

Electronic supplementary information (ESI)

Mechanistic Insight into Construction of Axially Chiral Biaryls via Palladium/Chiral
Norbornene Cooperative Catalysis: a DFT-Based Computational Study

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I. Comparison of four potential pathways of NBE* insertion into Pd–C bond.

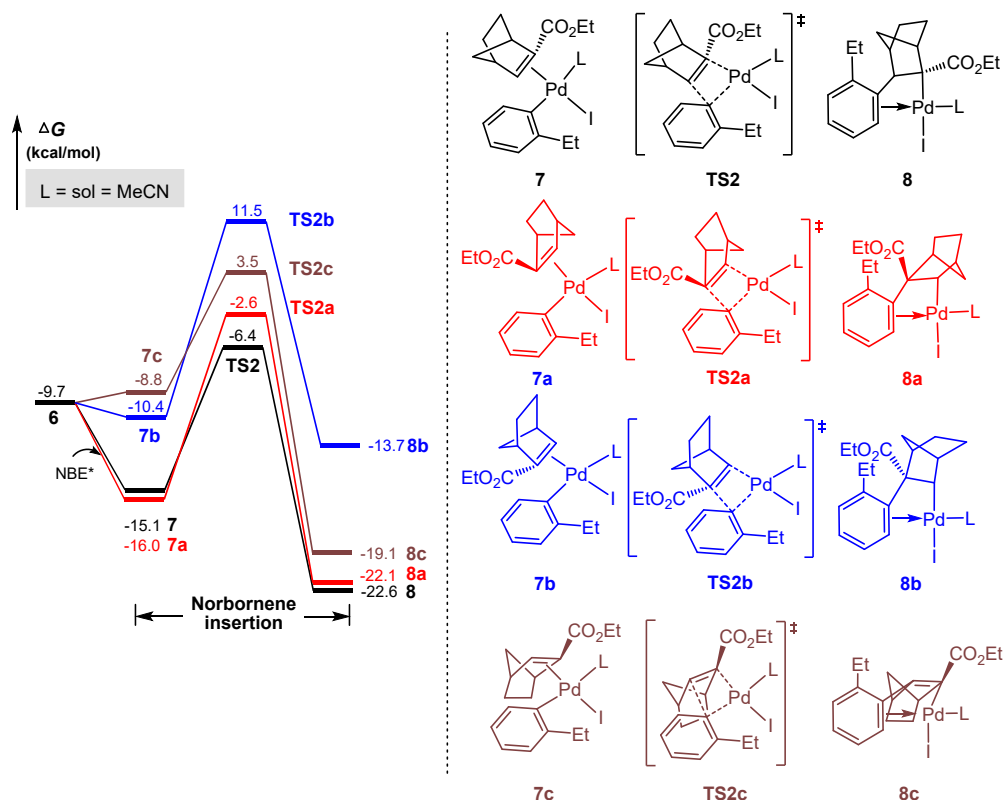


Fig. S1 Calculated Gibbs energy profiles for potential pathways of NBE* insertion into Pd–C bond.

II. Other oxidative addition pathways of aryl bromide on Pd(II).

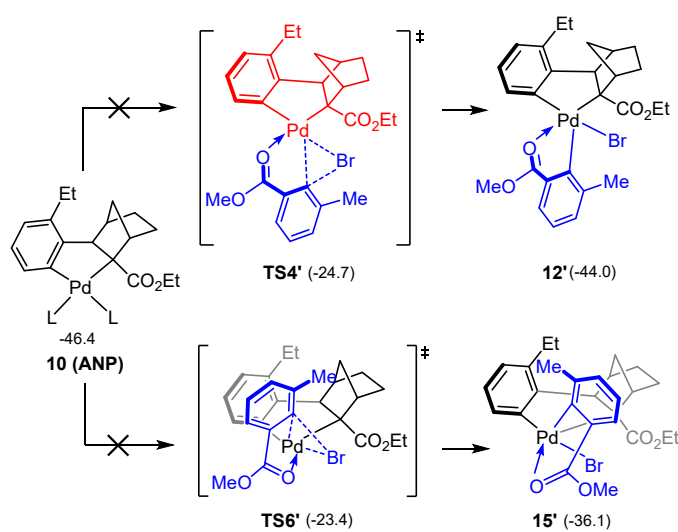


Fig. S2 Calculated Gibbs energy profiles for other two oxidative addition of aryl bromide on Pd(II).

