

Supporting Information

The Stabilizing Effect of the Transient Imine Directing Group in the Pd(II)-Catalyzed C(sp³)-H Arylation of Free Primary Amines

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I. Free energy profiles for the pivalate-assisted inner-sphere AMLA/CMD C(sp³)–H activation without the dissociation of pivalate

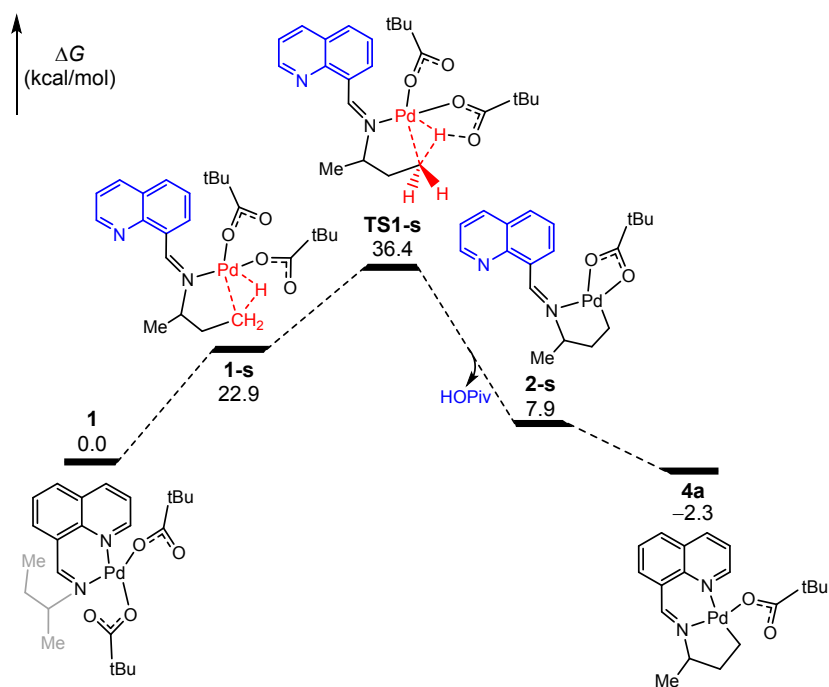


Fig. S1. Free energy profiles for the pivalate-assisted inner-sphere AMLA/CMD C(sp³)–H activation without the dissociation of pivalate.

II. Free energy profiles for the outer-sphere AMLA/CMD C(sp³)–H activation with the binuclear palladium species

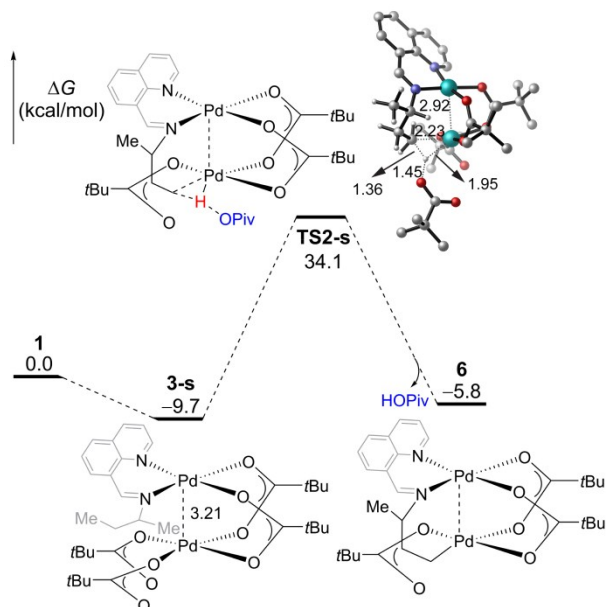


Fig. S2. Free energy profiles for the outer-sphere AMLA/CMD C(sp³)–H activation with the binuclear palladium species, and bond lengths are given in Å.

III. Cartesian coordinates of all the structures

Tables S1. Cartesian coordinates (in Å) of all the structures reported in the text of this manuscript

1a

C	1.7848670	-0.7258620	-0.0135130
H	1.7295300	-1.7651210	-0.3557240
H	1.9681480	-0.7388980	1.0691730
H	2.6455280	-0.2503200	-0.4958400
C	0.4924850	0.0284490	-0.3351170
H	0.3575890	0.0334060	-1.4262150
N	0.6545990	1.4404690	0.0688480
H	-0.1831750	1.9740110	-0.1546140
H	0.7653260	1.4946870	1.0818050
C	-0.7303860	-0.6756940	0.2906400
C	-2.0833150	-0.0734120	-0.1028250
H	-0.6197220	-0.6570040	1.3850620
H	-0.7110120	-1.7331530	-0.0066590
H	-2.9084220	-0.6360820	0.3486520
H	-2.1826250	0.9672090	0.2281140
H	-2.2252610	-0.0929040	-1.1908000

P

C	-3.8026150	-0.3252030	-0.5115640
H	-4.2939800	-1.3033020	-0.4766710
H	-4.4466480	0.4015290	-0.0047040
H	-3.7225800	-0.0245160	-1.5648230

C	-2.4175710	-0.3909300	0.1396780
H	-2.5438240	-0.7106260	1.1838680
N	-1.6390930	-1.4524480	-0.5312180
H	-1.4915680	-1.1972310	-1.5079000
H	-0.7120570	-1.5270350	-0.1193220
C	-1.7551750	1.0046850	0.1525280
H	-2.4965560	1.7221450	0.5283290
H	-1.5314180	1.3032210	-0.8813720
C	-0.4900570	1.1567400	1.0308340
H	-0.3247870	2.2312320	1.1837140
H	-0.6926720	0.7336740	2.0226980
C	0.7955510	0.5587780	0.4877670
C	1.4483810	-0.4933920	1.1496350
C	1.3838880	1.0679990	-0.6835830
C	2.6421620	-1.0311480	0.6535070
H	1.0172260	-0.8972560	2.0629830
C	2.5749620	0.5354970	-1.1831510
H	0.9059900	1.8923150	-1.2081360
C	3.2092050	-0.5202070	-0.5171900
H	3.1271390	-1.8467630	1.1835150
H	3.0110050	0.9471350	-2.0897950
H	4.1360000	-0.9342920	-0.9046220

Ar^QCHO

C	1.7405840	1.4040590	-0.0216750
C	1.3454310	0.0702190	-0.0069690
C	-0.0604240	-0.2454350	-0.0020210
C	-0.9977030	0.8418030	0.0051120
C	-0.5365500	2.1866020	0.0004130
C	0.8122400	2.4662010	-0.0156920

H	2.8040320	1.6302650	-0.0323710	N	0.8620850	1.3611680	-0.3633860
C	-2.3819350	0.5303850	0.0132300	C	-0.9996930	-1.0195390	-0.2284780
H	-1.2704590	2.9883360	0.0069470	H	-1.4021200	-2.0398760	-0.2604310
H	1.1646910	3.4926890	-0.0229570	C	-3.7578380	-1.6061070	-0.5634940
C	-2.7782060	-0.7870790	0.0090490	H	-4.8356160	-1.5676440	-0.7532400
C	-1.7778710	-1.7872600	-0.0083550	H	-3.6035540	-2.1769420	0.3602600
H	-3.1078430	1.3393040	0.0209160	H	-3.2990900	-2.1606460	-1.3896590
H	-3.8265650	-1.0674150	0.0149660	C	-3.2173660	-0.1736430	-0.4567650
H	-2.0695000	-2.8361510	-0.0197320	H	-3.4699740	0.3518370	-1.3906060
N	-0.4770430	-1.5426430	-0.0133700	N	-1.7638970	-0.0002740	-0.3152520
C	2.4603250	-0.9041270	0.0131690	C	-3.9156140	0.5933440	0.6899410
O	2.4056940	-2.1216040	0.1076930	C	-3.6391150	2.0989130	0.7198200
H	3.4504750	-0.4080330	-0.0606580	H	-3.6139930	0.1384070	1.6436830
1b				H	-4.9956600	0.4265890	0.5904590
C	1.0313190	-2.2769580	0.1747580	H	-4.1936080	2.5774200	1.5356880
C	0.4725290	-1.0231770	-0.0567200	H	-3.9517820	2.5760160	-0.2175430
C	1.3554170	0.1167300	-0.1037660	H	-2.5758280	2.3113870	0.8640470
C	2.7616800	-0.0910670	0.1122740	H₂O			
C	3.2684880	-1.3954620	0.3585030	O	0.0000000	0.0000000	0.1177710
C	2.4135720	-2.4736590	0.3848350	H	0.0000000	0.7693060	-0.4710840
H	0.3725850	-3.1412770	0.2008630	H	0.0000000	-0.7693060	-0.4710840
C	3.6194370	1.0390070	0.0680470	Pd₃(OPiv)₆			
H	4.3356780	-1.5223760	0.5203420	Pd	1.6254910	0.9513360	0.0089710
H	2.7912130	-3.4752350	0.5670540	C	-0.0326120	2.6542950	-1.8708770
C	3.0922530	2.2839570	-0.1847230	O	1.0734400	2.4018140	-1.3052350
C	1.6976330	2.3853300	-0.3996810	O	-1.1511950	2.1139480	-1.6009930
H	4.6849480	0.9006840	0.2327900	C	-2.3153340	-1.2584030	1.8633750
H	3.7159760	3.1712350	-0.2266070	O	-1.5233940	-2.0884440	1.3229180
H	1.2572830	3.3581420	-0.6139440				

O	-2.4163700	-0.0245770	1.5756250	C	0.3195800	2.9250890	4.3267440
Pd	-0.0026640	-1.8320480	0.0000400	C	1.1741760	4.7127270	2.7552920
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O	-2.6234560	-0.2353450	-1.3178430	H	-2.1265890	3.7254410	3.3118200
O	-1.2527370	-2.0165730	-1.5818430	H	-1.2653550	5.1508490	3.9205720
C	0.0392420	2.6543480	1.8695500	H	1.2870460	2.4153620	4.2953900
O	1.1559210	2.1099420	1.5999870	H	0.3298460	3.6323590	5.1634390
O	-1.0674590	2.4062880	1.3031910	H	-0.4591830	2.1795830	4.5230800
Pd	-1.6233980	0.9568220	-0.0100380	H	1.1862080	5.4522690	3.5635330
C	2.2778260	-1.3323370	1.8661490	H	2.1524920	4.2263560	2.7176570
O	2.6225310	-0.2422240	1.3174030	H	1.0198640	5.2475710	1.8110380
O	1.2469590	-2.0195260	1.5822340	C	-3.1737990	-1.8734630	-2.9997990
C	2.3122600	-1.2662330	-1.8630460	C	-4.4619150	-1.0463640	-3.1405090
O	2.4164870	-0.0325190	-1.5758860	C	-2.3565890	-1.7931920	-4.3104640
O	1.5177490	-2.0938320	-1.3225750	C	-3.5253300	-3.3442180	-2.6898210
C	-0.0352220	3.6926120	-3.0124780	H	-5.0605210	-1.0729870	-2.2244240
C	1.3164900	4.4196900	-3.1028270	H	-4.2472080	0.0001800	-3.3747260
C	-0.3061660	2.9257830	-4.3285700	H	-5.0676710	-1.4613080	-3.9538000
C	-1.1652370	4.7130810	-2.7592880	H	-1.4434380	-2.3922850	-4.2490120
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H	2.1371370	3.7260870	-3.3066690	H	-2.0773340	-0.7589950	-4.5419610
H	1.2774550	5.1516280	-3.9173450	H	-4.1529870	-3.7453760	-3.4932820
H	-1.2737990	2.4161710	-4.3001530	H	-2.6274980	-3.9632060	-2.6122140
H	-0.3139900	3.6332490	-5.1651290	H	-4.0841780	-3.4295100	-1.7506910
H	0.4730590	2.1802460	-4.5228840	C	3.2213880	-1.7833460	-2.9974720
H	-1.1747450	5.4529660	-3.5672470	C	3.2084910	-3.3198530	-3.0583200
H	-2.1436530	4.2267040	-2.7249150	C	2.6718500	-1.2042520	-4.3228240
H	-1.0138760	5.2474950	-1.8143190	C	4.6604080	-1.2791650	-2.7615970
C	0.0449150	3.6921570	3.0115960	H	3.5730710	-3.7625060	-2.1255280
C	-1.3065520	4.4191780	3.1059180	H	2.2047600	-3.7097710	-3.2488470

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H	3.2888420	-1.5579420	-5.1564450	H	-5.0605820	-1.6301870	1.8071340
H	1.6414740	-1.5306190	-4.5027010	1			
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H	4.7071260	-0.1869910	-2.7579450	C	3.2191170	0.9894310	-0.4137220
H	5.0570220	-1.6420110	-1.8063460	C	3.0679980	-0.3972360	-0.0870960
C	3.1680560	-1.8803380	3.0007640	C	4.1952310	-1.2645910	-0.2450340
C	4.4565920	-1.0542220	3.1435090	C	5.3876460	-0.7753720	-0.8450770
C	2.3495240	-1.8004390	4.3106040	C	5.4917720	0.5450110	-1.2224290
C	3.5189080	-3.3510970	2.6900070	H	4.5430050	2.4832570	-1.1805350
H	5.0563550	-1.0807190	2.2281830	C	4.1015840	-2.5946390	0.2347330
H	4.2422960	-0.0076560	3.3780330	H	6.2173660	-1.4632450	-0.9805150
H	5.0610160	-1.4700270	3.9573500	H	6.4029240	0.9221580	-1.6752950
H	1.4361220	-2.3989920	4.2478300	C	2.9449080	-3.0092620	0.8527720
H	2.9545920	-2.1820670	5.1405310	C	1.8500790	-2.1278160	0.9087570
H	2.0705930	-0.7662180	4.5424030	H	4.9530860	-3.2599600	0.1237970
H	4.1453410	-3.7533480	3.4938760	H	2.8409540	-4.0052640	1.2685830
H	2.6207140	-3.9693720	2.6108490	H	0.9081270	-2.4376740	1.3463950
H	4.0788020	-3.4360030	1.7514630	N	1.8887930	-0.8856350	0.4221240
C	-3.2251800	-1.7727310	2.9984840	C	2.2701080	2.0288270	-0.0246590
C	-3.2146050	-3.3091960	3.0612750	H	2.6984980	3.0300990	-0.0059340
C	-2.6747220	-1.1928600	4.3231050	N	1.0473240	1.8741320	0.3412380
C	-4.6634450	-1.2667190	2.7619320	C	0.3067380	3.0344880	0.9287650
H	-3.5799160	-3.7525250	2.1290960	H	-0.7395740	2.8411880	0.6990540
H	-2.2114490	-3.7003930	3.2522270	C	0.4930820	2.9853420	2.4522170
H	-3.8706470	-3.6397020	3.8742130	H	1.5333560	3.1990200	2.7246050
H	-2.6952600	-0.0988970	4.3187190	H	-0.1511010	3.7330280	2.9264320
H	-3.2920470	-1.5447810	5.1572290	H	0.2234440	2.0023010	2.8492100
H	-1.6447500	-1.5204090	4.5031730	C	0.6729850	4.4130830	0.3499910

H	1.7017860	4.6877580	0.6162710	H	-3.2192550	3.7239310	-0.7422590
H	0.0335420	5.1281040	0.8816880	H	-2.8154030	2.6564190	-2.1020630
C	0.4483670	4.5723110	-1.1577840	H	-4.4801730	3.2303390	-1.8828320
H	0.6570180	5.6028040	-1.4665110	H	-4.6392260	-0.3862460	-0.8179390
H	1.0945520	3.9152030	-1.7497580	H	-5.2990000	0.8123140	-1.9436040
H	-0.5886570	4.3457700	-1.4283760	H	-3.6297140	0.2389850	-2.1373890
Pd	0.1062610	0.0921500	0.0985410	H	-5.9192040	2.3454070	-0.0322290
C	-2.6425940	1.1769450	0.2658110	H	-5.2966980	1.1594560	1.1319470
O	-2.6547560	0.9795780	1.4880680	H	-4.7162660	2.8285840	1.1781780
O	-1.6058300	1.0125590	-0.5071680				
C	-1.3414580	-2.5236850	0.3682540	OPIv			
O	-1.2422770	-2.4967720	1.6069610	C	-1.0529970	0.0251020	-0.0276510
O	-0.8163870	-1.6531390	-0.4378410	O	-1.6207060	-1.1208340	-0.0211200
C	-2.0711820	-3.7096590	-0.3215200	O	-1.6353780	1.1669690	-0.0237630
C	-1.1327790	-4.9352200	-0.2233230	C	0.5193760	0.0064500	-0.0068540
C	-3.3765450	-4.0056010	0.4431250	C	1.0360610	-1.0131400	-1.0401150
C	-2.3875270	-3.4260430	-1.7992630	C	1.1167660	1.3913990	-0.3124610
H	-0.1898110	-4.7601030	-0.7548500	C	0.9624260	-0.4353420	1.4122630
H	-0.9007530	-5.1736780	0.8199710	H	0.6401790	-2.0131870	-0.8368740
H	-1.6137660	-5.8117120	-0.6744980	H	0.7377550	-0.7333240	-2.0624390
H	-4.0674010	-3.1555310	0.3987210	H	2.1377870	-1.0655560	-1.0235930
H	-3.8812410	-4.8729680	0.0006430	H	0.7737780	2.1438350	0.4036740
H	-3.1763130	-4.2221140	1.4960240	H	2.2139980	1.3505370	-0.2666070
H	-2.9096510	-4.2859950	-2.2369750	H	0.8336280	1.7407950	-1.3170520
H	-3.0321800	-2.5480400	-1.9102950	H	2.0534380	-0.4785190	1.4808650
H	-1.4781450	-3.2483700	-2.3806690	H	0.6021390	0.2683790	2.1754470
C	-3.9135370	1.6580020	-0.4907090	H	0.5661710	-1.4288570	1.6545470
C	-3.5799610	2.8902240	-1.3563600				
C	-4.3944160	0.5076390	-1.4027730	2			
C	-5.0239270	2.0171120	0.5098740	C	-4.2283010	0.9638320	-0.0852070

