67144500	1.25716100	1.20198200
C	3.52262600	-0.75337100	-0.08927600	H	-1.49613700	-2.66417000	1.08763600
C	3.25128600	-1.43854800	1.26176200	O	-1.81967800	-1.62984800	3.56243700
C	4.54860600	-1.57602900	-0.88535000	O	-2.97439800	-1.27840300	3.69165000
H	4.02410200	0.19569700	0.12314500	C	0.98144900	4.46980000	-2.01084000
C	4.54532200	-1.58947800	2.07233800	C	0.23087300	4.80382200	-0.77528200
H	2.81681300	-2.43099000	1.08283100	C	-0.90446500	3.92736000	-0.40699600
H	2.51453300	-0.87338700	1.84223200	C	-1.24256200	2.86962400	-1.16133000
C	5.85820800	-1.68582000	-0.08755400	C	-0.48831800	2.53120700	-2.38679300
H	4.17504300	-2.58837000	-1.06543400	C	0.64535900	3.41071700	-2.76395000
H	4.74534200	-1.12040900	-1.86108500	H	1.81074000	5.12335300	-2.26372000
C	5.62286900	-2.33816800	1.27975600	H	-1.43808200	4.17866800	0.50390600
H	4.33577000	-2.10707900	3.01590500	H	-2.05063900	2.20495600	-0.88106200
H	4.91779000	-0.58984500	2.33608500	H	1.18281200	3.14871200	-3.67008700
H	6.59123500	-2.26291600	-0.66345200	O	0.54449000	5.77252800	-0.08563200
H	6.28466700	-0.68305000	0.05380700	O	-0.78223600	1.54878000	-3.06800900
H	6.55811500	-2.37718900	1.85090800				
H	5.30037700	-3.37789500	1.12836700	6 ^s _BQ			
C	1.34746500	-1.62440000	-0.99398400	C	1.56654600	1.20217900	0.43142500
C	1.84233700	-2.59982600	-1.85939400	C	2.22871700	2.39364700	0.78375700
N	0.27362800	-1.93825900	-0.21789800	C	1.83472500	3.12863600	1.88943200
C	1.37055900	-3.91305900	-1.78929700	C	0.77804700	2.68275500	2.69240400
H	2.62970300	-2.36513200	-2.55706800	C	0.14793200	1.51943500	2.27660200
C	-0.12911000	-3.21970900	-0.09046000	N	0.51782800	0.82589700	1.17904300
C	0.41843000	-4.25637900	-0.84744200	H	2.35822900	4.04744500	2.13805800
H	1.78031700	-4.66804100	-2.45223500	H	3.06851200	2.74659300	0.20193600
H	0.05615400	-5.26803600	-0.71434100	H	-0.71213800	1.12947500	2.80699100
O	-1.10584300	-3.50831600	0.77817900	C	2.15875400	0.35057100	-0.71482700

C	2.39009000	1.30537400	-1.91206000	H	-1.70397600	-2.86999500	-1.78294000
H	3.07109700	2.11158800	-1.64154800	C	-3.68279200	-0.01708200	1.28196100
H	2.83581100	0.80840200	-2.76925200	O	-2.47621700	0.50677800	1.39327700
H	1.44973900	1.75211600	-2.23638900	O	-4.66075100	0.43212700	1.86731000
C	3.56822400	-0.13009900	-0.12024800	H	-0.59971000	-3.31843800	1.18894600
C	3.41458000	-1.07714700	1.08180500	O	-0.71349700	-1.57846000	2.27588500
C	4.56946600	-0.72545100	-1.12234700	O	-1.28055200	-2.77183600	2.28894900
H	4.03042000	0.79211900	0.24961300	C	-1.35459000	4.16437800	-0.57785100
C	4.76577100	-1.31696700	1.76813700	C	-0.97735700	4.83035100	-1.84835400
H	3.01041000	-2.03745300	0.73973000	C	-0.78513800	3.97009200	-3.04280100
H	2.69678100	-0.67477600	1.80389000	C	-0.89524500	2.63446900	-2.96000500
C	5.93062800	-0.94777100	-0.44389600	C	-1.17742100	1.98124400	-1.66583900
H	4.20321800	-1.68710200	-1.49641600	C	-1.47170100	2.82928400	-0.49547300
H	4.69465300	-0.06746100	-1.98770700	H	-1.53887500	4.81200200	0.27372400
C	5.80505900	-1.86018100	0.78125000	H	-0.54413700	4.47522300	-3.97299600
H	4.63754500	-2.00940700	2.60849200	H	-0.74465400	1.98025300	-3.81276200
H	5.12667300	-0.36911400	2.19126400	H	-1.77468700	2.32303800	0.41356000
H	6.63531300	-1.37482900	-1.16721300	O	-0.84071200	6.04809300	-1.91350700
H	6.34422600	0.02210800	-0.13442600	O	-1.13472700	0.74412000	-1.58826600
H	6.77797000	-1.97397500	1.27415800				
H	5.49731200	-2.86252800	0.45165400				
C	1.44829000	-0.94124400	-1.19185100				
C	1.87446200	-1.51958900	-2.37937200				
N	0.61476200	-1.66090300	-0.37195100				
C	1.57808200	-2.86270500	-2.65997500				
H	2.49963900	-0.97784200	-3.07021900				
C	0.43638300	-2.99498600	-0.56086000				
C	0.91868200	-3.62646600	-1.72787600				
H	1.91976300	-3.30382600	-3.59103200				
H	0.72111100	-4.68295600	-1.86310200				
O	-0.20541600	-3.74357500	0.30144600				
C	0.32805700	3.42561800	3.91771500				
H	-0.52253500	2.92933400	4.39160000				
H	1.13868200	3.49428600	4.65144500				
H	0.03204600	4.44938600	3.66399200				
Pd	-0.96681300	-0.55122600	0.49032900				
C	-4.87968500	-2.77111900	-1.02140400				
C	-4.93713900	-1.77927700	-0.04587100				
C	-3.74073700	-1.17351800	0.33493600				
C	-2.53761300	-1.59236800	-0.23687200				
C	-2.59078300	-2.55534000	-1.24392700				
N	-3.73999000	-3.13982500	-1.62609600				
H	-5.78531000	-3.27712000	-1.34934100				
H	-5.87673100	-1.46462500	0.39711300				