III. Potential pathways for *tert*-butyl acrylate insertion into Pd–C_{phenyl}/Pd–C_{norborneyl} bond.

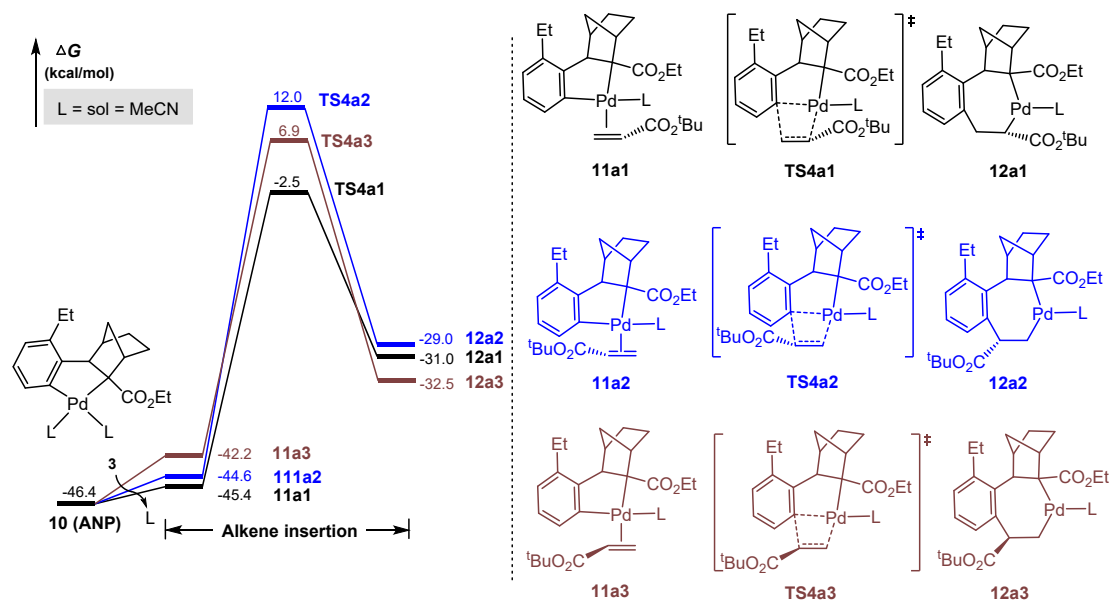


Fig. S3 Calculated Gibbs energy profiles for *tert*-butyl acrylate insertion into the Pd–C_{phenyl} bond.

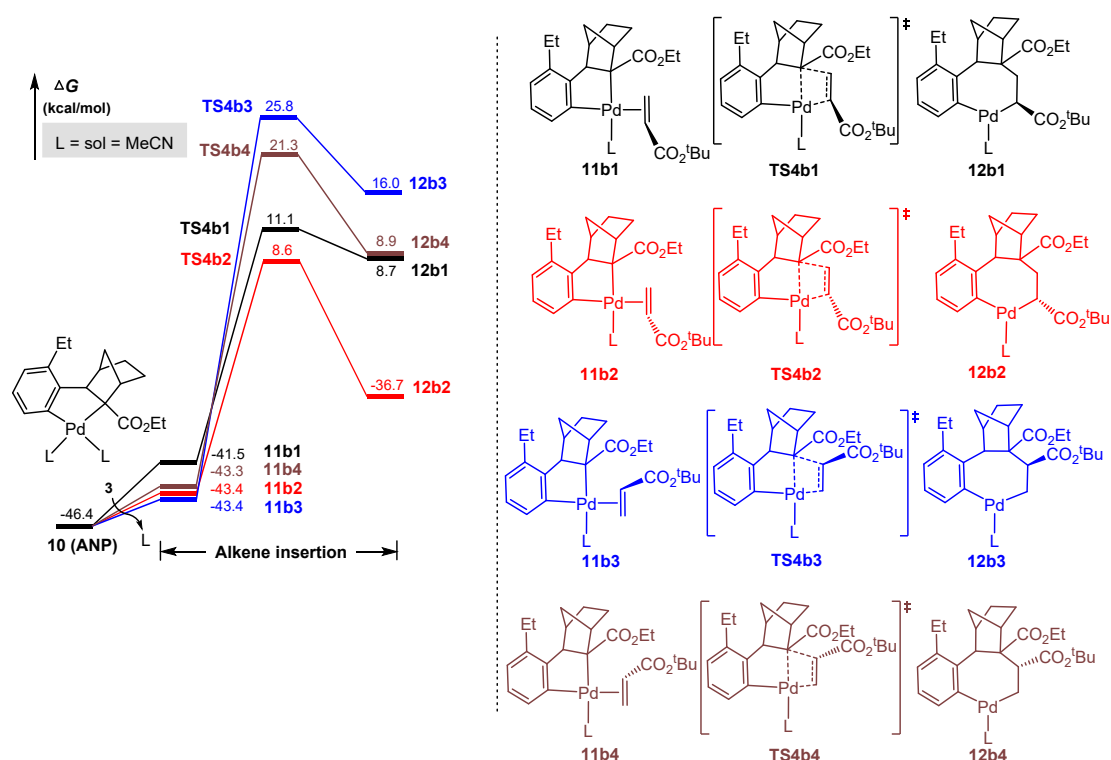


Fig. S4 Calculated Gibbs energy profiles for *tert*-butyl acrylate insertion into the Pd–C_{norborneyl} bond.

IV. Calculated energies and imaginary frequencies.

Stationary point	Thermal correction to Gibbs free energy at B3LYP-D3/LANL2DZ/6-31G(d,p) (in a.u.) (1)	Single-point energy at B3LYP-D3/SDD/6-311++G(d,p) (in a.u.) (2)	Gibbs free energies (G) (in a.u.) (3)=(1)+(2)+ $aRT \cdot \ln 31.4$ ($a=3.8088 \cdot 10^{-7}$)	Imaginary frequencies
1	0.111223	-321.819386	-321.7041447	
2	0.121678	-3073.174248	-3073.048552	
3	0.143798	-424.584747	-424.4369307	
L(MeCN)	0.021352	-132.81171	-132.7863397	
NBE*	0.187118	-540.136848	-539.9457117	
K₂CO₃	-0.017929	-1463.936561	-1463.950472	
OAc⁻	0.021233	-228.703667	-228.6784157	
I⁻	-0.016848	-11.607332	-11.62016172	
KOAc	0.017865	-828.596561	-828.5746777	
KI	-0.025616	-611.478998	-611.5005957	
KI-KHCO₃	-0.011317	-1476.050561	-1476.05786	
KHCO₃	-0.00244	-864.538127	-864.5365487	
KBr	-0.024326	-3174.204113	-3174.224421	
<i>o</i>-Bromotoluene	0.085587	-2845.22217	-2845.132565	
4	0.217456	-818.20877	-817.9872957	
5	0.144645	-582.597942	-582.4492787	
TS1	0.146018	-582.59786	-582.4478237	-54.32
6	0.144173	-582.631838	-582.4836467	
7	0.357163	-1122.799138	-1122.437957	
TS2	0.359306	-1122.787323	-1122.423999	-228.05
8	0.363198	-1122.817172	-1122.449956	
7a	0.355793	-1122.799232	-1122.439421	
TS2a	0.359136	-1122.781177	-1122.418023	-219.20
8a	0.360989	-1122.814174	-1122.449167	
7b	0.353482	-1122.788002	-1122.430502	
TS2b	0.359556	-1122.759091	-1122.395517	-211.93
8b	0.360599	-1122.800393	-1122.435776	