C	-2.8841950	0.5885560	-0.1065270	H	5.6899940	-2.0120690	-1.2463440
C	-2.5523680	-0.8014230	-0.0124280	H	4.0448010	-2.6763870	-1.2922390
C	-3.6162610	-1.7558280	0.0888520	H	6.2063430	0.0816330	0.0744810
C	-4.9672010	-1.3158150	0.1053250	H	4.9688270	0.9747730	-0.8261080
C	-5.2703900	0.0249380	0.0230200	H	4.9318260	0.9510110	0.9465690
H	-4.4722430	2.0198350	-0.1541630	C	-0.0836930	3.4539010	-1.8203500
C	-3.2986920	-3.1326450	0.1689610	H	0.6033650	4.2907600	-1.9803600
H	-5.7514720	-2.0630660	0.1832100	H	-1.1071980	3.8273520	-1.9343340
H	-6.3012420	0.3625960	0.0367120	H	0.1035530	2.7055230	-2.5970600
C	-1.9807440	-3.5285100	0.1500100	C	0.1491950	2.8679250	-0.4226090
C	-0.9850170	-2.5453260	0.0571720	H	1.1925910	2.5590620	-0.3470840
H	-4.1040180	-3.8576430	0.2430100	C	-0.1290620	3.8797980	0.7036180
H	-1.6897950	-4.5711080	0.2068250	H	-1.1762750	4.2044840	0.6602210
H	0.0618780	-2.8248490	0.0472350	H	0.4749260	4.7658690	0.4743380
N	-1.2522130	-1.2373500	-0.0180550	C	0.2151910	3.3780840	2.1090690
C	-1.9307500	1.6754210	-0.2360880	H	0.0273500	4.1617250	2.8511330
H	-2.3879190	2.6608340	-0.3300000	H	1.2723610	3.0972420	2.1811840
N	-0.6457380	1.6038110	-0.2529620	H	-0.3836080	2.5048410	2.3909820
Pd	0.4097100	-0.0770710	-0.0979390				
C	2.8209930	-0.5949470	-0.0177420	3			
O	1.9219740	-1.5108900	0.0435350	C	4.3957450	-0.1446450	-0.4843340
O	2.3845510	0.6061140	-0.1246300	C	3.0422160	0.0000440	-0.1795220
C	4.2997910	-0.9320500	0.0208450	C	2.2455090	-1.1742760	0.0296660
C	4.5713160	-1.7885760	1.2787860	C	2.8972490	-2.4498080	-0.0136210
C	4.6265110	-1.7505500	-1.2522270	C	4.2749690	-2.5383500	-0.3518140
C	5.1452360	0.3516730	0.0558090	C	5.0121240	-1.4036270	-0.6026930
H	4.3210620	-1.2402880	2.1938680	H	4.9927900	0.7521220	-0.6210520
H	3.9943560	-2.7177470	1.2631870	C	2.1543120	-3.6146100	0.2949330
H	5.6352890	-2.0453070	1.3159410	H	4.7302080	-3.5233150	-0.3957970
H	4.4226930	-1.1715610	-2.1598450	H	6.0642660	-1.4684760	-0.8590880

C	0.8264120	-3.5027670	0.6341460	H	-4.8791250	-2.6960390	-1.2844370
C	0.2285780	-2.2336450	0.6040970	H	-3.3801280	-1.9810060	-1.9042550
H	2.6503600	-4.5801480	0.2662270	H	-6.0116300	-1.7988260	0.7609520
H	0.2225230	-4.3638790	0.8965670	H	-4.5324160	-2.0156560	1.7130930
H	-0.8277140	-2.1185310	0.8029330	H	-5.3246230	-0.4304820	1.6608970
N	0.8959710	-1.1180900	0.2959360	C	-1.0769160	2.6921240	-0.8486260
C	2.5884190	1.3695630	0.0199850	H	-0.7955790	2.0666080	-1.7059750
H	3.3837380	2.1119020	0.0495020	H	-2.0300200	3.1504420	-1.1328370
C	2.2064190	4.1017490	0.7482180	H	-1.4166780	2.1200540	0.0646380
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H	2.7753160	4.2538540	-0.1753120	TS1			
H	2.8826560	3.7445620	1.5313190	C	4.4678650	0.1727960	-0.2082720
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H	0.4863500	3.0653550	1.4999440	C	2.3801450	-1.0666320	0.0333380
N	1.3767070	1.7549640	0.1971890	C	3.1488920	-2.2760480	-0.0083170
C	0.0151330	3.7064300	-0.4884230	C	4.5558330	-2.2271720	-0.2036270
H	0.5500640	4.0089820	-1.3958220	C	5.2067130	-1.0199710	-0.3170440
H	-0.4357420	4.6062700	-0.0597240	H	4.9935560	1.1224950	-0.2428520
Pd	-0.2167530	0.5744740	-0.0093850	C	2.4878940	-3.5165670	0.1629700
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O	-1.8746820	-0.5335920	-0.3688990	H	6.2811080	-0.9782450	-0.4623190
O	-3.0038200	0.6656330	1.1544510	C	1.1282540	-3.5374200	0.3665170
C	-4.2494830	-0.9435750	-0.1770460	C	0.4276470	-2.3203260	0.3520990
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C	-5.0772370	-1.3154710	1.0686360	H	-0.6496190	-2.3093390	0.4574500
H	-5.3081610	0.9554900	-0.4903940	N	1.0134890	-1.1335210	0.1793810
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4a

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H	0.0173290	-4.4310240	-0.0488380	H	-3.9900210	-2.8698650	0.6733000
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C	2.6620310	1.3009540	0.1528920	H	-1.8804480	2.5622540	-0.9807890
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C	1.2377370	3.2534120	0.3411820	C	-3.5724020	-0.2387380	0.4983230
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Pd	-0.2257810	0.7383640	-0.0886770	H	-6.7560020	-0.0817270	1.7951310
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H	-0.3874840	-1.6505360	-4.8757190	O	2.5499160	-0.5287930	-0.9299550
C	-0.9239200	-0.4188730	-3.1850380	C	1.9936980	-1.6079510	-1.3138420
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C	-1.3395500	0.8353300	-3.9768950	O	1.3169930	2.6307410	1.2852860
H	-2.3726690	0.7271030	-4.3300650	C	1.2921460	4.7983680	0.1221050
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C	1.1875080	-1.3282980	2.1908740	H	1.2916230	5.0886200	2.2962150
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TS2

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H	1.6427080	4.9118270	-3.3388150	H	-3.9465960	-4.2218670	-1.2216110
H	0.2443040	5.0465730	-2.2514280	C	-4.5430240	-0.3754290	2.3567630
H	1.4788350	6.3189250	-2.2692190	H	-6.3824840	-2.1785010	1.6580360
H	2.2040270	4.5357810	0.9581350	H	-6.0971940	-4.0056880	-0.0151930
H	1.8511620	6.1061660	0.2163800	C	-3.4958970	0.4784500	2.6051330
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H	4.2176380	4.2721900	-0.6466020	H	-3.5865860	1.3241480	3.2774790
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C	3.6577560	-3.6318920	-0.0080950	H	-1.9867190	-3.4898710	-1.8848150
C	1.5673950	-4.9557180	0.4844000	C	0.3094470	-3.9900370	-2.5872570
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H	2.6454490	-3.7077260	-2.5875860	H	0.3261220	-4.7492440	-1.7980130
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H	4.1466740	-2.9176090	-0.6760470	N	-0.6265310	-2.3189120	-0.9218890
H	2.1465350	-5.8839500	0.4288340	C	0.3298980	-1.5054610	-3.1299950
H	1.5636480	-4.6204570	1.5262870	H	-0.4294320	-1.8341940	-3.8587910
H	0.5360540	-5.1805840	0.1966670	H	1.2960930	-1.5841770	-3.6425330
				Pd	-0.0615070	-1.1326170	0.6156960
6				C	0.0293560	-0.0399500	-2.7916430
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C	1.3318420	1.1471490	1.9178670	H	-2.9323060	3.0047840	-0.3282130
O	1.6456920	1.6198250	0.8026880	H	-3.8687520	4.2332210	-1.2020550
O	0.5926930	0.1030000	2.1190450	H	-3.2951130	2.7826800	-2.0448340
C	1.7992960	1.8632130	3.2098730	H	-2.2385360	6.0025550	-0.4070260
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C	2.3574510	0.8345340	4.2140250	H	-0.5101580	5.8756310	-0.7899200
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H	3.7610550	2.4472910	2.4292130	H	5.1953530	-3.7684750	-0.2715940
H	2.5063800	3.6710000	2.1935850	H	3.5313840	-3.8340400	0.3425870
Pd	0.9147510	0.8472020	-1.1978640	H	6.2209200	-1.5851840	-0.9968030
O	1.9411850	-1.7137760	0.5122020	H	4.9110690	-1.3508700	-2.1681820
O	2.6113560	-0.3657150	-1.1641490	H	5.2779540	-0.0825140	-0.9903310
C	2.8279200	-1.2366660	-0.2765170				
C	-0.5214480	3.3295140	-1.7898490	7a			
O	0.4993180	3.7216420	-2.3830260	C	-2.8704520	-3.8570440	-0.4481470
O	-0.6573710	2.1742910	-1.2205640	C	-2.0871760	-2.7114630	-0.3173570
C	-1.7454560	4.2812670	-1.6565520	C	-2.4055390	-1.7687280	0.7135060
C	-1.9554160	5.0283870	-2.9880260	C	-3.4666320	-2.0843470	1.6228740
C	-3.0331690	3.5265340	-1.2839340	C	-4.2482030	-3.2552630	1.4266070
C	-1.4074690	5.2987990	-0.5419010	C	-3.9679140	-4.1203600	0.3930960
H	-1.0607200	5.5886090	-3.2726850	H	-2.6085480	-4.5766920	-1.2181800
H	-2.1884020	4.3303110	-3.8014650	C	-3.7048570	-1.2251790	2.7231190

H	-5.0594310	-3.4553740	2.1205130	H	-2.3507680	6.2536840	-0.5728820
H	-4.5595440	-5.0173290	0.2425280	H	-1.6030730	3.6614510	2.0208710
C	-2.9143850	-0.1137680	2.9012980	H	-2.2861590	5.2706430	1.7272130
C	-1.9347020	0.1783350	1.9387950	H	-3.1859320	3.8267310	1.2330740
H	-4.5046320	-1.4656400	3.4174400	H	-0.0996620	5.9024020	0.5136460
H	-3.0438650	0.5581160	3.7420490	H	0.5365660	4.2655420	0.7775700
H	-1.3445150	1.0831100	2.0059070	H	0.4640590	4.9382340	-0.8620110
N	-1.7052700	-0.5967920	0.8766780	C	1.1078350	0.7572730	-2.3034360
C	-0.9085090	-2.6515740	-1.1743480	H	0.0009250	0.9815440	-2.1591220
H	-0.6975990	-3.5760460	-1.7079360	H	1.3361700	1.6297510	-2.9265670
C	1.3781580	-3.1001170	-2.8013100	H	1.7443940	0.8299610	-1.4102130
H	2.3464480	-3.0639100	-3.3093520	C	3.9937390	-0.4527710	0.4838750
H	0.6079860	-3.2826240	-3.5600680	O	3.4991220	0.6288010	0.0475230
H	1.4073730	-3.9486200	-2.1105060	O	3.5757960	-1.6167460	0.2086560
C	1.1783990	-1.7699950	-2.0788520	C	5.2312670	-0.3169950	1.4399950
H	1.9563460	-1.6623740	-1.3045310	C	5.7283990	-1.6849790	1.9351290
N	-0.1045600	-1.6600480	-1.3140690	C	6.3687480	0.3883420	0.6704660
C	1.2981080	-0.5715010	-3.0306860	C	4.8264590	0.5456610	2.6541370
H	0.5830780	-0.6701250	-3.8571010	H	4.9491000	-2.2183690	2.4897780
H	2.3040850	-0.5984400	-3.4625740	H	6.0356940	-2.3260120	1.1023280
Pd	-0.4909570	0.1606830	-0.5825080	H	6.5919920	-1.5565500	2.6018590
C	-1.3928180	2.9092390	-0.6687040	H	6.0494250	1.3725870	0.3142580
O	-1.8299570	2.6352860	-1.7942410	H	7.2475160	0.5238080	1.3151650
O	-0.7960650	2.0419630	0.1098380	H	6.6837000	-0.2003080	-0.2008260
C	-1.4896310	4.3313020	-0.0652610	H	5.6774600	0.6786960	3.3354290
C	-2.2935750	5.2465180	-1.0021610	H	4.4824580	1.5343220	2.3357040
C	-2.1819870	4.2610900	1.3126390	H	4.0153250	0.0731760	3.2230710
C	-0.0572080	4.8872790	0.1011540				
H	-1.8246500	5.3219450	-1.9877700	TS3a			
H	-3.3152130	4.8790360	-1.1444250	C	-4.4125500	-2.1060620	-0.1631090

C	-3.1505920	-1.5147250	-0.1105120	O	0.6210330	1.8007530	-0.1668970
C	-2.9623270	-0.3591280	0.7210580	C	1.0429470	4.1192250	-0.6159200
C	-4.0667350	0.0928580	1.5162800	C	0.4059900	5.2981030	-1.3692470
C	-5.3347810	-0.5394510	1.4084610	C	1.0304420	4.4073070	0.8994870
C	-5.5107770	-1.6148630	0.5678070	C	2.5007560	3.9283850	-1.0945150
H	-4.5455110	-2.9876260	-0.7835540	H	0.4151400	5.1350190	-2.4509130
C	-3.8673520	1.1671060	2.4179860	H	-0.6343760	5.4543270	-1.0638250
H	-6.1544460	-0.1599570	2.0118340	H	0.9641440	6.2178590	-1.1566570
H	-6.4764670	-2.1024210	0.4827490	H	1.5068120	3.6010600	1.4638940
C	-2.6252090	1.7480380	2.5165440	H	1.5732660	5.3373960	1.1073160
C	-1.5991960	1.2896600	1.6727580	H	0.0063710	4.5305590	1.2725530
H	-4.7003470	1.5089570	3.0256250	H	3.0745700	4.8462830	-0.9180690
H	-2.4212550	2.5598230	3.2057580	H	2.9916020	3.1093490	-0.5602150
H	-0.6228470	1.7580260	1.6853020	H	2.5401670	3.7092240	-2.1682660
N	-1.7568010	0.2971680	0.7959680	C	1.1556900	-0.4562500	-2.2166280
C	-2.1061740	-2.2198150	-0.8489200	H	0.4847630	0.2796670	-2.6781140
H	-2.4239670	-3.1743030	-1.2640180	H	2.1535020	-0.0888760	-2.4822350
C	-0.4122200	-4.0359590	-2.2541090	H	1.6930910	-0.5749910	-0.9839730
H	0.4258730	-4.5800050	-2.7012210	C	2.9285940	-1.6701990	0.7385880
H	-1.1601080	-3.8748720	-3.0396020	O	2.8301670	-0.7600450	-0.1730970
H	-0.8424070	-4.6812220	-1.4810100	O	2.0949740	-2.5781920	0.9357140
C	0.1238100	-2.7257720	-1.6872210	C	4.2002910	-1.5610190	1.6293290
H	0.8331470	-2.9374690	-0.8763720	C	4.2902160	-2.7434810	2.6073140
N	-0.8880560	-1.8512720	-1.0189290	C	5.4532260	-1.5423260	0.7279940
C	0.8639380	-1.8768550	-2.7354530	C	4.1190960	-0.2391380	2.4247560
H	0.2671700	-1.8326760	-3.6558160	H	3.4250100	-2.7786680	3.2769640
H	1.7951830	-2.3980480	-2.9801360	H	4.3378630	-3.6999800	2.0759810
Pd	-0.1858960	-0.0413740	-0.5362230	H	5.1941210	-2.6513540	3.2224180
C	0.2703570	2.8077360	-0.9179610	H	5.4273600	-0.6993550	0.0315750
O	-0.5818210	2.7473990	-1.8170980	H	6.3592460	-1.4561180	1.3408690