7c	0.356902	-1122.788962	-1122.428042	
TS2c	0.36025	-1122.77262	-1122.408352	-229.13
8c	0.361045	-1122.809476	-1122.444413	
9	0.369674	-2586.810158	-2586.436466	
TS3	0.364657	-2586.761182	-2586.392507	-127.28
9'	0.410869	-1339.928936	-1339.514049	
TS3'	0.404484	-1339.899034	-1339.490532	-1227.29
9''	0.374664	-1975.279102	-1974.90042	
TS3''	0.3693	-1975.248561	-1974.875243	-642.31
9'''	0.403805	-1951.437746	-1951.029923	
TS3'''	0.398061	-1951.412722	-1951.010643	-596.13
10(ANP)	0.392841	-1243.56362	-1243.166761	
TS1'	0.156018	-3333.946869	-3333.786833	-99.02
7'	0.314397	-1007.25341	-1006.934995	
TS2'	0.315349	-1007.232211	-1006.912844	-241.56
8'	0.319199	-1007.268303	-1006.945086	
11	0.460123	-4051.10108	-4050.636939	
TS4	0.461584	-4051.086662	-4050.62106	-196.24
12	0.463184	-4051.122002	-4050.6548	
TS5	0.46165	-4051.088202	-4050.622534	-290.58
13	0.463578	-4051.136762	-4050.669166	
14	0.458753	-4051.098745	-4050.635974	
TS6	0.460734	-4051.084257	-4050.619505	-186.95
15	0.462185	-4051.112759	-4050.646556	
TS7	0.462411	-4051.072511	-4050.606082	-184.63
16	0.463225	-4051.135676	-4050.668433	
TS4'	0.460186	-4051.072221	-4050.608017	-200.50
12'	0.462134	-4051.104975	-4050.638823	
TS6'	0.459803	-4051.069837	-4050.606016	-194.67
15'	0.462529	-4051.092778	-4050.626231	
TS8	0.351241	-1110.668864	-1110.313605	-247.44
TS9	0.487294	-1432.542095	-1432.050783	-224.04
TS4''	0.46114	-3955.938962	-3955.473804	-226.04
11a1	0.521665	-1535.341568	-1534.815885	
TS4a1	0.522933	-1535.274282	-1534.747331	-171.70
12a1	0.524972	-1535.321901	-1534.792911	

11a2	0.523214	-1535.34167	-1534.814438	
TS4a2	0.522523	-1535.250907	-1534.724366	-34.22
12a2	0.527544	-1535.321364	-1534.789802	
11a3	0.522544	-1535.337289	-1534.810727	
TS4a3	0.523335	-1535.259824	-1534.732471	-210.84
12a3	0.522199	-1535.321412	-1534.795195	
11b1	0.520665	-1535.334292	-1534.809609	
TS4b1	0.524164	-1535.253986	-1534.725804	-188.62
12b1	0.52601	-1535.259557	-1534.729529	
11b2	0.523087	-1535.339764	-1534.812659	
TS4b2	0.523173	-1535.256955	-1534.729764	-191.67
12b2	0.523784	-1535.329981	-1534.802179	
11b3	0.523088	-1535.339765	-1534.812659	
TS4b3	0.523553	-1535.229782	-1534.702211	-206.69
12b3	0.525698	-1535.247701	-1534.717985	
11b4	0.523386	-1535.339917	-1534.812513	
TS4b4	0.523802	-1535.237343	-1534.709523	-234.73
12b4	0.527174	-1535.260436	-1534.729244	
TS10	0.460658	-4051.112423	-4050.647747	-228.67
17	0.458486	-4051.12759	-4050.665086	
18	0.414945	-3935.576429	-3935.157466	
TS11	0.414956	-3935.568058	-3935.149084	-232.53
19	0.419633	-3935.593777	-3935.170126	
21	0.414993	-3935.57603	-3935.157019	
TS14	0.415881	-3935.569148	-3935.149249	-212.19
22	0.418563	-3935.600174	-3935.177593	
18'	0.416093	-3935.577799	-3935.157688	
TS11'	0.4161	-3935.563253	-3935.143135	-264.38
19'	0.418078	-3935.595719	-3935.173623	
21'	0.415881	-3935.57883	-3935.158931	
TS14'	0.41691	-3935.555343	-3935.134415	-281.03
22'	0.418607	-3935.580037	-3935.157412	
20	0.45473	-4068.421643	-4067.962895	
TS12	0.453535	-4068.414306	-4067.956753	-548.33
TS13	0.450404	-4068.404638	-4067.950216	-441.93
23	0.455337	-4068.41195	-4067.952595	

TS15	0.450486	-4068.407565	-4067.953061	-545.71
TS16	0.451519	-4068.395099	-4067.939562	-289.78
P	0.407239	-1232.829535	-1232.418278	
P'	0.406908	-1232.822707	-1232.411781	
TS_{rot}	0.412103	-1232.779996	-1232.363875	-15.14
P''	0.406883	-1232.828634	-1232.417733	

V. Cartesian coordinates of all the structures.

1

C	-0.48027000	-0.45179800	-0.03478200
C	-1.02155700	-1.71239600	0.23303400
C	-1.28754500	0.66575800	-0.29944900
C	-2.40664100	-1.87830600	0.24608900
H	-0.36876100	-2.55593500	0.42813000
C	-2.67760400	0.46097100	-0.27744800
C	-3.23735400	-0.78633700	-0.00926500
H	-2.82741100	-2.85773500	0.45264800
H	-3.32414900	1.31085700	-0.47966900
H	-4.31658000	-0.90571700	-0.00367000
I	1.64735700	-0.29569700	-0.03039600
C	-0.75056400	2.05400900	-0.55545700
H	-1.48517500	2.60891100	-1.14792200
H	0.16475300	1.99460000	-1.15269600
C	-0.46631000	2.81999900	0.74559500
H	-0.07857100	3.82055300	0.52717700
H	-1.38024400	2.92964800	1.33881100
H	0.27328800	2.29533000	1.35830500

2

C	0.73212400	0.14940000	-0.03071400
C	1.91162300	0.90789700	0.01921200
C	-0.53447900	0.74940300	-0.10372600
C	1.78556100	2.30297400	-0.01723000
C	-0.61424600	2.14969700	-0.11643800
C	0.54020000	2.92295800	-0.08202900
H	2.68895100	2.90455400	0.01269000
H	-1.59006700	2.61772200	-0.16743200
H	0.47035900	4.00547800	-0.10423500
C	-1.80418100	-0.03068800	-0.22740600
O	-1.95141900	-1.04127000	-0.88517900
O	-2.79898300	0.55618100	0.46517700
C	-4.09272500	-0.06933000	0.34235900

H	-4.76525400	0.52894100	0.95608100
H	-4.42322100	-0.06595400	-0.69897600
H	-4.05603900	-1.09760700	0.70901300
C	3.27162600	0.27246500	0.11397200
H	3.36667200	-0.32474300	1.02701200
H	3.45234900	-0.40477700	-0.72728900
H	4.05114200	1.03729800	0.11775900
Br	0.90386600	-1.75568200	0.08135400

3

C	2.27038700	-0.74723700	0.00002600
C	3.49107500	-0.20847500	-0.00010100
H	2.11390200	-1.82138300	0.00052900
H	4.38451200	-0.82482900	0.00028100
H	3.62049300	0.87014600	-0.00045500
C	1.05562900	0.11020300	-0.00020900
O	1.07251100	1.33074900	0.00022500
O	-0.04573700	-0.65846500	-0.00086000
C	-1.40437600	-0.07476300	-0.00000300
C	-2.29937400	-1.31096100	0.00034900
H	-2.11422000	-1.92164700	0.88892600
H	-3.34990800	-1.00748200	0.00049100
H	-2.11454800	-1.92192000	-0.88810900
C	-1.61348200	0.74665300	1.27143300
H	-1.39177100	0.14103300	2.15572600
H	-0.97984300	1.63383200	1.28179800
H	-2.65983300	1.06217000	1.32787500
C	-1.61450900	0.74687200	-1.27113200
H	-1.39451900	0.14111100	-2.15574800
H	-2.66059100	1.06352700	-1.32622700
H	-0.97995900	1.63341700	-1.28218100

L(MeCN)

N	-1.43772400	0.00017600	-0.00028000
C	-0.27661700	-0.00038400	0.00062900
C	1.17873300	0.00010900	-0.00013600
H	1.55025900	1.02760600	-0.04466100
H	1.55095900	-0.47520400	0.91160900
H	1.55015600	-0.55198800	-0.86794700

NBE*

C	-1.30566000	1.30301800	0.40568700
C	-1.13123500	-0.66039700	-0.81269900
C	-2.65687700	0.65141400	0.21721300

C	-0.39067000	0.52732400	-0.21002900
C	-2.47009400	0.01703300	-1.18197300
H	-3.25984200	-0.69571700	-1.44021500
H	-2.36770500	0.76120900	-1.97703700
C	-1.58111500	-1.54150700	0.39901400
H	-2.03938000	-2.46824900	0.04110200
H	-0.73602200	-1.80871100	1.03856700
C	-2.62705400	-0.63705600	1.11610800
H	-3.61746200	-1.10173500	1.12416300
H	-2.35587400	-0.40506400	2.14901600
H	-0.60316600	-1.20069000	-1.59722300
H	-3.52679000	1.28941900	0.37617600
C	1.06335100	0.71347900	-0.11898400
O	1.61622200	1.69525100	0.35389600
O	1.72762700	-0.34525700	-0.63523100
C	3.17476600	-0.30559100	-0.56154600
H	3.50629400	-0.96423600	-1.36689600
H	3.51200100	0.71258500	-0.76747900
H	-1.09921900	2.16275400	1.03333900
C	3.66575600	-0.79124600	0.78990800
H	4.76043100	-0.81878500	0.79519900
H	3.33412900	-0.12197100	1.58814300
H	3.29480000	-1.79959500	0.99763200

K₂CO₃

C	0.00021900	0.83794500	-0.00057700
O	0.00102900	-0.48992000	-0.00203100
O	1.12719700	1.46512400	-0.03482100
O	-1.12803800	1.46304900	0.03531100
K	2.51847400	-0.64570400	0.00702600
K	-2.51862200	-0.64554200	-0.00619500

OAc⁻

C	-0.20507500	0.00083800	-0.00030800
O	-0.81438400	-1.10146900	0.00006200
O	-0.69650300	1.16188400	0.00008000
C	1.34931400	-0.05666600	-0.00006400
H	1.74622600	0.47019400	-0.87722600
H	1.74513700	0.46467000	0.88098300
H	1.73029900	-1.08321900	-0.00266300