H	5.5340450	-2.4656800	0.1408650	H	0.5950190	-0.5652630	4.0942070
H	5.0010110	-0.1291450	3.0683140	H	2.2704430	-0.2487170	3.6342100
H	4.0736930	0.6237800	1.7537500	H	2.2358240	-2.1490070	5.1742710
H	3.2303280	-0.2162070	3.0676260	H	1.0832240	-3.0353010	4.1717920
				H	2.7274320	-2.7395900	3.5789440
7b				C	1.6775150	3.6699770	1.3433880
C	-3.4613930	-1.4199580	-0.0423340	C	0.8760270	2.5826980	0.9918740
O	-2.5729260	-0.7326990	-0.7171940	C	-0.2020230	2.7799730	0.0632710
O	-3.3689800	-1.6115800	1.1784980	C	-0.3877580	4.0957940	-0.4790400
C	-4.6181330	-1.9877850	-0.8920750	C	0.4570810	5.1661030	-0.0795260
C	-5.6569180	-2.6654900	0.0158880	C	1.4743720	4.9602120	0.8235190
C	-5.2854870	-0.8429390	-1.6845310	H	2.4916810	3.5052940	2.0429280
C	-4.0287890	-3.0257970	-1.8745110	C	-1.4186800	4.3190900	-1.4227680
H	-5.2139220	-3.4866490	0.5874150	H	0.2804110	6.1471360	-0.5106940
H	-6.0920070	-1.9570620	0.7286150	H	2.1220300	5.7750130	1.1294890
H	-6.4692590	-3.0741020	-0.5964090	C	-2.2255780	3.2749520	-1.8061410
H	-4.5821860	-0.3732430	-2.3782880	C	-2.0110810	2.0137760	-1.2314590
H	-6.1259120	-1.2374060	-2.2675730	H	-1.5520120	5.3164170	-1.8314360
H	-5.6771240	-0.0690480	-1.0132630	H	-3.0233170	3.3942480	-2.5303510
H	-4.8320540	-3.4596200	-2.4814190	H	-2.6336700	1.1687240	-1.4975400
H	-3.2987970	-2.5671290	-2.5482010	N	-1.0521080	1.7699230	-0.3338060
H	-3.5329580	-3.8434710	-1.3381990	C	1.2449280	1.3182600	1.6075450
C	-0.0983720	-2.0603340	1.8092120	H	2.1305910	1.3418280	2.2416220
H	-0.4398720	-2.0695000	0.7388670	N	0.6294270	0.2044890	1.4592100
H	-0.9440330	-1.8925680	2.4799710	Pd	-0.9565540	-0.1481780	0.3754230
H	0.2269510	-3.0997050	1.9121990	C	3.6327780	-1.6592030	-0.9349760
C	1.0671920	-1.0884660	2.0516210	O	2.5343280	-1.8108060	-1.5439510
H	1.9416960	-1.4032200	1.4585200	O	3.7801780	-1.6232490	0.3241270
C	1.4500400	-0.9673980	3.5344840	C	4.9094000	-1.4845130	-1.8322940
C	1.8964590	-2.3025600	4.1441720	C	5.0015700	-2.6721770	-2.8124670

C	4.7536320	-0.1733690	-2.6327370	H	-1.5245750	-0.8512980	0.6633380
C	6.1975980	-1.4165790	-0.9961760	H	-0.9352760	-0.0568680	2.6254160
H	5.1105420	-3.6221400	-2.2735830	H	-2.0467400	-1.3139340	2.1367230
H	4.1021040	-2.7392910	-3.4314930	C	0.0634050	-1.9434730	2.0625980
H	5.8707960	-2.5628040	-3.4748720	H	-0.2593780	-2.8721140	1.5780300
H	4.6703360	0.6927780	-1.9635800	C	0.5602090	-2.2219680	3.4876890
H	5.6233210	-0.0091730	-3.2830060	C	-0.5282610	-2.8344510	4.3765950
H	3.8569870	-0.2014360	-3.2599620	H	0.9200870	-1.2825650	3.9276720
H	7.0691620	-1.2804410	-1.6509230	H	1.4159230	-2.9070400	3.4438150
H	6.1720790	-0.5839480	-0.2858770	H	-0.1265160	-3.0572200	5.3710810
H	6.3496910	-2.3352310	-0.4191660	H	-1.3759490	-2.1533970	4.5073060
				H	-0.9099490	-3.7707350	3.9519590
TS3b				C	4.4656870	-1.8187230	-0.0607160
C	-1.3129440	2.6979800	0.8441360	C	3.2593860	-1.1330320	0.0864260
O	-0.8838610	1.8727760	-0.0704690	C	3.0810410	0.1235640	-0.5987910
O	-0.9901360	2.6420550	2.0404210	C	4.1706850	0.6077400	-1.3984080
C	-2.3061730	3.7669590	0.3195000	C	5.3743460	-0.1389440	-1.5125330
C	-2.5530860	4.8392510	1.3929860	C	5.5219800	-1.3383240	-0.8551500
C	-1.7508790	4.4320580	-0.9564970	H	4.5883710	-2.7622550	0.4630890
C	-3.6361320	3.0494210	-0.0085740	C	4.0353340	1.8426470	-2.0794080
H	-2.9635660	4.4038240	2.3087170	H	6.1714710	0.2629280	-2.1314020
H	-1.6282910	5.3632690	1.6583110	H	6.4394110	-1.9113930	-0.9401870
H	-3.2673480	5.5816230	1.0167110	C	2.8653110	2.5543690	-1.9700410
H	-1.5953600	3.7002060	-1.7539580	C	1.8313870	2.0260470	-1.1806430
H	-2.4571830	5.1880350	-1.3206900	H	4.8635970	2.2053610	-2.6813290
H	-0.7964490	4.9364660	-0.7613590	H	2.7154760	3.5019180	-2.4753250
H	-4.3777610	3.7791050	-0.3559480	H	0.8867670	2.5470130	-1.0794090
H	-3.5007500	2.2979940	-0.7921570	N	1.9222370	0.8690170	-0.5224770
H	-4.0456710	2.5485800	0.8766450	C	2.2853270	-1.7821410	0.9563280
C	-1.0569110	-0.8950740	1.9302720	H	2.6058360	-2.7105530	1.4317310

N	1.1073080	-1.3427870	1.1916020	H	-3.7126810	-2.0212970	-1.7811550
Pd	0.2280520	0.2477240	0.5123830	H	-5.4214890	-1.5530860	-1.7628340
C	-2.3649330	-2.3483620	-0.8679540	H	-4.1684440	-0.3408170	-2.0896920
O	-2.3211520	-1.1259980	-0.4460970	H	-5.7295640	-2.5278870	0.5339040
O	-1.7797870	-3.3077770	-0.3242920	H	-4.0294450	-3.0251480	0.5876000
C	-3.2219850	-2.5649630	-2.1476200	H	-4.6936190	-2.0142690	1.8828660
C	-4.6730700	-2.1252130	-1.8553430	C	-0.6909760	2.6225390	0.1016010
C	-2.6408450	-1.6959960	-3.2841850	H	-1.0950890	3.0291960	-0.8306410
C	-3.2101960	-4.0410520	-2.5750120	H	-1.3588890	2.8406470	0.9385340
H	-5.1100950	-2.7141790	-1.0393950	C	0.7883270	3.0028710	0.3500900
H	-4.7168640	-1.0693820	-1.5732120	H	0.9577910	3.3515690	1.3781260
H	-5.2984640	-2.2712680	-2.7449290	C	1.4058790	4.0069120	-0.6325970
H	-1.6034050	-1.9750540	-3.5074770	C	0.8415490	5.4192550	-0.4465300
H	-3.2275310	-1.8304780	-4.2015810	H	1.2182240	3.6566000	-1.6560550
H	-2.6564400	-0.6352350	-3.0174960	H	2.4941880	4.0277790	-0.4933550
H	-3.8136590	-4.1709050	-3.4821790	H	1.2873420	6.1119580	-1.1688210
H	-2.1944580	-4.3883560	-2.7901660	H	-0.2441840	5.4415890	-0.5915190
H	-3.6250740	-4.6893530	-1.7962550	H	1.0539310	5.8016100	0.5592010
				C	4.4413960	-0.2665650	0.4633310
4b				C	3.0682860	-0.1093570	0.2703550
C	-2.9314400	-0.4575580	0.4661380	C	2.2699590	-1.2832590	-0.0171030
O	-2.0922020	-0.1923580	-0.4848270	C	2.9451470	-2.5490990	-0.0963940
O	-2.6884210	-0.3414860	1.6814070	C	4.3479320	-2.6406360	0.1090150
C	-4.3415450	-0.9309050	0.0140030	C	5.0877420	-1.5145090	0.3882750
C	-5.3360660	0.2018630	0.3580150	H	5.0340890	0.6180390	0.6796050
C	-4.4091230	-1.2261130	-1.4936920	C	2.1897050	-3.7141800	-0.3854750
C	-4.7186710	-2.1998970	0.8054220	H	4.8179390	-3.6176350	0.0408280
H	-5.3256000	0.4241730	1.4297830	H	6.1594120	-1.5777160	0.5482930
H	-5.0925860	1.1233380	-0.1846440	C	0.8332610	-3.6158880	-0.5834490
H	-6.3553470	-0.0926370	0.0788980	C	0.2363310	-2.3452970	-0.4833900

H	2.7015210	-4.6705250	-0.4455720	H	-1.3610700	-1.0663450	4.3381540
H	0.2197010	-4.4814850	-0.8086300	H	-2.8963360	-0.9721260	3.4412960
H	-0.8322730	-2.2227770	-0.6297420	C	-1.2883120	0.1887350	2.5382760
N	0.9081200	-1.2302500	-0.2110040	H	-2.0308950	0.7072310	1.9097010
C	2.5940200	1.2716650	0.3817420	N	-0.6668370	-0.8020430	1.6228310
H	3.3558710	2.0187970	0.6175120	C	-0.1840630	1.2060600	2.9093930
N	1.3801170	1.6459780	0.2271580	H	0.3463480	1.5584370	1.9823880
Pd	-0.2335600	0.6310780	-0.0855290	H	-0.6782190	2.1289740	3.2330740
				Pd	0.6659370	0.1260950	0.5204100
7c				C	0.8407240	0.7508840	3.9493370
C	-0.8328060	-4.3374030	0.8409070	H	1.3103120	-0.1997150	3.6755340
C	-0.4353420	-3.0171800	0.6304040	H	0.3671660	0.6285850	4.9288310
C	0.3692840	-2.7057050	-0.5167550	H	1.6343210	1.4968010	4.0554580
C	0.6872560	-3.7691200	-1.4259980	C	3.1346730	1.4992610	0.0452950
C	0.2657150	-5.0983790	-1.1524030	O	3.4760680	0.9808430	1.1165750
C	-0.4742670	-5.3836310	-0.0280650	O	1.9744600	1.2725630	-0.5206360
H	-1.4496780	-4.5583610	1.7070230	C	4.0417520	2.4775090	-0.7344720
C	1.4142950	-3.4772770	-2.6048140	C	5.3916870	2.6331640	-0.0161930
H	0.5370650	-5.8781670	-1.8578480	C	4.2720160	1.9302820	-2.1601290
H	-0.7987710	-6.3971100	0.1830110	C	3.3317730	3.8480990	-0.8124690
C	1.7991770	-2.1833870	-2.8632240	H	5.2647500	3.0234510	0.9983650
C	1.4969330	-1.1900530	-1.9197670	H	5.9216430	1.6778930	0.0574700
H	1.6496820	-4.2846140	-3.2919560	H	6.0259950	3.3321540	-0.5738490
H	2.3425480	-1.9092800	-3.7602860	H	3.3327070	1.8494300	-2.7148640
H	1.8182790	-0.1670240	-2.0683580	H	4.9360350	2.6049550	-2.7131670
N	0.8306570	-1.4359530	-0.7884820	H	4.7451150	0.9411530	-2.1351070
C	-0.9549110	-2.0496870	1.5864780	H	3.9638410	4.5634060	-1.3519210
H	-1.6640600	-2.4446620	2.3121060	H	2.3745710	3.7721750	-1.3364160
C	-2.0063930	-0.4115480	3.7431390	H	3.1427550	4.2550360	0.1880360
H	-2.3437940	0.4089970	4.3849300	C	-3.5542300	1.8458380	-0.4002510

O	-3.7420420	1.1992450	0.6738180	H	2.7393250	2.6579570	-3.0173810
O	-2.5175500	2.5111640	-0.6882650	H	0.8848770	1.9063230	-1.5417330
C	-4.6951350	1.8290460	-1.4788130	N	1.9069330	0.3258410	-0.7282100
C	-5.9068350	1.0008890	-1.0207610	C	2.1516220	-2.2204690	0.9365940
C	-5.1442160	3.2811000	-1.7457830	H	2.4279000	-3.1324840	1.4671310
C	-4.1317440	1.2254240	-2.7827820	C	0.2563030	-3.0072350	3.1586580
H	-5.6310920	-0.0412230	-0.8274310	H	-0.6488710	-3.3038040	3.6993180
H	-6.3418950	1.4017790	-0.0991890	H	0.8492260	-2.3564640	3.8095070
H	-6.6860670	1.0082900	-1.7951470	H	0.8300540	-3.9182870	2.9594660
H	-4.3053860	3.8928600	-2.0913920	C	-0.1519350	-2.3059880	1.8678290
H	-5.9305550	3.3071130	-2.5120180	H	-0.6752410	-3.0083430	1.2077390
H	-5.5487040	3.7454080	-0.8373610	N	0.9631580	-1.7641120	1.0619300
H	-4.8992330	1.2189090	-3.5683350	C	-1.0802310	-1.0680670	2.0026680
H	-3.2755160	1.8034550	-3.1436920	H	-1.6143700	-0.7086510	0.7902160
H	-3.8013510	0.1896620	-2.6315980	H	-2.1043000	-1.4520070	2.0842360
				Pd	0.2313180	-0.0744670	0.4418990
TS3c				C	-0.8485030	-0.1466250	3.2076840
C	4.4098270	-2.3032860	0.1081260	H	0.1889700	0.1878280	3.3024300
C	3.1948580	-1.6181270	0.1139900	H	-1.1239160	-0.6565830	4.1405800
C	3.0600210	-0.4292720	-0.6900530	H	-1.4752500	0.7471050	3.1293000
C	4.1825050	-0.0337790	-1.4926010	C	-0.3362780	2.7849320	0.6988700
C	5.3970110	-0.7707740	-1.4528740	O	0.6058170	2.8317140	1.5053000
C	5.5139590	-1.8875450	-0.6578830	O	-0.6890560	1.7194370	0.0366860
H	4.4976310	-3.1992680	0.7156020	C	-1.2201140	4.0281950	0.4107800
C	4.0647610	1.0986890	-2.3356270	C	-0.6025580	5.2834100	1.0482360
H	6.2254950	-0.4315580	-2.0679300	C	-1.3589430	4.2370460	-1.1115520
H	6.4391660	-2.4533970	-0.6243180	C	-2.6160420	3.7685730	1.0222240
C	2.8803240	1.7938570	-2.3779630	H	-0.4992560	5.1747520	2.1318670
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H	4.9156380	1.3948450	-2.9424520	H	-1.2409090	6.1529450	0.8500000

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H	-1.9863130	5.1141830	-1.3117380	C	-2.5770420	-3.4199950	0.1218910
H	-0.3832640	4.4125780	-1.5813290	H	-5.2122160	-3.0447870	0.2619140
H	-3.2685440	4.6323620	0.8457060	H	-6.3960760	-0.8500790	0.2331820
H	-3.0861260	2.8873290	0.5756150	C	-1.2058270	-3.4637670	0.0426310
H	-2.5530370	3.6114510	2.1057260	C	-0.5060810	-2.2465040	-0.0570380
C	-3.0507060	-1.8341970	-0.6256250	H	-3.1675010	-4.3287490	0.1989290
O	-2.5752500	-2.9341970	-0.2696500	H	-0.6575990	-4.3995490	0.0538670
O	-2.6461830	-0.6862790	-0.1931020	H	0.5764860	-2.2373920	-0.1288150
C	-4.2123230	-1.7745580	-1.6590080	N	-1.0923900	-1.0536400	-0.0778630
C	-4.6325690	-3.1865250	-2.0969830	C	-2.5798850	1.6354130	-0.1165330
C	-5.4151990	-1.0555050	-1.0113010	H	-3.2876810	2.4686370	-0.1118480
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H	-3.4486630	0.0443150	-2.6138080	H	1.1437050	2.7859290	-1.5561910
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4c				C	1.8840540	3.2042070	0.4310040
C	-4.5627560	0.2861330	0.0721490	H	1.6353650	3.0485910	1.4856450
C	-3.1699120	0.2987600	-0.0122730	H	2.0536590	4.2836970	0.2869070
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C	-3.2437480	-2.1678680	0.1039180	C	2.7932550	-0.5943790	0.4383080
C	-4.6609320	-2.1115660	0.1865170	O	2.5459470	-0.3857940	1.6398010
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				C	4.1223150	-1.2744440	0.0007340

C	5.0681290	-1.4408590	1.2008070	H	1.7233450	-0.0558530	-2.1645110
C	3.7887240	-2.6644680	-0.5861740	C	3.1986340	-1.3239780	1.2139280
C	4.8092380	-0.4131620	-1.0797880	H	1.7236920	-0.0555170	2.1645900
H	5.3282150	-0.4729920	1.6423610	C	3.7243180	-1.7780970	0.0000030
H	4.6169950	-2.0535650	1.9872810	H	3.6093050	-1.6747920	-2.1559650
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H	3.1325410	-2.5794510	-1.4578400	H	4.5487450	-2.4850120	0.0000040
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C	2.1358580	-0.4136010	1.2280080	H	2.4269910	-2.9957630	4.3116150
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H	0.8643180	-2.2358870	2.5323970	C	-1.4958750	-5.0799460	0.5963480
N	2.1988050	-1.1906430	1.3475320	H	-0.4983230	-5.1125540	-1.3209320
C	1.5589090	-0.4890350	3.5599750	H	-0.6713680	-2.6578360	-1.6626460
C	0.6226800	0.4669360	2.8169790	H	-2.6895060	-2.2825820	2.1471580
H	2.5180750	0.0012170	3.7718350	H	-2.5158550	-4.7395080	2.4713160
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H	-1.6881740	3.7214260	-0.8533340	C	-4.1957190	-0.5637250	2.2658580
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9