I⁻

I	0.00000000	0.00000000	0.00000000
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KOAc

C	0.99669300	-0.00006600	-0.02030500
O	0.41568700	-1.12668700	-0.01486300
O	0.41602700	1.12676400	-0.01487500
K	-1.92312300	0.00002600	0.00786500
C	2.52918400	-0.00013900	0.01365100
H	2.93403700	0.89429100	-0.46736100
H	2.86220800	0.00245800	1.05912000
H	2.93410800	-0.89662200	-0.46337300

KI

I	0.00000000	0.00000000	0.88208700
K	0.00000000	0.00000000	-2.46055900

KI-KHCO₃

H	2.87126700	0.91079600	1.85145800
C	2.39661100	-0.11670500	0.30089900
O	2.01178700	0.00308500	-0.89478600
O	2.53670500	-1.15367200	0.98087900
O	2.64042700	1.10876700	0.92927800
I	-1.88804600	0.01256100	0.19894800
K	0.65864500	-2.27211500	-0.57472200
K	0.67315100	2.24360200	-0.60022700

KHCO₃

H	2.67788200	-0.86138800	0.00679800
C	1.02132400	0.04027100	-0.00226100
O	0.45670600	1.16046500	-0.00474100
O	0.48410800	-1.10347800	-0.00544000
O	2.40547700	0.07014000	0.00582100
K	-1.87242900	-0.02090800	0.00219200

KBr

K	0.00000000	0.00000000	-1.91836800
Br	0.00000000	0.00000000	1.04140000

***o*-Bromotoluene**

C	-0.11675900	-0.24313700	-0.00005700
C	-0.78733600	0.98716600	-0.00003600
C	-0.78281000	-1.46606100	-0.00004300
C	-2.18904900	0.93648700	0.00001600
C	-2.17769400	-1.47913400	0.00000000
C	-2.88097000	-0.27431600	0.00003700
H	-2.73916800	1.87313800	0.00001200

H	-2.70501900	-2.42785300	0.00005200
H	-3.96651500	-0.27552300	0.00011600
C	-0.06036400	2.30326600	-0.00002200
H	0.58553000	2.39919600	0.87951300
H	0.58623700	2.39886300	-0.87906400
H	-0.76859100	3.13476600	-0.00044300
Br	1.80564200	-0.26558900	0.00001700
H	-0.22004100	-2.39259000	-0.00014300

4

Pd	-1.28019400	-0.37879200	-0.37699700
N	-0.66594100	1.73319000	-0.33784700
C	-0.07358800	2.72946800	-0.30239800
C	0.68586500	3.96731300	-0.25467200
H	1.64338700	3.82933900	-0.76504100
H	0.12602800	4.76688100	-0.74782900
H	0.86983800	4.24540600	0.78688200
C	0.34885600	-1.58791800	-0.97613800
C	-0.76647900	-2.40423200	-0.66018400
H	0.61567500	-1.38271200	-2.00982300
H	-1.31981700	-2.88308300	-1.46531500
H	-0.77534800	-2.93863400	0.28778300
C	1.41619800	-1.34178000	0.01621000
O	1.44726700	-1.79420700	1.15458300
O	2.36170900	-0.52776700	-0.50984000
C	3.46059100	0.00641700	0.30627600
C	4.19849200	0.91632100	-0.67419700
H	3.53512000	1.70565400	-1.04162300
H	5.05456300	1.38484500	-0.18000000
H	4.56379900	0.34390500	-1.53239800
C	2.89893900	0.82001300	1.47347200
H	2.20950700	1.58605000	1.10520900
H	2.36935300	0.18136600	2.18101200
H	3.71946500	1.32169000	1.99614400
C	4.36903400	-1.13123400	0.77449600
H	4.70398400	-1.72519000	-0.08207300
H	5.25346600	-0.71502800	1.26755900
H	3.84854700	-1.78463600	1.47497800
N	-3.31027600	-0.03950100	0.25826200
C	-4.40193100	0.14439400	0.60265300
C	-5.77106000	0.36966700	1.03377400
H	-5.94944900	-0.15029300	1.97942500
H	-5.94428800	1.44056200	1.17292100
H	-6.46272900	-0.01231800	0.27746500

5

Pd	1.19465200	0.17225300	-0.13043700
C	-0.87373500	0.42205300	-0.38146100
C	-0.50754600	0.93423400	-1.65942200
C	-1.20682000	1.30772400	0.69200200
C	-0.50287600	2.32529800	-1.87458800
H	-0.37566200	0.25740200	-2.49559400
C	-1.18022900	2.67992300	0.42045700
C	-0.85295000	3.18899400	-0.84368300
H	-0.24776200	2.70684000	-2.85873400
H	-1.43211200	3.36461900	1.22644500
H	-0.86404500	4.26188600	-1.01010100
I	-1.49533000	-1.66828100	-0.30997700
C	-1.66681400	0.82470800	2.04823000
H	-1.28680600	1.51192600	2.81157700
H	-1.23805000	-0.15833900	2.25876300
C	-3.19868100	0.75564600	2.14763600
H	-3.50563300	0.39871100	3.13646700
H	-3.64326400	1.74358900	1.98832800
H	-3.61103400	0.07381000	1.39732000
N	3.19470100	-0.10598300	0.24593600
C	4.30212500	-0.32683100	0.51432500
C	5.68965700	-0.59852800	0.84651600
H	5.81767500	-1.66459100	1.05560300
H	6.33201600	-0.31678300	0.00711600
H	5.97747100	-0.02128900	1.73003500

TS1

Pd	-1.09398200	-0.21211100	-0.09284800
C	0.92615000	-0.46437900	-0.40392600
C	0.83627400	-1.04154400	-1.69907600
C	1.35491700	-1.23427600	0.71678600
C	1.14063500	-2.39468200	-1.87393900
H	0.58538400	-0.41927800	-2.55027200
C	1.64549000	-2.58650400	0.48505600
C	1.55171700	-3.16298700	-0.78414500
H	1.06654300	-2.83447600	-2.86422000
H	1.96012000	-3.19416300	1.33004900
H	1.79695200	-4.21220800	-0.91814400
I	1.12597400	1.78228700	-0.34891400
C	1.59193400	-0.64861800	2.09140200
H	1.28118800	-1.38074500	2.84453400
H	0.97220600	0.23962500	2.23316400

C	3.06999600	-0.29139100	2.31289100
H	3.21915600	0.13360000	3.31116800
H	3.70354700	-1.17995700	2.22222800
H	3.41071000	0.44320900	1.57652000
N	-3.13484100	-0.13055900	0.23149500
C	-4.27665600	-0.07307800	0.43091800
C	-5.70634300	-0.00558000	0.67917600
H	-6.02059600	1.03927000	0.75605900
H	-6.24639600	-0.48439200	-0.14278100
H	-5.94306900	-0.52245200	1.61380600

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Pd	0.49410500	0.76374200	-0.22617100
C	-1.43636400	0.55591400	-0.43267900
C	-1.94569800	0.37186800	-1.72250700
C	-2.27920400	0.81936500	0.65969600
C	-3.31675000	0.52343600	-1.95436700
H	-1.27993100	0.11979300	-2.54286000
C	-3.65154500	0.96331800	0.40018400
C	-4.16892900	0.82007400	-0.88819600
H	-3.71274200	0.39882900	-2.95838700
H	-4.31874800	1.19076700	1.22883700
H	-5.23595700	0.93248900	-1.05804900
I	0.67318500	-1.87449000	-0.10719600
C	-1.76292300	0.91723200	2.08167600
H	-2.28493600	1.73033500	2.59962200
H	-0.69807100	1.17692800	2.07442000
C	-1.95810900	-0.39215000	2.85843800
H	-1.58713100	-0.29549900	3.88456100
H	-3.01772100	-0.66556900	2.90375100
H	-1.41828500	-1.21241000	2.37461600
N	2.61058500	1.24194300	-0.04857200
C	3.74253300	1.46544200	0.04825700
C	5.16211900	1.74135100	0.16929200
H	5.69468900	0.81631500	0.40808900
H	5.53919600	2.14398000	-0.77494900
H	5.32715500	2.47114100	0.96685300

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Pd	-0.29520300	0.35029100	-0.09766300
C	-1.60816300	-0.88570900	0.76897100
C	-1.54959000	-0.98693200	2.16342500
C	-2.51860500	-1.65432200	0.03001200
C	-2.38923900	-1.87389600	2.84233300

H	-0.83188800	-0.39038200	2.71932500
C	-3.34859100	-2.54594800	0.73281400
C	-3.29121700	-2.66059200	2.12071700
H	-2.33316500	-1.95123800	3.92483900
H	-4.05027900	-3.15904700	0.17116800
H	-3.94435100	-3.35904600	2.63619300
I	-2.19275200	2.24516600	0.04711300
C	-2.64821200	-1.54968800	-1.47623300
H	-2.53435900	-2.54638200	-1.92118800
H	-1.83223100	-0.93496000	-1.86569500
C	-3.99003200	-0.95050500	-1.91907100
H	-4.04769300	-0.89206600	-3.01156700
H	-4.83108400	-1.55849800	-1.56965300
H	-4.11520500	0.05965300	-1.51637600
N	1.14773000	1.78593900	-0.90402300
C	2.03451600	2.49094900	-1.13795300
C	3.16277000	3.35810100	-1.41959300
H	2.89575800	4.07165300	-2.20381000
H	3.43741300	3.90334100	-0.51214800
H	4.01090100	2.75288400	-1.75145400
C	0.88566700	-1.94319300	0.04793900
C	2.34976100	-1.14110700	-1.57624600
C	0.77287100	-2.73053000	-1.23449400
C	1.82865700	-0.96515100	-0.15485400
C	1.08520200	-1.65274300	-2.29501600
H	1.29889600	-2.07717800	-3.27974000
H	0.30252500	-0.89375000	-2.37896100
C	3.19289100	-2.45887500	-1.51316700
H	3.70817000	-2.61015100	-2.46569300
H	3.94748300	-2.42073500	-0.72373500
C	2.11223400	-3.55507900	-1.27329600
H	2.07067400	-4.26672100	-2.10236000
H	2.27270000	-4.12038600	-0.35185300
H	2.86575000	-0.28390200	-2.00191100
H	-0.13264900	-3.32341800	-1.35241000
C	2.53569700	-0.25523700	0.94067800
O	2.15343900	-0.19628800	2.09787800
O	3.66636500	0.31271500	0.48632800
C	4.47735200	1.02993000	1.45598900
H	5.05718100	1.73101300	0.85309500
H	3.81467500	1.58692800	2.12174700
H	0.54050600	-2.28439800	1.01358800
C	5.37545900	0.07843100	2.22367700
H	6.02602400	0.65075900	2.89310300