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H	-4.9211950	0.0704540	0.3021840	N	1.0397190	-1.4332220	-0.0494410
H	-4.9018090	-0.1369980	-1.4623760	C	2.6886040	0.9269580	-0.9226380
C	0.6452840	3.5083220	3.3969990	H	3.4711000	1.5283020	-1.3854590
C	1.6833940	3.0788380	2.5656840	C	1.9503340	2.3785350	-3.3489260
C	1.4176550	2.2590420	1.4587900	H	1.5857060	3.1741240	-4.0063070
C	0.1015490	1.8727530	1.2005980	H	1.8589220	1.4243570	-3.8790110
C	-0.9473540	2.2965660	2.0184460	H	3.0080620	2.5765940	-3.1562730
C	-0.6676630	3.1158970	3.1216810	C	1.1092810	2.3739940	-2.0714840
H	0.8578520	4.1435490	4.2522060	H	1.2718220	3.3096000	-1.5219750
H	2.7089200	3.3751750	2.7703320	N	1.4653790	1.2555820	-1.1318690
H	2.2396910	1.9351070	0.8314990	C	-0.3813790	2.2077660	-2.3671440
H	-1.9705480	1.9967680	1.8173450	C	-1.2316370	2.1419020	-1.0986080
H	-1.4849020	3.4442080	3.7586960	H	-0.5275610	1.3132570	-2.9807220
				H	-0.7237710	3.0708870	-2.9530480
TS5				H	-2.1844770	1.6286670	-1.2139360
C	4.5379980	-0.1961840	0.1390380	H	-1.4119830	3.1414160	-0.7181140
C	3.1730160	-0.2061720	-0.1483260	Pd	-0.1311800	0.3457860	-0.3095100
C	2.3925830	-1.3619690	0.1922660	C	-2.5924500	-1.0636230	-0.6790260
C	3.0735560	-2.4858530	0.7644490	O	-2.3006520	-0.9484870	-1.8767870
C	4.4589630	-2.4061090	1.0723560	O	-1.8271390	-0.6271810	0.2938030
C	5.1805450	-1.2711290	0.7796700	C	-3.8944900	-1.7558780	-0.2058230
H	5.1223130	0.6716130	-0.1532820	C	-4.7371410	-2.1725730	-1.4222680
C	2.3484130	-3.6778580	1.0062840	C	-3.5228670	-3.0088240	0.6188590
H	4.9339050	-3.2682060	1.5316230	C	-4.7043000	-0.7806840	0.6753160
H	6.2396160	-1.2107370	1.0071570	H	-5.0197470	-1.3076550	-2.0308720

H	-4.1958870	-2.8725560	-2.0660190	H	6.0463150	-0.8973190	-1.4702910
H	-5.6557580	-2.6631220	-1.0802610	C	1.6702300	-3.5645060	1.2765320
H	-2.9405810	-2.7472960	1.5075480	C	0.7198170	-2.6313380	0.8372860
H	-4.4363470	-3.5177140	0.9476890	H	3.7503100	-4.1046820	1.2008790
H	-2.9423650	-3.7214960	0.0207810	H	1.3497880	-4.3869900	1.9056960
H	-5.6401300	-1.2586830	0.9875050	H	-0.3203430	-2.7368190	1.1209830
H	-4.1509000	-0.4988660	1.5753760	N	1.0235200	-1.5862210	0.0603110
H	-4.9639340	0.1330030	0.1274830	C	1.7892510	0.7570380	-1.6449750
C	-0.8472570	3.3324340	3.3650610	H	2.2775770	1.5266990	-2.2438220
C	0.3033500	3.4512810	2.5809040	C	-1.1048340	1.5559430	-3.1914100
C	0.3947830	2.8027070	1.3436450	H	-1.4888900	2.4200910	-3.7430840
C	-0.6696750	2.0038060	0.9003380	H	-1.9550620	1.0056130	-2.7823700
C	-1.8345540	1.8976900	1.6705360	H	-0.5733230	0.9104130	-3.8982580
C	-1.9136000	2.5552400	2.9022640	C	-0.1568240	2.0489190	-2.0903760
H	-0.9144370	3.8433680	4.3211190	H	0.6394390	2.6313480	-2.5688430
H	1.1404490	4.0545600	2.9220750	N	0.5213920	0.8776790	-1.4493320
H	1.2935930	2.9293060	0.7545710	C	-0.8565730	2.9688800	-1.0727740
H	-2.6677570	1.2992580	1.3274200	C	0.0667950	3.8056690	-0.1593760
H	-2.8188750	2.4562500	3.4954020	H	-1.5767200	2.3999190	-0.4790570
10				H	-1.4455830	3.6710040	-1.6746460
C	4.0242250	-0.1363250	-1.5459420	H	-0.5367570	4.6390780	0.2236030
C	2.6888970	-0.2767970	-1.1645340	H	0.8597850	4.2597060	-0.7659140
C	2.3184490	-1.3877910	-0.3429420	Pd	-0.5916410	-0.4500130	-0.4240840
C	3.3367520	-2.3088950	0.0670990	C	-2.9884560	-0.7415840	0.0864890
C	4.6806740	-2.1164430	-0.3522780	O	-2.5595360	0.2515940	-0.5993700
C	5.0208500	-1.0464420	-1.1490490	O	-2.0877140	-1.5612200	0.4987630
H	4.3009870	0.7094990	-2.1686160	C	-4.4636270	-0.9697940	0.3565630
C	2.9806020	-3.4051480	0.8882880	C	-4.6396840	-1.6092640	1.7479300
H	5.4293840	-2.8327840	-0.0270940	C	-5.2307880	0.3626850	0.2739390
				C	-4.9738330	-1.9420300	-0.7395090

H	-4.1122330	-2.5642240	1.8219450	C	4.3640710	-0.1703200	1.4638470
H	-4.2676490	-0.9483390	2.5385930	C	4.4810390	-1.1751010	-0.8564610
H	-5.7042590	-1.7910000	1.9290700	C	4.5005500	1.3405880	-0.5624280
H	-5.1306910	0.8280340	-0.7107440	H	3.9834990	0.6478310	2.0845210
H	-6.2942930	0.1767940	0.4570920	H	3.9944050	-1.1172760	1.8698070
H	-4.8768000	1.0749970	1.0269110	H	5.4572110	-0.1712590	1.5331170
H	-6.0394640	-2.1354310	-0.5764920	H	4.1868130	-1.0831530	-1.9077430
H	-4.8546190	-1.5132920	-1.7402180	H	5.5750490	-1.1877930	-0.8091890
H	-4.4425980	-2.8986180	-0.7044030	H	4.1108180	-2.1321780	-0.4783670
C	1.8523240	1.8582880	3.2924710	H	5.5948040	1.3200560	-0.5229420
C	2.6615940	2.4737890	2.3327710	H	4.2017310	1.5031600	-1.6033820
C	2.0836040	3.0875300	1.2149330	H	4.1541690	2.1922990	0.0300610
C	0.6923300	3.0982700	1.0301830	C	-3.9523690	0.0048200	0.0222180
C	-0.1088320	2.4815560	2.0074180	C	-4.3670290	-0.1659620	-1.4630260
C	0.4623420	1.8664380	3.1252340	C	-4.4816070	-1.1805300	0.8526310
H	2.2971980	1.3833100	4.1627250	C	-4.4971120	1.3365050	0.5706020
H	3.7418510	2.4800400	2.4534990	H	-3.9904840	0.6566470	-2.0799800
H	2.7226790	3.5691410	0.4779220	H	-3.9957740	-1.1097530	-1.8753050
H	-1.1906020	2.4896060	1.8974690	H	-5.4603450	-0.1700000	-1.5295070
H	-0.1780280	1.3997380	3.8694830	H	-4.1860800	-1.0942040	1.9039560
				H	-5.5757050	-1.1909790	0.8066920
Pd(OPiv)₂				H	-4.1140870	-2.1369060	0.4701910
Pd	-0.0000200	0.0125140	-0.0046580	H	-5.5914610	1.3190530	0.5326350
C	-2.4375870	0.0124850	0.0542670	H	-4.1959560	1.4924960	1.6120250
O	-1.7491750	1.0953110	0.0036400	H	-4.1487670	2.1900030	-0.0179430
O	-1.7458020	-1.0693450	0.0901320				
C	2.4376610	0.0132110	-0.0582350	11			
O	1.7486680	-1.0701770	-0.0122500	C	-1.6463180	-0.5221430	2.3016030
O	1.7465330	1.0946160	-0.0952960	C	-1.1830950	-0.8534890	1.0320460
C	3.9523590	0.0082650	-0.0210540	C	-2.0194650	-0.5512920	-0.1027990

C	-3.2617540	0.1349310	0.1222310	C	2.1509980	1.8095100	1.1581180
C	-3.6654690	0.4787750	1.4406620	C	2.7703460	1.1438440	0.0895250
C	-2.8738180	0.1424230	2.5154660	C	2.5619860	1.6432730	-1.2077080
H	-1.0285500	-0.7674620	3.1618250	C	1.7563830	2.7629910	-1.4294200
C	-4.0664350	0.4464120	-1.0049960	H	0.5141090	4.2841790	-0.5246890
H	-4.6084500	1.0006950	1.5812410	H	0.8719370	3.4267830	1.7884060
H	-3.1803720	0.3902480	3.5272320	H	2.2998890	1.4432420	2.1714170
C	-3.6519720	0.0682010	-2.2606850	H	3.0349900	1.1516640	-2.0543790
C	-2.4306550	-0.6374530	-2.3761230	H	1.6095460	3.1283300	-2.4426030
H	-5.0043100	0.9750750	-0.8551060				
H	-4.2395610	0.2873620	-3.1465510	12			
H	-2.0957790	-0.9718860	-3.3569820	Pd	-0.0006910	-0.0124760	-0.1259160
N	-1.6446720	-0.9370460	-1.3562770	C	-2.9028190	-0.6473840	-0.6122610
C	0.1608120	-1.4690110	0.9922490	O	-2.0333730	0.1727640	-0.1050970
H	0.5039280	-1.8030510	1.9853830	O	-2.6301050	-1.7251780	-1.1737440
C	2.2055550	-3.5994580	-0.4833660	C	-4.3726050	-0.1705920	-0.4726280
H	3.1643640	-4.1110080	-0.3426780	C	-5.3332680	-1.2245990	-1.0461960
H	2.0167090	-3.5076530	-1.5591060	C	-4.6890920	0.0565290	1.0214870
H	1.4162920	-4.2242310	-0.0516880	C	-4.5364810	1.1543420	-1.2495110
C	2.2319070	-2.2153990	0.1850150	H	-5.1365470	-1.4134970	-2.1059880
H	2.4286830	-2.3549130	1.2635640	H	-5.2458780	-2.1780240	-0.5154140
N	0.9280860	-1.5831990	-0.0216070	H	-6.3673870	-0.8729960	-0.9483230
C	3.3636930	-1.3547130	-0.4090070	H	-4.0453180	0.8278260	1.4535400
C	3.6897960	-0.0399810	0.3333770	H	-5.7322350	0.3735950	1.1390860
H	3.1372890	-1.1513770	-1.4628610	H	-4.5515910	-0.8654240	1.5992580
H	4.2706310	-1.9716620	-0.3983540	H	-5.5728440	1.5055320	-1.1767250
H	4.7040540	0.2585770	0.0346330	H	-3.8818940	1.9336500	-0.8489830
H	3.7390500	-0.2389090	1.4111840	H	-4.3014570	1.0227210	-2.3127120
C	1.1412450	3.4135250	-0.3533200	C	2.8977980	0.6219870	-0.5905900
C	1.3432020	2.9320070	0.9430140	O	2.0329000	-0.1951250	-0.0762530

O	2.6206660	1.6907330	-1.1701040	C	0.7464470	2.4619650	2.1612720
C	4.3850480	0.1997900	-0.4598360	H	0.5186710	2.9906010	3.0927460
C	4.5618310	-1.1233290	0.3019000	H	1.7572700	2.7499450	1.8489320
C	4.9552560	0.0532280	-1.8883120	H	0.7446610	1.3878060	2.3700680
C	5.1354990	1.3274000	0.2824300	C	-0.2857120	2.8209910	1.0919910
H	4.1724360	-1.0579860	1.3228780	H	-1.2776620	2.4968630	1.4267660
H	4.0505520	-1.9495470	-0.2012980	N	-0.0028970	2.0652050	-0.1648980
H	5.6284810	-1.3720160	0.3610660	H	-0.6926640	2.3160220	-0.8727690
H	4.8542750	0.9864550	-2.4499110	H	0.9252700	2.3017800	-0.5426720
H	6.0189950	-0.2089780	-1.8414160	C	-0.3214510	4.3399110	0.8322010
H	4.4379660	-0.7385480	-2.4436510	C	-1.4304260	4.8142260	-0.1142050
H	6.1994990	1.0763470	0.3662570	H	0.6593130	4.6540090	0.4482160
H	5.0473730	2.2782790	-0.2510490	H	-0.4477610	4.8332570	1.8041700
H	4.7424780	1.4660150	1.2969110	H	-1.4276900	5.9073820	-0.1895470
C	-0.7566100	-2.4837010	2.1502570	H	-1.3097360	4.4228120	-1.1313330
H	-0.5373690	-3.0184950	3.0802850	H	-2.4194290	4.5090760	0.2488400
H	-1.7703990	-2.7575580	1.8348440				
H	-0.7420800	-1.4103480	2.3626940	TS6			
C	0.2728720	-2.8518600	1.0814870	Pd	0.1682220	-0.4216310	-0.3019120
H	1.2678820	-2.5394910	1.4180200	C	2.5768600	0.1231140	-0.9972050
N	-0.0003730	-2.0901440	-0.1742710	O	2.1553700	-0.7871160	-0.1723720
H	-0.9274970	-2.3233130	-0.5567630	O	1.7329700	0.8790630	-1.5451730
H	0.6918000	-2.3414740	-0.8796400	C	4.0783670	0.2004300	-1.2824250
C	0.2908100	-4.3706210	0.8186330	C	4.4591770	-1.0487040	-2.1141800
C	1.3915680	-4.8569690	-0.1312260	C	4.4042280	1.4742420	-2.0790920
H	-0.6945320	-4.6727370	0.4366470	C	4.8585530	0.1947680	0.0493890
H	0.4136570	-4.8670120	1.7894950	H	4.2585870	-1.9720750	-1.5618630
H	1.3754840	-5.9499630	-0.2075140	H	3.9022940	-1.0828440	-3.0576290
H	1.2727430	-4.4632810	-1.1477010	H	5.5284110	-1.0175990	-2.3527310
H	2.3851470	-4.5642820	0.2292570	H	4.1369270	2.3765350	-1.5191130

H	5.4797540	1.5092050	-2.2861460	C	-0.0334260	4.4439300	1.8579270
H	3.8707090	1.4993160	-3.0338550	C	-1.4512310	4.8072650	1.4037960
H	5.9345810	0.2317300	-0.1557380	H	0.7021800	4.9056090	1.1827130
H	4.6024540	1.0646710	0.6648100	H	0.1450810	4.8718010	2.8539770
H	4.6521380	-0.7080650	0.6311480	H	-1.6014540	5.8929390	1.4196670
C	-2.8241970	-0.4993590	-0.7525950	H	-1.6516930	4.4669060	0.3813390
O	-1.7210900	0.1790780	-0.7094520	H	-2.2065890	4.3585740	2.0615910
O	-2.9422170	-1.6956390	-0.4183120	C	-0.6981700	-1.6711050	2.7869880
C	-4.0618380	0.2657600	-1.2848350	H	-0.3871810	-1.8769970	3.8161420
C	-3.7784150	1.7595210	-1.5104300	H	-1.7846490	-1.8063850	2.7275850
C	-4.4614850	-0.3934320	-2.6250650	H	-0.4692620	-0.6251110	2.5612750
C	-5.2092600	0.1038670	-0.2653700	C	0.0260150	-2.6109180	1.8248480
H	-3.4904220	2.2587750	-0.5795590	H	1.1074970	-2.4533510	1.9068420
H	-2.9770070	1.9157720	-2.2386430	N	-0.3448990	-2.2749090	0.4173710
H	-4.6826550	2.2506480	-1.8895230	H	0.0925200	-2.9349500	-0.2256040
H	-4.6989240	-1.4530040	-2.4893940	H	-1.3667450	-2.3209290	0.2622130
H	-5.3456240	0.1073800	-3.0370170	C	-0.2832110	-4.0898820	2.1326980
H	-3.6547350	-0.3146320	-3.3636160	C	0.5369250	-5.1081260	1.3318830
H	-6.1112880	0.6042790	-0.6366580	H	-1.3571290	-4.2656740	1.9814360
H	-5.4438630	-0.9510110	-0.0975380	H	-0.0902210	-4.2392900	3.2023330
H	-4.9481740	0.5536000	0.7001790	H	0.3143110	-6.1267710	1.6683320
C	1.6485120	2.6577880	2.4903630	H	0.3193760	-5.0730350	0.2578070
H	1.7683840	3.1085130	3.4817670	H	1.6130420	-4.9418020	1.4636190
H	2.4188020	3.0839280	1.8339840				
H	1.8352290	1.5822930	2.5758360	13			
C	0.2502840	2.9271320	1.9274210	C	0.9427330	2.8776460	1.6539510
H	-0.4902730	2.4780530	2.6044510	H	1.5076390	3.7591980	1.9706660
N	0.1125460	2.2272090	0.6350840	H	1.6143850	2.0134040	1.6686350
H	0.7615420	2.6134350	-0.0492490	H	0.1474790	2.7123290	2.3896980
H	-0.8240520	2.3376250	0.2533580	C	0.3539170	3.0987490	0.2614600