H	4.78412800	-0.61516700	2.82711200
H	6.00619600	-0.49638400	1.53858000
TS2			
Pd	0.02890900	-0.39308200	-0.09089200
C	1.41597400	0.92469300	0.76285500
C	1.35074000	0.85501600	2.16677600
C	2.63264100	1.21979100	0.11620600
C	2.49290300	1.03458300	2.94180300
H	0.38907400	0.68717300	2.64220400
C	3.76619000	1.41534100	0.92241500
C	3.70782200	1.32108300	2.31173500
H	2.43335000	0.96702500	4.02416200
H	4.71958600	1.62099400	0.44367400
H	4.60744100	1.47302600	2.90118800
I	1.93667400	-2.46596800	-0.21994300
C	2.79149400	1.23998500	-1.38803000
H	1.81743600	1.10189500	-1.85419600
H	3.38579500	0.36280100	-1.67468600
C	3.46440500	2.50291700	-1.94029100
H	3.50343900	2.46443700	-3.03390700
H	2.91671400	3.40625200	-1.65296500
H	4.49107300	2.60828400	-1.57653800
N	-1.46306900	-1.71845900	-0.76620900
C	-2.35280800	-2.38881800	-1.07599500
C	-3.47013900	-3.22843000	-1.46479400
H	-3.16229600	-3.89704000	-2.27367300
H	-3.79578900	-3.82365100	-0.60721000
H	-4.29726400	-2.60051600	-1.80701100
C	-0.29673900	2.07562800	0.20400200
C	-1.98254200	1.50286600	-1.35839800
C	-0.18487300	2.85713000	-1.08566200
C	-1.39681600	1.17212500	0.01702500
C	-0.71297800	1.87065000	-2.14727400
H	-0.93382000	2.36297400	-3.09820300
H	-0.05958500	1.01323400	-2.32244700
C	-2.63713500	2.90634700	-1.18958800
H	-3.18818300	3.16851900	-2.09738100
H	-3.33880300	2.93626900	-0.35197500
C	-1.40572000	3.83833000	-0.98601800
H	-1.32602300	4.58041300	-1.78476800
H	-1.42688700	4.37415000	-0.03339000
H	-2.63110100	0.73797100	-1.77942400
H	0.76786600	3.34991500	-1.26364400

C	-2.25905600	0.78773500	1.16793200
O	-1.95671500	0.90633200	2.34640400
O	-3.42466400	0.27008600	0.74898800
C	-4.32134400	-0.22308300	1.77663500
H	-3.78722200	-0.96610900	2.37622200
H	-4.59836800	0.60885400	2.43068200
H	-0.15512800	2.58449300	1.14600600
C	-5.52260700	-0.81896300	1.07628000
H	-6.22952000	-1.19533200	1.82215900
H	-6.03318400	-0.06769900	0.46592100
H	-5.22611000	-1.65196100	0.43185100

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Pd	-0.24104900	0.35395200	-0.03115200
C	-0.49572800	-1.79970700	0.75427600
C	-0.60050300	-1.17440400	2.03573100
C	-1.70310000	-2.28949400	0.15479900
C	-1.80977500	-1.06455500	2.72188900
H	0.31827400	-0.86138700	2.52038300
C	-2.89237900	-2.17868300	0.88434900
C	-2.96088500	-1.58839100	2.14679600
H	-1.83514000	-0.59720400	3.70091800
H	-3.80146600	-2.56944700	0.43572500
H	-3.91205400	-1.53711000	2.66775700
I	-2.79830200	1.64103700	-0.01968300
C	-1.84890800	-2.89376400	-1.22719400
H	-2.50256200	-3.76939100	-1.14281000
H	-0.90499000	-3.24991600	-1.62332600
C	-2.48180900	-1.90605000	-2.22158400
H	-2.56878400	-2.36472100	-3.21223800
H	-3.48153500	-1.60461700	-1.89453800
H	-1.87877500	-0.99717600	-2.31176000
N	0.58541700	2.01759600	-0.91769500
C	1.11466100	2.93965900	-1.37125700
C	1.78811700	4.09328300	-1.93599400
H	1.52408000	4.19192100	-2.99265800
H	1.48123800	4.99543800	-1.39936200
H	2.86993000	3.96311900	-1.84136900
C	0.98811000	-2.04338200	0.33374200
C	2.16854000	-0.81309700	-1.42555300
C	1.35535800	-2.86731400	-0.91864600
C	1.55883100	-0.65332500	-0.02910600
C	1.22044100	-1.84191600	-2.06572700
H	1.59252400	-2.22234400	-3.02192900

H	0.21251300	-1.44956800	-2.20284400
C	3.45600100	-1.66545700	-1.25037300
H	4.00550300	-1.69285300	-2.19665900
H	4.13062300	-1.26030700	-0.49242300
C	2.89216700	-3.06941100	-0.87929000
H	3.18898800	-3.82142600	-1.61594400
H	3.23179400	-3.41462600	0.10187200
H	2.32067000	0.12221800	-1.96117100
H	0.81158000	-3.80623900	-1.01257900
C	2.39023300	0.04126900	1.00088600
O	2.42306500	-0.24035200	2.19160000
O	3.11676400	1.03886000	0.46142400
C	3.95206100	1.80930200	1.36194400
H	4.06653400	2.77454700	0.86444800
H	3.41837600	1.95141800	2.30425200
H	1.48644200	-2.46171000	1.21220500
C	5.29325100	1.13280000	1.57746300
H	5.92552500	1.76494900	2.20991800
H	5.16671600	0.16667100	2.07310700
H	5.80758100	0.97757100	0.62400800