H	-0.2718180	4.0026820	0.2871580	H	-5.4867010	0.6743850	0.6780640
N	-0.5721600	1.9729670	-0.0807830	C	3.4576760	-2.0393520	0.0922670
H	-1.0065560	2.1664210	-0.9853570	C	3.7858670	-2.0960740	1.6062650
H	-1.3410510	1.9098010	0.5984140	C	3.2920210	-3.4652400	-0.4608890
C	1.3961600	3.2695200	-0.8532160	C	4.5836570	-1.2988210	-0.6578160
C	2.2412130	4.5409710	-0.7149010	H	3.9164730	-1.0927370	2.0240850
H	2.0475480	2.3887590	-0.8735660	H	2.9942490	-2.6051780	2.1668130
H	0.8656990	3.2968940	-1.8150400	H	4.7185030	-2.6521660	1.7516570
H	2.8612050	4.5241560	0.1879520	H	3.0503580	-3.4546810	-1.5291430
H	2.9138260	4.6466890	-1.5730940	H	4.2314740	-4.0132730	-0.3307140
H	1.6117580	5.4386570	-0.6741250	H	2.5023420	-4.0128220	0.0614500
Pd	0.0630400	0.0202390	-0.1703390	H	5.5226840	-1.8501110	-0.5384060
C	2.1583780	-1.2627110	-0.0513680	H	4.3664750	-1.2263140	-1.7293230
O	1.0288800	-1.8395430	-0.2226440	H	4.7280770	-0.2873620	-0.2678430
O	2.1355690	0.0196110	0.0351210				
C	-2.8518440	-0.1820380	0.2784540	TS7			
O	-1.8493250	-0.5364340	-0.4760710	C	2.3636640	4.1986580	0.6907380
O	-2.7849400	0.6566710	1.1929680	H	2.0828770	5.2409240	0.8744280
C	-4.1729150	-0.9138640	-0.0645810	H	3.0172760	4.1700950	-0.1894230
C	-4.5164560	-0.6659650	-1.5495220	H	2.9343350	3.8456210	1.5568670
C	-3.9694760	-2.4260270	0.1795050	C	1.1097790	3.3477230	0.4726970
C	-5.3138800	-0.3965800	0.8255910	H	0.4753460	3.4015790	1.3650310
H	-4.6397840	0.4043220	-1.7553910	N	1.4874130	1.9059010	0.3277580
H	-3.7351090	-1.0535280	-2.2094110	H	2.0102280	1.6095890	1.1536720
H	-5.4591110	-1.1660690	-1.8013060	H	2.1179050	1.7675460	-0.4677560
H	-3.6976180	-2.6256810	1.2230030	C	0.2941910	3.7922960	-0.7444540
H	-4.8994290	-2.9663030	-0.0341080	C	-1.0416660	3.0628490	-0.8839790
H	-3.1812470	-2.8307340	-0.4619160	H	0.8983500	3.6617820	-1.6522940
H	-6.2407530	-0.9280610	0.5795430	H	0.1018010	4.8667400	-0.6453240
H	-5.0994870	-0.5581670	1.8864980	H	-1.6193230	3.4303760	-1.7392650

H	-0.9089110	1.9786380	-1.1267630	H	-4.3507220	-3.3808230	0.2976740
H	-1.6592140	3.1525030	0.0124240	H	-2.6455610	-3.1131650	-0.1174470
Pd	-0.0391590	0.5728250	0.0338060	H	-5.9145910	-1.4359310	0.6473280
C	-2.6318540	-0.3607590	0.2411580	H	-4.8461370	-0.7723310	1.8974100
O	-1.5124090	-0.7764410	-0.2791270	H	-5.3376900	0.2376800	0.5305790
O	-2.7111010	0.7194760	0.8557520				
C	2.2914850	-1.1160900	-0.3107710	14			
O	1.2178520	-0.9681730	0.4203020	C	-3.2898070	3.7753220	0.0229470
O	2.6596080	-0.3302730	-1.1944120	H	-3.3073670	4.8181810	-0.3103720
C	3.0815700	-2.4102060	0.0209940	H	-3.4389860	3.7609260	1.1092130
C	4.4074440	-2.4287620	-0.7562530	H	-4.1311940	3.2559280	-0.4489160
C	3.3641880	-2.4726600	1.5365200	C	-1.9594730	3.1234900	-0.3564100
C	2.2156580	-3.6202550	-0.3975060	H	-1.8438610	3.1384370	-1.4459780
H	4.2406370	-2.3986970	-1.8371540	N	-1.9528510	1.6745080	0.0291500
H	5.0413320	-1.5759480	-0.4913970	H	-2.6670920	1.1734200	-0.5010390
H	4.9577670	-3.3472680	-0.5202360	H	-2.2068380	1.5610390	1.0138130
H	2.4364130	-2.5004760	2.1143610	C	-0.7464590	3.8119770	0.2742380
H	3.9410790	-3.3754540	1.7690720	C	0.5718580	3.1164570	-0.0741500
H	3.9495200	-1.6068030	1.8690710	H	-0.8711830	3.8536050	1.3639490
H	2.7653710	-4.5504550	-0.2109140	H	-0.7134350	4.8471000	-0.0829660
H	1.2803540	-3.6546490	0.1688370	H	1.4477080	3.6847650	0.2577190
H	1.9695060	-3.5834600	-1.4652740	H	0.7481960	2.1877000	0.5588640
C	-3.8467790	-1.2834310	0.0172420	H	0.6914950	2.9492570	-1.1494470
C	-4.1835940	-1.2694600	-1.4922890	Pd	-0.1394660	0.7459490	-0.1979070
C	-3.4900870	-2.7199870	0.4551470	C	2.6100140	0.0052510	0.3363230
C	-5.0549290	-0.7783180	0.8223290	O	1.6293460	-0.1852210	-0.5015890
H	-4.4281910	-0.2572470	-1.8358070	O	2.5425530	0.7396940	1.3338760
H	-3.3460920	-1.6417830	-2.0903060	C	-1.8257770	-1.5272720	0.3239850
H	-5.0528840	-1.9092440	-1.6853440	O	-1.0367980	-1.0165120	-0.5831460
H	-3.2273730	-2.7569120	1.5189940	O	-2.1037040	-0.9832580	1.4017060

C	-2.4024430	-2.9239990	-0.0266750	H	-2.2584650	4.1088800	1.6426810
C	-3.9229980	-2.8978380	0.2302270	H	-3.3147710	4.0777530	0.2136810
C	-2.1303140	-3.3281220	-1.4851900	C	-1.2771440	3.4111780	-0.1699320
C	-1.7315440	-3.9397100	0.9264930	H	-1.3392130	3.6005020	-1.2479150
H	-4.1446110	-2.6258620	1.2658950	N	-1.5844910	1.9573780	0.0032700
H	-4.4240690	-2.1774760	-0.4278120	H	-2.3891180	1.6879810	-0.5636280
H	-4.3512170	-3.8875220	0.0327420	H	-1.8413730	1.7398680	0.9699480
H	-1.0588630	-3.3751520	-1.6995260	C	0.1691010	3.6153960	0.2732580
H	-2.5601060	-4.3188690	-1.6762220	C	1.0956310	2.6187450	-0.4365060
H	-2.5840320	-2.6232980	-2.1902100	H	0.2376780	3.4934710	1.3627320
H	-2.1185210	-4.9461790	0.7276430	H	0.4719270	4.6466320	0.0492180
H	-0.6450350	-3.9616660	0.7838420	H	2.1404450	2.9201990	-0.2824220
H	-1.9357050	-3.6946940	1.9734760	H	1.6812100	1.5035790	0.2500900
C	3.8977480	-0.7779450	-0.0244340	H	0.9696200	2.6495540	-1.5267230
C	5.0067700	-0.4760630	0.9953560	Pd	-0.0038970	0.7062160	-0.3615950
C	3.5764490	-2.2888910	-0.0108950	C	2.5992590	-0.3305650	0.0671780
C	4.3625830	-0.3571950	-1.4359820	O	1.5650480	-0.6211290	-0.6149820
H	5.2610850	0.5887110	1.0087200	O	2.6885050	0.7757100	0.6970860
H	4.7087460	-0.7614800	2.0091790	C	-2.1574070	-1.1773140	0.3563730
H	5.9110110	-1.0387240	0.7338850	O	-1.2843420	-0.8918600	-0.5633800
H	2.8112220	-2.5389640	-0.7513860	O	-2.3124980	-0.5336040	1.4091590
H	4.4802400	-2.8663060	-0.2402590	C	-3.0409290	-2.4093990	0.0240810
H	3.2153440	-2.6082610	0.9740960	C	-3.9596300	-2.7478110	1.2087750
H	5.2853100	-0.8879720	-1.6995200	C	-3.9000450	-2.0666140	-1.2140170
H	3.6053840	-0.5909230	-2.1899540	C	-2.1361080	-3.6189530	-0.2927560
H	4.5709370	0.7186680	-1.4815590	H	-3.3825710	-2.9961290	2.1056860
				H	-4.6201050	-1.9116060	1.4581180
				H	-4.5845260	-3.6130510	0.9561610
				H	-3.2731050	-1.8497950	-2.0842280
				H	-4.5528810	-2.9118410	-1.4635000
TS8							
C	-2.2960530	4.2843820	0.5607240				
H	-2.0882640	5.3444010	0.3800320				

H -4.5392440 -1.1954240 -1.0247580
H -2.7518300 -4.4989880 -0.5149340
H -1.4954090 -3.4196060 -1.1561100
H -1.4914820 -3.8669420 0.5591600
C 3.7353400 -1.3558030 0.1622360
C 3.3797080 -2.2991320 1.3391800
C 3.8306340 -2.1653730 -1.1443730
C 5.0736500 -0.6505190 0.4457830
H 3.2989980 -1.7476090 2.2822290
H 2.4339670 -2.8213300 1.1606990
H 4.1689350 -3.0510010 1.4517260
H 4.0530430 -1.5160180 -1.9987670
H 4.6378010 -2.9013470 -1.0599580
H 2.9000140 -2.6986700 -1.3549970
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H 5.3298150 0.0545100 -0.3528530
H 5.0475730 -0.0997640 1.3899210

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C -4.8857330 -0.8653760 0.0588360
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H -4.9577090 -0.9716870 1.1484970
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C -3.5635400 -0.2148310 -0.3404280
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N -2.3829140 -1.0576230 0.0579080
H -2.3449920 -1.9104850 -0.5020800
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C -3.2997920 1.1569570 0.2758200
C -1.8781930 1.5962490 -0.0920970

H -3.4053280 1.0796230 1.3670580
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H -1.4875410 2.3807030 0.5669520
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Pd -0.6160840 0.0213460 -0.0101480
C 1.9357060 -0.1095440 -0.0139790
O 1.2482170 0.9772270 -0.0509370
O 1.3298460 -1.2229080 0.0237090
C 3.4679680 -0.0526680 0.0049860
C 4.0098720 -0.9735780 -1.1095930
C 3.9769020 1.3824460 -0.2085080
C 3.9374840 -0.5745150 1.3833770
H 3.6707050 -2.0043160 -0.9724870
H 3.6813700 -0.6341120 -2.0990590
H 5.1059690 -0.9659030 -1.0963560
H 3.6170710 2.0593450 0.5723680
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H 3.6551110 1.7829900 -1.1754880
H 5.0325700 -0.5600290 1.4304780
H 3.5549710 0.0531500 2.1967570
H 3.5999470 -1.6014940 1.5543270

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C -2.0237560 -4.1628950 -2.6425310
H -1.8431490 -4.5207430 -3.6621810
H -3.1058320 -4.0391190 -2.5124110
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C -1.2926440 -2.8435550 -2.3979000
H -0.2143660 -2.9999730 -2.5213860
N -1.4750500 -2.3630930 -0.9877260

C	-1.7201100	-1.6887370	-3.3052930	C	-2.8240940	4.6262540	0.1954630
C	-1.0433970	-0.3958620	-2.8276600	C	-0.4174960	4.3686280	-0.4868310
H	-2.8127610	-1.5830760	-3.2557550	H	-1.5362420	4.2750900	-3.0285480
H	-1.4718910	-1.9225440	-4.3518500	H	-3.2277030	4.4802450	-2.5355110
H	-1.4716310	0.4981630	-3.2949180	H	-2.0427530	5.7622610	-2.2069360
H	0.0351670	-0.4120930	-3.0391320	H	-2.6251840	4.1915960	1.1825310
Pd	-1.3323740	-0.3060630	-0.8159640	H	-2.6908860	5.7123710	0.2717230
H	-2.4197590	-2.5338790	-0.6252770	H	-3.8684880	4.4238300	-0.0591190
H	-0.8513400	-2.8618120	-0.3533260	H	-0.2817270	5.4557930	-0.4247010
C	-2.6333720	-1.0879420	1.8626860	H	-0.1549770	3.9394240	0.4855790
O	-1.7513330	-0.3145640	1.3364120	H	0.2907940	3.9832410	-1.2272780
O	-3.2717140	-1.9785250	1.2526340	C	2.3223940	-3.8070450	0.9381690
C	-2.9030220	-0.8433890	3.3769900	C	1.9157610	-2.4679300	0.9795720
C	-1.5677640	-0.8856870	4.1493350	C	2.1936760	-1.6629400	-0.1248430
C	-3.5418660	0.5550530	3.5294370	C	2.8508470	-2.1361880	-1.2602840
C	-3.8570960	-1.9056290	3.9461110	C	3.2514510	-3.4774020	-1.2784530
H	-1.0819440	-1.8648650	4.0499460	C	2.9879010	-4.3088830	-0.1848710
H	-0.8743370	-0.1242150	3.7811370	H	2.1165480	-4.4509900	1.7883310
H	-1.7407890	-0.7066410	5.2180410	H	1.3996580	-2.0731750	1.8478520
H	-4.4862320	0.6211020	2.9757000	H	3.0487470	-1.4893460	-2.1081560
H	-3.7562580	0.7624260	4.5855720	H	3.7665730	-3.8667090	-2.1518810
H	-2.8744560	1.3362920	3.1534570	H	3.3004380	-5.3486740	-0.2086190
H	-4.0418190	-1.7120520	5.0103900	I	1.5676440	0.3947660	-0.0740080
H	-4.8195570	-1.8989620	3.4256880	C	3.5222140	1.1517090	0.5513930
H	-3.4374130	-2.9132070	3.8533520	C	4.4143210	1.5891250	-0.4277260
C	-2.1376520	2.5184690	-0.9749560	C	3.8109410	1.2252450	1.9139410
O	-3.2816510	2.1153460	-1.2477380	C	5.6502750	2.1053280	-0.0190940
O	-1.1134200	1.7511090	-0.7680890	H	4.1628720	1.5336020	-1.4820540
C	-1.8708960	4.0464270	-0.8714750	C	5.0517900	1.7431690	2.3042320
C	-2.1911290	4.6759820	-2.2450650	H	3.0962110	0.8889170	2.6581850

C	5.9674410	2.1804480	1.3411630	H	-2.0103680	-1.9563450	1.4243460
H	6.3591890	2.4495430	-0.7669170	H	-2.1165020	-4.2401150	0.4882480
H	5.2962150	1.8050380	3.3609950	H	-1.2580330	-4.7037800	-1.8102780
H	6.9273880	2.5830180	1.6514320	I	-2.1509600	1.0031600	-0.0670980
TS9				C	-4.0747030	0.1922660	-0.5034450
C	2.1171650	-3.4189610	3.5561120	C	-4.9093980	-0.1871430	0.5522560
H	1.7824260	-3.6368150	4.5764090	C	-4.4763270	0.0749370	-1.8375760
H	3.1321860	-3.0075180	3.6119440	C	-6.1784660	-0.6971530	0.2574910
H	2.1617110	-4.3663150	3.0063350	H	-4.5848080	-0.0868650	1.5827790
C	1.1675510	-2.4322920	2.8782270	C	-5.7473570	-0.4396430	-2.1146430
H	0.1625420	-2.8685310	2.8359300	H	-3.8183440	0.3768180	-2.6457100
N	1.5617080	-2.1729770	1.4546700	C	-6.5962800	-0.8244250	-1.0713130
C	1.0704810	-1.0640600	3.5546770	H	-6.8361790	-0.9935040	1.0697350
C	0.2193810	-0.1329660	2.6843910	H	-6.0701400	-0.5364290	-3.1473370
H	2.0817500	-0.6512720	3.6750660	H	-7.5827840	-1.2208710	-1.2937490
H	0.6493380	-1.1711720	4.5659530	C	3.4250820	-0.9080310	-1.0095550
H	0.2719740	0.9120870	3.0054890	O	2.2549650	-0.3865010	-1.0256440
H	-0.8302160	-0.4464540	2.6621770	O	3.9229490	-1.5435370	-0.0443450
Pd	1.0102620	-0.2762670	0.8097110	C	4.2971990	-0.7226500	-2.2866300
H	2.5808720	-2.1299040	1.3107050	C	5.5236140	0.1327890	-1.8970460
H	1.2208940	-2.9147080	0.8433420	C	4.7729860	-2.1096030	-2.7680310
C	-0.6611600	-2.6569880	-2.1564610	C	3.5271890	-0.0234580	-3.4190160
C	-0.5923060	-1.3561950	-1.6418320	H	5.2187910	1.1239050	-1.5397760
C	-1.0158890	-1.1486300	-0.3278440	H	6.1037690	-0.3499200	-1.1046560
C	-1.6232270	-2.1514530	0.4312470	H	6.1784910	0.2744120	-2.7658870
C	-1.6807080	-3.4422950	-0.1078280	H	3.9241390	-2.7472120	-3.0453440
C	-1.1973470	-3.7018650	-1.3959020	H	5.4154730	-2.0049010	-3.6512850
H	-0.3019270	-2.8392770	-3.1659900	H	5.3412990	-2.6235580	-1.9873810
H	-0.1795040	-0.5504120	-2.2354740	H	4.1805460	0.1045330	-4.2916610
				H	2.6561380	-0.6075470	-3.7346530

H	3.1716020	0.9647230	-3.1121120	H	1.7845280	-1.8155940	-1.9180660
C	1.3897560	2.6037350	0.7018940	H	1.3696630	-2.7715990	-0.4733740
O	2.4041610	2.3694380	1.3729040	Pd	0.0071780	-0.5315440	-0.6014530
O	0.5364450	1.6819550	0.3432410	C	-1.2746250	-1.5926340	3.3115930
C	1.0353610	4.0382210	0.2344920	C	-1.2385330	-1.1748670	1.9718970
C	2.2005230	4.9961930	0.5308320	C	-0.0288020	-1.2486200	1.2846110
C	0.7453050	4.0339650	-1.2811110	C	1.1399920	-1.7055650	1.8900120
C	-0.2203210	4.5027550	1.0064040	C	1.0816460	-2.1160560	3.2303640
H	2.4351480	5.0242750	1.5990760	C	-0.1210000	-2.0671040	3.9403620
H	3.1090810	4.6978900	-0.0027450	H	-2.2146410	-1.5337600	3.8541770
H	1.9359340	6.0114320	0.2111780	H	-2.1363550	-0.7780090	1.5093950
H	-0.1114000	3.3995260	-1.5248250	H	2.0805220	-1.7285620	1.3515780
H	0.5263400	5.0526540	-1.6234710	H	1.9900030	-2.4716020	3.7100940
H	1.6089160	3.6660200	-1.8475030	H	-0.1566530	-2.3874790	4.9778660
H	-0.4831820	5.5265980	0.7139090	H	-1.9475790	-1.1247760	-2.0400300
H	-1.0809330	3.8593220	0.7971310	H	-2.4588080	-1.3562610	-0.5175560
H	-0.0449360	4.4977490	2.0888950	C	2.9024510	0.3842690	-0.2631570
				O	1.6243140	0.6485670	-0.3642630
17				O	3.3943070	-0.7440520	-0.1608390
C	-2.5512580	-3.6863930	-2.1345450	C	3.7790540	1.6653830	-0.2856300
H	-2.3416110	-4.7529670	-2.2669330	C	3.5674760	2.3851200	-1.6358620
H	-2.6916280	-3.2412600	-3.1270260	C	3.3489620	2.5906370	0.8730550
H	-3.4899570	-3.5939220	-1.5772560	C	5.2614740	1.2923960	-0.1263180
C	-1.4025600	-3.0139930	-1.3886670	H	3.8379540	1.7366740	-2.4783530
H	-1.2844590	-3.4663040	-0.3988000	H	2.5262600	2.6948160	-1.7628180
N	-1.6807680	-1.5619060	-1.1519130	H	4.2000700	3.2794860	-1.6859380
C	-0.0595250	-3.0202490	-2.1160530	H	3.4660260	2.0917210	1.8426260
C	0.9652880	-2.2152980	-1.3165880	H	3.9732640	3.4922890	0.8821920
H	-0.1978210	-2.5897180	-3.1173380	H	2.3040380	2.8962270	0.7719190
H	0.2988160	-4.0488100	-2.2555530	H	5.8734070	2.2020900	-0.1442730

H	5.4457630	0.7769340	0.8217090	H	-0.9422820	-3.4370950	2.6335170
H	5.6011730	0.6373670	-0.9349530	H	-1.4257500	-0.7749810	2.3298730
C	-2.3718750	1.4711040	-0.0735300	H	-2.5131420	-2.0099660	1.6749610
O	-1.1033830	1.3275280	-0.2524430	Pd	-0.1958900	-0.5662000	0.1108570
O	-3.1971900	0.5302520	-0.0089270	C	-0.6923530	2.2761150	-0.0844250
C	-2.8474540	2.9421140	0.0776150	O	-0.5754700	1.3116050	0.7855490
C	-2.1522840	3.5551550	1.3133050	O	-0.7313700	2.1151780	-1.3112280
C	-2.4403150	3.7281710	-1.1875630	C	-0.8097270	3.7014800	0.5219490
C	-4.3723260	3.0101990	0.2569490	C	0.2898580	4.5801820	-0.1117930
H	-2.4032850	3.0005000	2.2256640	C	-2.1983550	4.2594560	0.1393130
H	-1.0643930	3.5464660	1.1999190	C	-0.6539400	3.7116050	2.0521160
H	-2.4774950	4.5934890	1.4519620	H	1.2896690	4.2007330	0.1289550
H	-2.9116950	3.3082100	-2.0850010	H	0.1914230	4.6122300	-1.2007400
H	-2.7601100	4.7739130	-1.1013170	H	0.2169100	5.6047010	0.2726920
H	-1.3562160	3.7107530	-1.3316840	H	-3.0049390	3.6565940	0.5733860
H	-4.6886500	4.0557450	0.3567600	H	-2.3069300	5.2840900	0.5152100
H	-4.8972050	2.5771410	-0.6009410	H	-2.3315400	4.2753590	-0.9466550
H	-4.6968440	2.4701800	1.1522530	H	-0.7357360	4.7408240	2.4228260
				H	-1.4280670	3.1138640	2.5435080
TS10				H	0.3201070	3.3183590	2.3606060
C	0.7650720	-4.6974140	0.8003090	H	1.4170850	-2.4212300	-0.2125840
H	0.3004860	-5.4566420	1.4383230	H	0.2257480	-2.7635780	-1.3096200
H	1.7018040	-4.3797640	1.2720290	C	-4.6916540	-0.6890950	-1.5299740
H	1.0044050	-5.1654590	-0.1609510	C	-4.3777990	0.1962040	-0.4912930
C	-0.1845550	-3.5158990	0.6088800	C	-3.1704070	0.0783940	0.1973430
H	-1.1198430	-3.8764520	0.1710920	C	-2.2473570	-0.9271270	-0.1448630
N	0.3878090	-2.5020700	-0.3366160	C	-2.5786620	-1.8310080	-1.1697590
C	-0.4994330	-2.7545930	1.8952110	C	-3.7868020	-1.6990010	-1.8651980
C	-1.5004570	-1.6230410	1.6494290	H	-5.6308700	-0.5933630	-2.0673640
H	0.4329270	-2.3660080	2.3192890	H	-5.0732900	0.9846890	-0.2159270

H	-2.9446490	0.7656740	1.0040240	H	1.5176410	0.4130640	-1.3358960
H	-1.9143940	-2.6388190	-1.4505530	H	2.4600450	-1.0496960	-1.6024350
H	-4.0143910	-2.3943070	-2.6689210	H	3.3327800	1.3064870	0.1722970
C	2.8579390	-0.4417090	-0.2613830	H	3.7015020	1.1753010	-1.5381500
O	1.7250360	0.1771130	-0.2305900	Pd	-1.2015350	0.2711160	-0.1126630
O	3.0103280	-1.6727120	-0.0934770	H	0.1598250	-1.7784360	-0.8029750
C	4.1066130	0.4345610	-0.5390360	H	-0.2298040	-1.8147130	0.7847960
C	5.1304350	0.1826220	0.5888050	C	7.2036980	-1.5612860	0.2504890
C	4.7004540	-0.0223280	-1.8909800	C	6.6729800	-0.6627870	1.1809650
C	3.7663410	1.9314530	-0.6034170	C	5.4851540	0.0224860	0.8983180
H	4.7277820	0.4821000	1.5640240	C	4.8051430	-0.1753670	-0.3132760
H	5.4073490	-0.8740330	0.6434790	C	5.3552200	-1.0752400	-1.2427670
H	6.0386030	0.7691250	0.4060330	C	6.5393400	-1.7639450	-0.9654910
H	3.9873810	0.1297960	-2.7101500	H	8.1251000	-2.0952840	0.4668860
H	5.6020860	0.5587520	-2.1188460	H	7.1815770	-0.4934560	2.1266950
H	4.9726470	-1.0819710	-1.8657600	H	5.0800460	0.7195200	1.6285570
H	4.6786530	2.5081750	-0.7986630	H	4.8530610	-1.2370140	-2.1940310
H	3.0487900	2.1488430	-1.3996760	H	6.9463040	-2.4550460	-1.6993350
H	3.3387740	2.2848350	0.3400430	C	-2.8320090	-2.1429210	0.3041630
18				O	-2.1108160	-2.4670380	1.2625950
C	2.3148860	-2.1216500	0.9086920	O	-2.6179040	-1.1154450	-0.4701700
H	3.3413940	-1.8908440	1.2034520	C	-4.1112240	-2.9384510	-0.0568980
H	2.3485310	-2.9064790	0.1435430	C	-5.3295010	-2.0681440	0.3315140
H	1.7922200	-2.5171030	1.7873980	C	-4.1442270	-3.2264760	-1.5719270
C	1.6063650	-0.8713020	0.3761660	C	-4.1504860	-4.2615490	0.7243810
H	1.5610320	-0.1167720	1.1689760	H	-5.3215930	-1.8269860	1.4010210
N	0.1858710	-1.2230540	0.0556920	H	-5.3430730	-1.1300250	-0.2319160
C	2.2547520	-0.2533280	-0.8741550	H	-6.2573650	-2.6110930	0.1155310
C	3.5299510	0.5847250	-0.6288980	H	-3.2744970	-3.8168440	-1.8847260
				H	-5.0450550	-3.7995670	-1.8212140

H	-4.1547250	-2.3009970	-2.1537440	H	-4.1170610	-1.9463300	-1.6092570
H	-5.0629640	-4.8133680	0.4692980	H	-3.9177570	-2.6255060	0.0162450
H	-3.2917820	-4.8965400	0.4807430	H	-5.4474850	-1.8571620	-0.4422750
H	-4.1445630	-4.0914850	1.8050410	H	-3.8862540	0.6960910	1.8449420
C	-1.2395910	2.7250430	0.0218940	H	-5.2990980	-0.3464130	1.5915420
O	-0.1567720	2.0460010	0.1519940	H	-3.7454260	-1.0633320	2.0600600
O	-2.3104320	2.0532090	-0.1837380	H	-5.6156710	0.6474020	-0.7424470
C	-1.2632500	4.2435370	0.1038610	H	-4.1994520	1.6881330	-0.5011870
C	-2.1806470	4.6443000	1.2833680	H	-4.2885940	0.6235650	-1.9186140
C	0.1540590	4.7974050	0.3235170	C	1.5723500	-2.5440060	1.6037710
C	-1.8488510	4.7857670	-1.2209630	H	2.1773640	-2.8447780	2.4646370
H	-3.1977250	4.2664050	1.1440030	H	1.0668030	-3.4366360	1.2158220
H	-1.7962610	4.2589210	2.2344590	H	0.8090790	-1.8404740	1.9508900
H	-2.2250370	5.7366620	1.3525920	C	2.4636480	-1.9145630	0.5370100
H	0.8241840	4.5280930	-0.4990380	H	2.9279950	-1.0056530	0.9367890
H	0.1096940	5.8904850	0.3804710	N	1.6176090	-1.4737710	-0.6247280
H	0.5928470	4.4265790	1.2550600	H	1.1753010	-2.3018140	-1.0342490
H	-1.8835630	5.8800280	-1.1810850	H	2.2177970	-1.0942900	-1.3594140
H	-1.2294260	4.4968880	-2.0777150	C	3.5715020	-2.8740940	0.0676250
H	-2.8640230	4.4146300	-1.3890500	C	4.5952480	-2.2623110	-0.8956710
19				H	3.1024530	-3.7571740	-0.3887100
Pd	0.0775890	-0.1370960	-0.2954460	H	4.0900230	-3.2275070	0.9667610
C	-2.3633230	-0.3259010	-0.1699540	H	5.3830960	-2.9875520	-1.1249600
O	-1.7601610	0.8036410	-0.0583710	H	4.1478530	-1.9646430	-1.8522560
O	-1.6123690	-1.3491800	-0.3618070	H	5.0760420	-1.3792810	-0.4570900
C	-3.8721880	-0.4332560	-0.0431280	C	1.0280800	2.2122990	2.0563520
C	-4.3592040	-1.8010820	-0.5512140	H	0.6948400	3.0571000	2.6665200
C	-4.2140440	-0.2748960	1.4608350	H	2.0326480	1.9271300	2.3933030
C	-4.5276160	0.7058080	-0.8523770	H	0.3495890	1.3729410	2.2382860
				C	1.0386690	2.6074110	0.5817210

H	0.0242160	2.8688120	0.2627090	C	1.4981970	2.2452900	-1.9303590
N	1.4331710	1.4153560	-0.2438140	H	2.2092050	2.6784260	-2.6408350
H	1.5544550	1.6987020	-1.2184660	H	0.5829770	2.8490400	-1.9561910
H	2.3502220	1.0905200	0.0720310	H	1.2491560	1.2331220	-2.2664240
C	1.9728790	3.7995390	0.3084760	C	2.1037030	2.2281120	-0.5283680
C	1.9218900	4.3505330	-1.1209950	H	3.0073010	1.6071200	-0.5313220
H	3.0015580	3.5127100	0.5681100	N	1.1460800	1.5694530	0.4206360
H	1.6852580	4.5928360	1.0086830	H	0.3055840	2.1487530	0.4909280
H	2.5440460	5.2479360	-1.2055210	H	1.5515490	1.5538950	1.3568450
H	2.2953950	3.6341390	-1.8626000	C	2.4787220	3.6419860	-0.0487130
H	0.8991230	4.6272880	-1.4032540	C	3.2161360	3.7053970	1.2940800

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Pd	0.4190420	-0.3642050	-0.0125760	H	3.5020340	4.7377630	1.5225330
C	-2.4040780	-0.1627200	0.1405060	H	2.5989720	3.3537850	2.1299270
O	-1.4183740	0.5399110	-0.2642160	H	4.1341280	3.1050390	1.2743720
O	-2.2405080	-1.3653510	0.5277310	C	3.5616540	-3.3613330	0.4009760
C	-3.8153040	0.4322230	0.1294150	H	3.6865770	-4.3330150	-0.0879220
C	-4.4678810	0.1825880	1.5060800	H	3.3922760	-3.5386360	1.4698970
C	-3.7840240	1.9387490	-0.1740180	H	4.4987990	-2.8052860	0.2857600
C	-4.6124590	-0.3084710	-0.9715990	C	2.3896450	-2.6054350	-0.2212940
H	-4.5244490	-0.8852360	1.7341990	H	2.5850090	-2.4345200	-1.2858470
H	-3.9069350	0.6779160	2.3069970	N	2.2402190	-1.2404690	0.3864900
H	-5.4846050	0.5896370	1.5033280	H	2.2912980	-1.3250210	1.4054650
H	-3.3412460	2.1448060	-1.1528940	H	3.0239470	-0.6458900	0.1123130
H	-4.8082010	2.3270310	-0.1755150	C	1.0381550	-3.2961270	-0.0740330
H	-3.2154410	2.4906550	0.5816920	C	-0.0820530	-2.4262490	-0.6568150
H	-5.6331300	0.0875860	-1.0058260	H	0.8501540	-3.5087340	0.9872520
H	-4.1587060	-0.1618360	-1.9584090	H	1.0723010	-4.2642990	-0.5893040
H	-4.6671130	-1.3824410	-0.7704950	H	-1.0026910	-3.0215100	-0.7225980

H -1.0279490 -1.7056770 0.1352630
H 0.1221030 -2.1411820 -1.6973330

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Pd -0.5435270 -0.4892030 0.0603190
C 2.3594560 -0.2638620 -0.4245150
O 1.4722560 -0.3945470 0.5074970
O 2.1105990 -0.1646750 -1.6417320
C 3.8398280 -0.2750910 0.0537480
C 4.6265430 0.8148600 -0.7005680
C 3.9649240 -0.0422060 1.5691910
C 4.4183820 -1.6646490 -0.3015990
H 4.5712740 0.6655180 -1.7823210
H 4.2348350 1.8149300 -0.4764730
H 5.6818170 0.7946090 -0.4017000
H 3.4417050 -0.8140500 2.1405220
H 5.0223610 -0.0569660 1.8620900
H 3.5498240 0.9289000 1.8615990
H 5.4707740 -1.7250230 0.0025270
H 3.8735340 -2.4655480 0.2122150
H 4.3637480 -1.8514930 -1.3792500
C -1.3942440 2.4288660 1.9893890
H -2.1687660 2.9975500 2.5148290
H -0.4171160 2.7904230 2.3347850
H -1.4829100 1.3753760 2.2749420
C -1.5344690 2.6016070 0.4765140
H -2.5211000 2.2327930 0.1664700
N -0.5340630 1.7355110 -0.2070560
H 0.4029010 2.0209030 0.0826590
H -0.5686570 1.8978490 -1.2130940

C -1.4238620 4.0815240 0.0638770
C -1.7251280 4.3601840 -1.4132780
H -0.4156650 4.4408760 0.3153420
H -2.1233510 4.6553250 0.6855190
H -1.6714150 5.4342300 -1.6238190
H -1.0125890 3.8650660 -2.0836610
H -2.7326270 4.0200280 -1.6840810
C -4.3872980 -2.5098480 -0.3725420
H -4.7040410 -3.4863460 0.0101580
H -4.3663750 -2.5669670 -1.4681800
H -5.1465560 -1.7744150 -0.0809110
C -3.0132740 -2.1373490 0.1810630
H -3.0632660 -2.0771760 1.2747300
N -2.5768060 -0.7735640 -0.2783680
H -2.7213050 -0.7057710 -1.2887020
H -3.1687790 -0.0538130 0.1377440
C -1.8785980 -3.0835340 -0.2088690
C -0.5459200 -2.5121240 0.2979300
H -1.8621930 -3.1723040 -1.3050000
H -2.0814860 -4.0901470 0.1855540
H 0.3166460 -2.9525090 -0.2167360
H -0.4237580 -2.6886520 1.3773600

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Pd -0.1491490 -0.1472790 0.2776610
C 2.4148080 -1.1744490 -0.6089220
O 1.6319360 -1.0822850 0.4361300
O 2.1474960 -0.7004320 -1.7196690
C 3.7191940 -1.9717800 -0.3482170
C 4.7048840 -1.7563320 -1.5083520

C	4.3687110	-1.5236090	0.9768230	H	4.1887170	5.3825530	0.6710470
C	3.3451470	-3.4697320	-0.2609630	C	2.5923320	3.9043520	0.5144930
H	4.2741190	-2.0694010	-2.4635950	H	1.8228080	4.6570740	0.2940440
H	4.9901890	-0.7026670	-1.5993160	N	2.4931990	3.6195490	1.9600100
H	5.6160680	-2.3405980	-1.3335420	H	3.2391180	2.9783450	2.2318480
H	3.7037460	-1.6956090	1.8276820	H	2.6483180	4.4748240	2.4912260
H	5.2958070	-2.0844710	1.1455460	C	2.2648170	2.6333880	-0.2881370
H	4.6223720	-0.4571440	0.9544330	C	0.8222120	2.1531680	-0.0942720
H	4.2481670	-4.0701190	-0.0980360	H	2.9655280	1.8406530	0.0042490
H	2.6564080	-3.6620380	0.5680930	H	2.4407810	2.8306430	-1.3515970
H	2.8741520	-3.8166720	-1.1880400	H	0.6678880	1.2820540	-0.7860170
C	-1.0652480	-3.1357580	-1.2186200	H	0.6307020	1.9478130	0.9657250
H	-1.7160660	-3.6622060	-1.9235930	H	0.0850520	2.8928560	-0.4197290
H	-0.2663360	-3.8235240	-0.9165400	C	-2.5951130	1.0835640	-0.6715870
H	-0.6127310	-2.2873470	-1.7403740	O	-1.9619520	0.7285420	0.4141880
C	-1.8770420	-2.6736490	-0.0119470	O	-2.1779140	0.8819230	-1.8198820
H	-2.6544360	-1.9755200	-0.3374220	C	-3.9384770	1.8233310	-0.4402990
N	-0.9937730	-1.8999530	0.9219070	C	-5.0220370	1.1403190	-1.3000590
H	-0.2115940	-2.4885900	1.2200070	C	-4.3710370	1.8190330	1.0355240
H	-1.5162020	-1.6501400	1.7629350	C	-3.7456660	3.2813570	-0.9160210
C	-2.5396560	-3.8517010	0.7264810	H	-4.7511980	1.1512690	-2.3596080
C	-3.5106390	-3.4533770	1.8441790	H	-5.1713980	0.0968490	-0.9970470
H	-1.7537370	-4.5099160	1.1225120	H	-5.9776340	1.6647120	-1.1815190
H	-3.0822030	-4.4348650	-0.0274380	H	-3.6320180	2.3106340	1.6752700
H	-3.9837870	-4.3427190	2.2745450	H	-5.3218950	2.3555020	1.1402700
H	-3.0125710	-2.9261350	2.6671300	H	-4.5166080	0.8005710	1.4109670
H	-4.3076220	-2.8038530	1.4628840	H	-4.6828950	3.8381310	-0.7978920
C	3.9572430	4.4757120	0.0997360	H	-2.9740430	3.7932190	-0.3288240
H	3.9750070	4.7347060	-0.9661490	H	-3.4548240	3.3175480	-1.9703930
H	4.7566160	3.7462370	0.2852510				

TS12

			H	-1.6843570	-5.0386290	0.3314020	
Pd	0.1863700	-0.1270060	-0.1054170	H	-2.5569710	-4.8579960	2.6300440
C	3.0720810	0.0240690	-0.2445060	H	-1.9239020	-3.2248940	2.8186300
O	2.1303330	-0.8193860	-0.1291990	H	-3.2317130	-3.5387720	1.6628950
O	2.8296150	1.2615390	-0.4375760	C	-0.4220780	4.8965210	1.2397420
C	4.5308090	-0.4377520	-0.1743800	H	-1.1197420	5.3481520	0.5232080
C	5.2668880	0.4213640	0.8771480	H	0.5117160	5.4741320	1.2130810
C	4.6243500	-1.9242120	0.2048630	H	-0.8548780	5.0021290	2.2422480
C	5.1570630	-0.2099240	-1.5706080	C	-0.1585800	3.4165910	0.9130920
H	5.2440800	1.4825340	0.6139250	H	-1.1184530	2.8859950	0.9054410
H	4.8192340	0.3032890	1.8706600	N	0.6769880	2.7492860	1.9330610
H	6.3133330	0.1028490	0.9369040	H	1.5867780	3.2080590	1.9822920
H	4.1228480	-2.5610460	-0.5298670	H	0.2519250	2.8631110	2.8520300
H	5.6783300	-2.2196240	0.2483570	C	0.4867030	3.2716040	-0.4773840
H	4.1781160	-2.1175240	1.1857980	C	0.3976800	1.8811100	-1.1457470
H	6.2026000	-0.5365340	-1.5557220	H	1.5355450	3.5926300	-0.4001170
H	4.6320510	-0.7867260	-2.3406330	H	0.0005100	3.9920500	-1.1501590
H	5.1307820	0.8468990	-1.8521970	H	0.9112560	1.9055320	-2.1176550
C	-0.0349820	-3.4877670	-1.0973120	H	1.5922070	1.3390450	-0.5993120
H	-0.5392570	-4.2597540	-1.6874320	H	-0.6433110	1.6769560	-1.3936430
H	0.9136660	-3.9036380	-0.7358900	C	-2.6570960	0.1543580	-0.7737720
H	0.1878080	-2.6439670	-1.7570080	O	-1.7793560	0.3611550	0.1649550
C	-0.9259470	-3.0581320	0.0669740	O	-2.3963760	-0.2994150	-1.8988840
H	-1.8488920	-2.6235080	-0.3299330	C	-4.1139810	0.5617240	-0.4184850
N	-0.2534820	-1.9632820	0.8357150	C	-5.0681910	-0.5620240	-0.8703930
H	0.6266670	-2.3180820	1.2161320	C	-4.3018830	0.8239160	1.0851970
H	-0.8302310	-1.7062400	1.6368430	C	-4.4294840	1.8526770	-1.2095470
C	-1.2830620	-4.2479620	0.9776040	H	-4.9639410	-0.7632580	-1.9401300
C	-2.3027180	-3.9439400	2.0819790	H	-4.8703340	-1.4945500	-0.3279690
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H -4.0658310 -0.0643250 1.6813780
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22

Pd -1.2114970 -0.8466130 0.4136660
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O -0.7053040 1.3664410 2.4959370
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C -0.4432050 3.3422470 1.0788870
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C 0.6925030 -2.6061580 1.9143790
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C -0.6724870 -3.1635160 2.3359940
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H -1.3668040 -2.6564090 0.2387420
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C 3.2158640 -0.2427750 -0.7922840
O 2.4522190 -0.5895950 -1.7320840
O 2.9142730 -0.2672420 0.4465730

C	4.6495410	0.2514920	-1.1799380	H	-5.1454610	-2.3722110	1.0725950
C	5.4715820	0.6614330	0.0528530	H	-4.0861570	-2.6879100	2.4529400
C	5.3749370	-0.8929640	-1.9196440	C	1.2240260	3.2077220	-1.4027600
C	4.5112000	1.4636680	-2.1255900	H	1.7318450	4.0683860	-0.9556470
H	4.9884050	1.4744780	0.6043430	H	1.1332700	3.3960190	-2.4804690
H	5.6005600	-0.1760220	0.7462740	H	1.8530340	2.3284400	-1.2483310
H	6.4686240	1.0048940	-0.2540720	C	-0.1516660	3.0291180	-0.7647140
H	4.8189370	-1.1978760	-2.8115890	H	-0.0345930	2.8011300	0.3006600
H	6.3787850	-0.5759180	-2.2314430	N	-0.8395050	1.8411500	-1.3704540
H	5.4887200	-1.7735990	-1.2744520	H	-0.8594900	1.9602730	-2.3854700
H	5.5003500	1.8244280	-2.4369960	H	-1.8141060	1.8315830	-1.0656990
H	3.9436410	1.1994240	-3.0230100	C	-1.0085920	4.3014430	-0.9084500
H	3.9926000	2.2945360	-1.6310600	C	-2.3518000	4.2741480	-0.1701920
TS13				H	-1.1707320	4.5005920	-1.9775070
Pd	-0.2777800	-0.1322020	-0.8965970	H	-0.4092190	5.1365780	-0.5253260
C	-2.7150550	-1.0509360	0.6443030	H	-2.8535080	5.2446280	-0.2547800
O	-2.5557480	-2.2231840	0.2588490	H	-3.0415200	3.5247430	-0.5766170
O	-1.9678950	-0.0450870	0.2976910	H	-2.2145430	4.0613050	0.8967570
C	-3.8671200	-0.6777010	1.6136980	C	0.6112280	-4.1741950	-1.8114960
C	-3.2559720	-0.0835890	2.9022320	H	1.2463470	-4.6409690	-2.5723570
C	-4.7735120	0.3733870	0.9365540	H	-0.4280230	-4.2250480	-2.1585350
C	-4.6977020	-1.9225570	1.9647350	H	0.6967630	-4.7649620	-0.8927010
H	-2.5904920	-0.8033700	3.3937030	C	1.0381570	-2.7274920	-1.5737590
H	-2.6800660	0.8218310	2.6899860	H	2.0701450	-2.7129270	-1.2050600
H	-4.0534110	0.1735740	3.6099020	N	0.2097460	-2.0881430	-0.4941610
H	-5.2063160	-0.0141800	0.0062090	H	-0.6838360	-2.5615460	-0.3258580
H	-5.6017590	0.6393420	1.6043960	H	0.7658920	-2.0373990	0.3738530
H	-4.2182310	1.2858090	0.7012180	C	0.9552870	-1.8402970	-2.8183050
H	-5.5079580	-1.6454690	2.6498050	C	1.2238190	-0.3686470	-2.4456810
				H	-0.0468270	-1.9383110	-3.2544530

H	1.6711570	-2.1890980	-3.5746150	H	-4.0699160	-4.0152160	0.6394820
H	0.7854290	0.3351670	-3.1581770	H	-5.5230350	-2.1887380	1.5129710
H	1.5425880	-0.0625500	-1.0832950	C	-0.4740800	-3.3997670	-1.1063530
H	2.3010330	-0.1596220	-2.4656060	C	-0.0381460	-2.0662820	-1.0716720
C	2.8381190	-0.3847930	0.9683500	H	-2.0416300	-4.7389640	-0.4955710
O	2.6109300	0.2319930	-0.1411020	H	0.1640020	-4.1514470	-1.5568160
O	2.2243820	-1.4023570	1.3672450	H	0.9393510	-1.7932650	-1.4476070
C	3.9552360	0.2362690	1.8523750	N	-0.7620720	-1.0774470	-0.5405720
C	4.2940800	-0.6838640	3.0362480	C	-2.6615860	1.1360570	0.2181390
C	5.2206260	0.4688820	1.0012090	H	-3.5393780	1.7560950	0.3862380
C	3.4331780	1.5895970	2.3873080	C	-2.7895840	3.9379790	-0.2339250
H	3.4215560	-0.8564860	3.6732290	H	-2.6312770	4.9728390	-0.5510390
H	4.6555850	-1.6600150	2.6950210	H	-3.0397360	3.9481350	0.8327590
H	5.0806240	-0.2270980	3.6495270	H	-3.6431200	3.5500980	-0.7980780
H	5.0167930	1.1380890	0.1606230	C	-1.5076820	3.1556450	-0.5103930
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H	5.6051360	-0.4757610	0.5970930	N	-1.5712320	1.6979620	-0.1646700
H	4.1893040	2.0594750	3.0282040	C	-0.2870180	3.7832880	0.1750950
H	3.2034320	2.2781940	1.5684180	H	-0.4625730	3.8507760	1.2551330
H	2.5235920	1.4537070	2.9851350	H	-0.1845610	4.8055070	-0.2034200
I				Pd	0.1727270	0.7227430	-0.2814640
C	-4.1331950	-0.6322850	0.9449330	C	2.8277520	-0.0760480	0.5477020
C	-2.8918680	-0.2896830	0.4086160	O	2.5800690	0.5274730	1.5987300
C	-2.0157260	-1.3333040	-0.0359060	O	1.9794820	-0.1724030	-0.4487240
C	-2.4869560	-2.6851910	0.0160270	C	4.1736320	-0.7975730	0.3006820
C	-3.7514900	-2.9778940	0.5958470	C	5.1394020	-0.5164940	1.4628750
C	-4.5565410	-1.9681670	1.0722830	C	3.9016460	-2.3162470	0.2108840
H	-4.7987830	0.1658200	1.2611290	C	4.7905030	-0.2976310	-1.0231700
C	-1.6833950	-3.7143560	-0.5312970	H	5.3512250	0.5532890	1.5589310
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II

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III

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H	2.9717560	1.7648240	1.6701950	N	1.3077460	0.7722440	-0.1733540
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				Pd	0.9894510	-1.1443650	0.0496480
IV				C	3.3202490	-1.0692310	0.6804560
C	-1.8225940	2.5976620	0.2923650	H	2.6456930	-1.1746420	1.5448510
C	-1.0396390	1.4576740	0.1067680	H	4.1662830	-1.7197750	0.9241810
C	-1.6882520	0.1892590	-0.0101110	H	2.9523890	-1.5554980	-0.2621410
C	-3.1163760	0.1253920	0.0241990				
C	-3.8634980	1.3186600	0.2261530	1-s			
C	-3.2266810	2.5319700	0.3706670	C	1.9452600	-0.1499390	1.7744850
H	-1.3295200	3.5617070	0.3706900	C	2.5523510	-0.6816030	0.6447140
C	-3.7460060	-1.1304930	-0.1482340	C	3.8979770	-0.2870280	0.3201870
H	-4.9466480	1.2493620	0.2578770	C	4.5682110	0.6578670	1.1605810
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C	-2.9863400	-2.2665510	-0.3395410	C	2.6184930	0.7734100	2.6052900
C	-1.5909540	-2.1435810	-0.3333430	H	0.9398960	-0.4596450	2.0382060
H	-4.8303900	-1.1838800	-0.1269860	C	5.8858700	1.0442390	0.8014750
H	-3.4331840	-3.2435890	-0.4805930	H	4.4233420	1.8890420	2.9374350
H	-0.9434930	-3.0116600	-0.4470800	H	2.1114540	1.1661010	3.4810060
N	-0.9818150	-0.9663910	-0.1707030	C	6.4671080	0.5026560	-0.3232900
C	0.3858880	1.6631280	-0.0540060	C	5.7245580	-0.4316230	-1.0850190
H	0.6955430	2.7048590	-0.1130250	H	6.4164400	1.7641230	1.4193820
C	3.0126720	2.5843450	-0.6710840	H	7.4718540	0.7737720	-0.6312260
H	4.0599820	2.6994840	-0.9650560	H	6.1701780	-0.8784020	-1.9720460
H	2.8699250	3.1129120	0.2769950	N	4.4925960	-0.8138620	-0.7893430
H	2.3989240	3.0535060	-1.4456710	C	1.9318880	-1.7264010	-0.1745690
C	2.7359990	1.0898700	-0.5404020	H	2.6387380	-2.4103830	-0.6375300
H	2.8528260	0.6212660	-1.5251180	C	1.2745010	-4.0034740	-1.7461290

H	0.7795710	-4.8089590	-2.2974520	C	-0.1450120	1.9297310	-0.2457950
H	1.9506880	-4.4646200	-1.0177730	O	-0.3277810	0.7836850	-0.8521730
H	1.8667360	-3.4262080	-2.4631990	O	-0.2180770	2.1103850	0.9715830
C	0.1949510	-3.1520640	-1.0819600	C	0.1669840	3.0876650	-1.2352090
H	-0.4842190	-2.7822880	-1.8593960	C	1.2893340	2.6701780	-2.2074090
N	0.6752400	-1.9230670	-0.3745790	C	-1.1232790	3.3917020	-2.0300990
C	-0.6357240	-3.9596590	-0.0643220	C	0.5989820	4.3402340	-0.4563990
H	0.0315590	-4.3400410	0.7186280	H	2.2074550	2.4098770	-1.6677520
H	-1.0597680	-4.8271390	-0.5820390	H	0.9962600	1.8073010	-2.8117750
Pd	-0.9720720	-0.8395300	0.1495270	H	1.5227030	3.5009860	-2.8844300
C	-3.7499530	-0.0902900	-0.0336290	H	-1.9447400	3.6730060	-1.3608790
O	-2.6767630	0.1011730	0.6789880	H	-0.9489200	4.2276590	-2.7183020
O	-3.8052030	-0.8084630	-1.0445760	H	-1.4423940	2.5250720	-2.6169380
C	-5.0180880	0.6475710	0.4698870	H	0.8015010	5.1577670	-1.1588320
C	-6.0798390	-0.4221750	0.8083900	H	-0.1796170	4.6704400	0.2375810
C	-4.7438750	1.5139540	1.7099300	H	1.5097580	4.1576650	0.1238530
C	-5.5337930	1.5397410	-0.6795480				
H	-6.3068110	-1.0435690	-0.0631880	TS1-s			
H	-5.7402370	-1.0795250	1.6181540	C	2.0022050	-0.0672970	1.6559640
H	-7.0073400	0.0624200	1.1362280	C	2.5645230	-0.7316790	0.5745880
H	-3.9940790	2.2842550	1.5045570	C	3.9477210	-0.4963110	0.2507270
H	-5.6690510	2.0147220	2.0208490	C	4.7002750	0.4315340	1.0391550
H	-4.3844840	0.9138340	2.5518140	C	4.0763820	1.0910820	2.1323670
H	-6.4551760	2.0487390	-0.3721820	C	2.7546540	0.8409530	2.4337470
H	-4.7976850	2.3072420	-0.9457620	H	0.9674200	-0.2526460	1.9209830
H	-5.7485600	0.9472070	-1.5736790	C	6.0567070	0.6537960	0.6849290
C	-1.7735670	-3.1474960	0.5533180	H	4.6590080	1.7927220	2.7238360
H	-1.3785250	-2.3199850	1.2275920	H	2.2783050	1.3413770	3.2708900
H	-2.3362840	-3.7117670	1.3055660	C	6.5968590	-0.0221830	-0.3860570
H	-2.4936270	-2.7938390	-0.1901200	C	5.7722140	-0.9247720	-1.1003750

H	6.6494050	1.3562200	1.2652740	H	-6.8188620	0.8114910	-1.1259720
H	7.6296280	0.1209910	-0.6873460	H	-5.2501510	0.6786030	-1.9403390
H	6.1821540	-1.4747970	-1.9457150	H	-6.0473490	-0.7775270	-1.3091510
N	4.5025790	-1.1553980	-0.8080750	C	-1.6034050	-2.6859400	0.8828440
C	1.8514900	-1.7520070	-0.2000230	H	-0.9570660	-2.4571520	1.7377770
H	2.4985010	-2.5022430	-0.6475070	H	-2.5005990	-3.1088330	1.3542570
C	0.9976570	-4.0398180	-1.6818990	H	-2.6297900	-1.9049800	0.2897240
H	0.4258610	-4.8291690	-2.1811700	C	-0.0564470	2.0989930	-0.1338930
H	1.6276330	-4.5170810	-0.9230480	O	-0.1977420	0.9761090	-0.7768280
H	1.6411170	-3.5710600	-2.4337200	O	-0.2319110	2.2522720	1.0827670
C	0.0046080	-3.0520460	-1.0763690	C	0.3643600	3.2852850	-1.0482730
H	-0.6008140	-2.6285600	-1.8862120	C	1.6473960	2.9097820	-1.8190980
N	0.5831800	-1.8589830	-0.3875680	C	-0.7797000	3.5604700	-2.0488610
C	-0.9598730	-3.7115010	-0.0646370	C	0.6218740	4.5450200	-0.2061280
H	-0.4101210	-4.4633680	0.5182360	H	2.4712500	2.6844810	-1.1312150
H	-1.7291180	-4.2478600	-0.6312740	H	1.4872240	2.0346870	-2.4550580
Pd	-1.0162840	-0.6895870	0.1054130	H	1.9612360	3.7461720	-2.4559650
C	-3.8256300	-0.2444720	0.2187290	H	-1.7094640	3.8189530	-1.5278790
O	-2.7457720	0.3948960	0.4144470	H	-0.5153620	4.4029980	-2.6999590
O	-3.8293650	-1.5050740	0.0083000	H	-0.9740630	2.6879440	-2.6798330
C	-5.1663320	0.4989280	0.2452640	H	0.9118470	5.3761680	-0.8607690
C	-6.0284950	-0.1132300	1.3729770	H	-0.2709390	4.8457470	0.3509510
C	-4.9632020	2.0010530	0.4970630	H	1.4282590	4.3854380	0.5172530
C	-5.8591290	0.2831480	-1.1194320				
H	-6.2126870	-1.1778090	1.2019590	2-s			
H	-5.5445860	0.0014000	2.3497680	C	1.2557760	-0.7484960	-1.3710810
H	-6.9944630	0.4023590	1.4121630	C	2.0706390	-0.0680860	-0.4762790
H	-4.3554100	2.4623310	-0.2870730	C	3.2623790	-0.7088550	0.0098480
H	-5.9385960	2.4999400	0.5099090	C	3.5652050	-2.0396730	-0.4219660
H	-4.4726300	2.1863810	1.4573650	C	2.6922510	-2.6993690	-1.3288680

C	1.5623390	-2.0617790	-1.7948460	C	-4.8457650	-1.6218160	1.5107730
H	0.3750630	-0.2555860	-1.7714320	H	-5.0990360	-1.1611100	-1.2009180
C	4.7413570	-2.6487860	0.0891430	H	-3.9767510	-2.4068270	-1.7800480
H	2.9330480	-3.7100860	-1.6480090	H	-5.4408580	-2.8772240	-0.8985280
H	0.9005110	-2.5611050	-2.4959930	H	-2.7611140	-3.4386610	1.6703320
C	5.5387860	-1.9500400	0.9675720	H	-4.1093480	-4.1811120	0.7883100
C	5.1542760	-0.6367200	1.3325150	H	-2.6015510	-3.7848530	-0.0571570
H	4.9940910	-3.6598670	-0.2197190	H	-5.6555140	-2.3532990	1.6172040
H	6.4449350	-2.3818150	1.3803860	H	-4.3246940	-1.5529690	2.4730160
H	5.7740340	-0.0665220	2.0224170	H	-5.2907880	-0.6465530	1.2918160
N	4.0650020	-0.0343140	0.8847130	C	-1.7861700	2.9267500	-0.3883090
C	1.8186570	1.3231180	-0.0767830	H	-2.4526120	2.9120160	-1.2579500
H	2.7106660	1.9179590	0.1026290	H	-2.3654030	3.1895570	0.5068030
C	1.8397310	4.1523350	0.2519110				
H	1.6030040	5.2011410	0.4582810	3-s			
H	2.2744090	4.0968810	-0.7529700	C	-5.1189820	-2.0027550	-2.1002330
H	2.5967850	3.8429720	0.9792850	C	-3.9347620	-1.5037370	-1.5625510
C	0.5531150	3.3390990	0.3615200	C	-3.8851940	-0.1338520	-1.1501160
H	0.1827600	3.3942300	1.3939700	C	-5.0177230	0.7027540	-1.4018890
N	0.6622740	1.8718010	0.0676770	C	-6.2129160	0.1345930	-1.9224200
C	-0.5655900	3.8241900	-0.5680930	C	-6.2709270	-1.2035720	-2.2432400
H	-0.2023580	3.7834160	-1.6032270	H	-5.1431480	-3.0350060	-2.4377040
H	-0.8000760	4.8739570	-0.3434790	C	-4.9059710	2.0915610	-1.1467100
Pd	-1.1991810	1.0314310	-0.0382100	H	-7.0700310	0.7839040	-2.0759500
C	-2.7662690	-1.0170380	0.2681180	H	-7.1804770	-1.6374470	-2.6454410
O	-1.5547950	-1.2931420	0.4809580	C	-3.7155720	2.6015320	-0.6810700
O	-3.0985480	0.1872560	-0.0592460	C	-2.6676480	1.7129670	-0.3873440
C	-3.8828750	-2.0646400	0.3854780	H	-5.7580960	2.7367120	-1.3401950
C	-4.6447390	-2.1258780	-0.9570370	H	-3.5726390	3.6617030	-0.5055400
C	-3.2982840	-3.4469310	0.7167570	H	-1.7357260	2.0811930	0.0212150

N	-2.7569750	0.3947790	-0.5742500	H	0.6387480	3.3586640	3.8143880
C	-2.7637100	-2.3688140	-1.6388980	H	-0.6935580	4.1359120	2.9470210
H	-2.8961780	-3.2441870	-2.2761020	Pd	1.4404330	0.7616220	0.4067610
C	-0.7862330	-4.5157880	-0.8850070	O	-0.1428790	-2.0574240	1.3865310
H	-1.6255690	-4.9971390	-1.4008720	O	1.6680050	-0.7434570	1.7690310
H	-1.0166050	-4.4630100	0.1819700	C	0.9782460	-1.7881640	1.9370200
H	0.0970310	-5.1492410	-1.0144960	C	1.9834570	3.3219480	-0.8076080
C	-0.4965090	-3.1218800	-1.4540160	O	2.8703400	3.4771860	0.0429390
H	0.3908150	-2.7144680	-0.9699920	O	1.2069840	2.2792280	-0.8982030
N	-1.6087980	-2.1756060	-1.1063190	C	1.6990860	4.3973070	-1.8940200
C	-0.2406210	-3.1610810	-2.9736000	C	1.9683740	3.7815940	-3.2842190
H	-1.0943020	-3.6276850	-3.4833450	C	0.2226310	4.8384230	-1.8008170
H	0.6085020	-3.8398220	-3.1187830	C	2.6103220	5.6177460	-1.6880860
Pd	-1.3672520	-0.7931650	0.3371130	H	3.0085990	3.4472300	-3.3743840
C	0.0767420	-1.8052740	-3.6114010	H	1.3184080	2.9215450	-3.4698300
H	-0.7645640	-1.1077440	-3.5328050	H	1.7863280	4.5271490	-4.0682500
C	-0.7421460	1.3857780	2.3767090	H	-0.0096480	5.2417140	-0.8076290
O	0.3003020	1.7831680	1.7815970	H	0.0191030	5.6254650	-2.5374360
O	-1.4757350	0.4094970	2.0098390	H	-0.4543860	4.0023890	-1.9978850
C	-1.1648280	2.1208820	3.6671610	H	2.4019710	6.3691100	-2.4597020
C	-2.6914020	2.3334540	3.6801350	H	2.4472290	6.0808990	-0.7093440
C	-0.7584060	1.2126820	4.8533480	H	3.6682850	5.3455810	-1.7546870
C	-0.4476600	3.4762640	3.7860440	C	1.5080440	-2.8443160	2.9345660
H	-3.0141450	2.9651960	2.8446130	C	1.5729040	-4.2163980	2.2302120
H	-3.2295060	1.3837810	3.6194010	C	2.9055890	-2.4635500	3.4501680
H	-2.9817230	2.8349300	4.6101890	C	0.5193740	-2.9177070	4.1206460
H	0.3219470	1.0317700	4.8647790	H	0.5826680	-4.5457650	1.9057510
H	-1.0291390	1.7031870	5.7953610	H	2.2286850	-4.1827350	1.3543620
H	-1.2735340	0.2481460	4.8100660	H	1.9706210	-4.9626690	2.9278350
H	-0.7643660	3.9725560	4.7103840	H	2.8988050	-1.4982460	3.9647740

H	3.2488130	-3.2255330	4.1594730	C	-5.8388890	-2.3977130	-2.7499160
H	3.6325110	-2.4067790	2.6342830	H	-4.1803010	-3.7376990	-3.0717600
H	0.8678660	-3.6667410	4.8409790	C	-5.7100740	0.8447540	-0.9197890
H	0.4487990	-1.9563270	4.6417950	H	-7.2417960	-0.8197120	-2.3518630
H	-0.4832770	-3.2022720	3.7876670	H	-6.5257290	-2.9906750	-3.3447670
H	0.9429300	-1.3353910	-3.1345470	C	-4.7980150	1.5876870	-0.2079880
C	3.1820950	-1.1886670	-1.0799560	C	-3.5350580	1.0332260	0.0558510
O	2.5570040	-2.1909150	-0.7069170	H	-6.7122920	1.2153810	-1.1142650
O	2.8505900	0.0473240	-0.8508650	H	-5.0317650	2.5739030	0.1765300
C	4.5118080	-1.3231170	-1.8792390	H	-2.8196100	1.5717140	0.6603500
C	4.5110830	-0.3705070	-3.0916040	N	-3.1559720	-0.1725220	-0.3737550
C	5.6685240	-0.9443530	-0.9257860	C	-2.2240370	-2.6187550	-1.8228320
C	4.6990930	-2.7701850	-2.3633590	H	-2.0319080	-3.3570100	-2.5997570
H	3.6828010	-0.5967220	-3.7739130	C	0.1842140	-4.1870390	-1.8789210
H	4.4166730	0.6722420	-2.7783330	H	-0.1885500	-4.3024030	-2.9020530
H	5.4473440	-0.4800550	-3.6527560	H	-0.3824260	-4.8512880	-1.2180440
H	5.6895070	-1.5976480	-0.0451500	H	1.2277350	-4.5160960	-1.8753250
H	6.6307210	-1.0468450	-1.4428300	C	0.1400080	-2.7373420	-1.3823230
H	5.5744820	0.0897760	-0.5803390	H	0.6660270	-2.7048210	-0.4356820
H	5.6447210	-2.8574370	-2.9123760	N	-1.2447700	-2.2499290	-1.0759600
H	4.7219260	-3.4747370	-1.5268200	C	0.8539940	-1.7894480	-2.3705500
H	3.8895940	-3.0759240	-3.0353130	H	0.3642810	-1.9027530	-3.3494220
H	0.3043780	-1.9279070	-4.6762910	H	1.8746200	-2.1678640	-2.4803890
				Pd	-1.4764170	-0.9984120	0.4848180
TS2-s				C	0.8853010	-0.2901200	-2.0482070
C	-4.5107960	-2.8299530	-2.5748410	H	-0.1322250	0.0938260	-1.9642210
C	-3.5932860	-2.1229670	-1.7985260	C	-0.7113730	1.0792940	2.4922520
C	-4.0069020	-0.9038940	-1.1697340	O	0.3595380	1.3459220	1.8784520
C	-5.3311990	-0.4220770	-1.4265730	O	-1.6320010	0.2770570	2.0969960
C	-6.2365360	-1.2010670	-2.1975680	C	-0.9769560	1.7830030	3.8422080

C	-2.2680020	2.6214520	3.7060760	H	-1.5405560	4.8957120	0.0390220
C	-1.1753420	0.7012930	4.9267780	H	-0.0664440	5.8819310	0.0724730
C	0.1962570	2.6988460	4.2264060	C	1.9507300	-2.7393270	2.6650050
H	-2.1701640	3.3838630	2.9244570	C	2.8025720	-3.6841290	1.7850040
H	-3.1313720	1.9914300	3.4731240	C	2.8779510	-1.8450940	3.5149060
H	-2.4667900	3.1377880	4.6520200	C	1.0386310	-3.5691620	3.5832320
H	-0.2795150	0.0798430	5.0367210	H	2.1714790	-4.3367540	1.1708010
H	-1.3711390	1.1826910	5.8915450	H	3.4671990	-3.1204480	1.1238890
H	-2.0203960	0.0488100	4.6896110	H	3.4181060	-4.3221060	2.4290090
H	-0.0234110	3.1849560	5.1838480	H	2.2999790	-1.1617060	4.1472430
H	1.1282880	2.1362130	4.3357760	H	3.4899100	-2.4749100	4.1701930
H	0.3629380	3.4789790	3.4779040	H	3.5438000	-1.2477500	2.8870350
Pd	0.9338220	0.5866990	0.0030000	H	1.6586150	-4.1868600	4.2427670
O	-0.1310890	-2.0435650	1.6469940	H	0.4092490	-2.9300510	4.2107600
O	1.7624910	-0.9894470	1.0334100	H	0.3839110	-4.2340960	3.0121330
C	1.1260080	-1.8430100	1.7187450	H	2.0793000	-0.0680000	-1.4294480
C	0.6095630	3.3897570	-0.8117470	C	4.5108200	0.1719620	-1.1709090
O	1.5760200	3.7007550	-0.1084430	O	3.4721860	-0.3505810	-1.7340630
O	0.1345280	2.1818890	-0.9542940	O	4.4959450	0.9772720	-0.2224940
C	-0.1541290	4.4828440	-1.6129150	C	5.8714330	-0.2734340	-1.7953910
C	0.8772990	5.2671840	-2.4509680	C	7.0520430	0.3099310	-1.0031190
C	-1.2314470	3.9011790	-2.5432910	C	5.9606850	-1.8137230	-1.7884760
C	-0.8144130	5.4298070	-0.5861060	C	5.9301880	0.2389800	-3.2513300
H	1.6537070	5.7010900	-1.8148550	H	7.0226220	1.4037900	-0.9887840
H	1.3645690	4.6174340	-3.1878000	H	7.0452340	-0.0341340	0.0366330
H	0.3794300	6.0794450	-2.9944050	H	8.0008000	-0.0018170	-1.4583980
H	-1.9984940	3.3552240	-1.9857240	H	5.1465190	-2.2597440	-2.3670480
H	-1.7246390	4.7149200	-3.0896210	H	6.9129270	-2.1418820	-2.2247010
H	-0.7995080	3.2149800	-3.2790470	H	5.9078750	-2.2098190	-0.7667750
H	-1.3471130	6.2360680	-1.1049930	H	6.8796210	-0.0513060	-3.7192910

H	5.1128130	-0.1751660	-3.8498380
H	5.8593700	1.3330520	-3.2896010
H	1.3113430	0.2577000	-2.8966690