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Pd	0.79775500	0.32326700	0.07824200
C	-0.26661800	-1.24480700	-0.55579200
C	-0.60301100	-1.32647500	-1.91009900
C	-0.68615300	-2.23018500	0.34973600
C	-1.39885700	-2.37623600	-2.37646500
H	-0.25584300	-0.56669400	-2.60331300
C	-1.49281700	-3.27251300	-0.13851400
C	-1.85289800	-3.34982500	-1.48311800
H	-1.66239300	-2.42835800	-3.42953700
H	-1.83919400	-4.03377000	0.55724500
H	-2.47860000	-4.16616500	-1.83291800
I	3.00076500	-1.12863200	-0.45796100
C	-0.28718100	-2.22309400	1.81192400
H	-1.18328000	-2.33965600	2.43151200
H	0.14084600	-1.24794600	2.06502300
C	0.71791100	-3.33070000	2.15467200
H	0.97818400	-3.30415100	3.21873000
H	0.30511400	-4.32088500	1.93360800
H	1.63883000	-3.21368500	1.57506000
N	2.06826900	1.95388100	0.79385100
C	2.78646200	2.77505400	1.17914500
C	3.68964400	3.80439500	1.65981500

H	4.44482100	3.35427400	2.31024800
H	4.18317500	4.28310900	0.80939500
H	3.12623100	4.55464700	2.22152700
C	-0.78426300	2.22175400	0.51465800
C	-1.97203700	1.69276500	-1.41642000
C	-0.58830500	3.26853300	-0.56040700
C	-1.62078200	1.26446700	0.00070400
C	-0.67739400	2.41375900	-1.84419900
H	-0.80518700	3.01655700	-2.74749600
H	0.17167400	1.73333000	-1.96706600
C	-2.92308400	2.92155700	-1.21729300
H	-3.32190300	3.23541500	-2.18577700
H	-3.76821300	2.68293700	-0.56670400
C	-1.97586600	4.00342600	-0.61695700
H	-1.89505900	4.87446700	-1.27312600
H	-2.29555900	4.35200200	0.36838600
H	-2.35899500	0.90855100	-2.06217100
H	0.27246100	3.92414500	-0.43935200
C	-2.43013800	0.34596800	0.84114200
O	-2.28435800	0.19486100	2.04220000
O	-3.37419000	-0.26019400	0.10598300
C	-4.26016500	-1.17661800	0.79799400
H	-4.58952800	-1.86914100	0.02174500
H	-3.68452100	-1.72422700	1.54621900
H	-0.57968500	2.36693700	1.56883600
C	-5.42729100	-0.43384800	1.42122700
H	-6.11480500	-1.15170400	1.88066600
H	-5.08113300	0.25582600	2.19584800
H	-5.97714100	0.13266000	0.66328000

TS2a

Pd	0.88559000	0.47295200	0.12306500
C	-0.55809600	-0.96295700	-0.34084900
C	-0.68689900	-1.37568500	-1.67795000
C	-0.79017500	-1.87566900	0.71626000
C	-1.02571400	-2.68930100	-1.98446300
H	-0.51571100	-0.66720300	-2.48007700
C	-1.14885900	-3.18922900	0.37954800
C	-1.27139800	-3.59624900	-0.94794400
H	-1.10915600	-3.00120000	-3.02119400
H	-1.32733100	-3.90276700	1.18008200
H	-1.56011000	-4.61825800	-1.17533600
I	3.03692800	-1.28523500	-0.55193500
C	-0.60994300	-1.52876500	2.17952300

H	-1.48093100	-1.88998300	2.73819900
H	-0.57552600	-0.44496400	2.30498400
C	0.66243500	-2.14528700	2.78056800
H	0.73783400	-1.89711300	3.84490900
H	0.65946200	-3.23615800	2.68640400
H	1.55467600	-1.76618800	2.27407900
N	2.27548400	1.95003500	0.72136700
C	3.03013900	2.76296900	1.05034500
C	3.98212000	3.78013000	1.45679500
H	4.50423500	3.45239100	2.36014200
H	4.70960100	3.93943600	0.65584500
H	3.45479800	4.71614400	1.66111100
C	-0.70561700	1.80906000	0.38410900
C	-1.97347300	1.39872100	-1.56480600
C	-0.59266400	2.93672600	-0.63964700
C	-1.62249200	0.86026200	-0.18227700
C	-0.69576000	2.15732700	-1.96807900
H	-0.85729200	2.80813700	-2.83170500
H	0.16074400	1.50358800	-2.15602600
C	-2.92377600	2.60523800	-1.25596800
H	-3.33696500	2.96806000	-2.20068800
H	-3.76548700	2.32957600	-0.61573200
C	-1.97506100	3.65568200	-0.60772200
H	-1.93334200	4.57492200	-1.19949200
H	-2.27356100	3.92324100	0.40962600
H	-2.38768300	0.67168300	-2.25865700
H	0.26768800	3.59229300	-0.51020900
C	-2.72795600	0.25864300	0.64215400
O	-2.87412700	0.45799400	1.83360200
O	-3.54828800	-0.47797400	-0.11674300
C	-4.65589900	-1.13362700	0.55758300
H	-4.88831300	-1.98725100	-0.08129200
H	-4.30854300	-1.49424500	1.52803900
H	-0.75177300	2.03001100	1.44812800
C	-5.84166000	-0.19819100	0.69666000
H	-6.68216600	-0.74025600	1.14247900
H	-5.59828300	0.64994900	1.34197300
H	-6.15579400	0.17863200	-0.28150300

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Pd	-0.87416800	0.45516500	-0.04104300
C	0.89101300	-0.94871000	0.42675000
C	0.53220400	-1.45456500	1.70541500
C	0.53301100	-1.71407500	-0.73210600

C	-0.11394600	-2.67090500	1.85370500
H	0.79523300	-0.89098900	2.59023300
C	-0.11144400	-2.94966000	-0.54164300
C	-0.42370800	-3.43140300	0.72129500
H	-0.36686100	-3.03084900	2.84562700
H	-0.35637100	-3.54345100	-1.41699500
H	-0.91282800	-4.39477300	0.82737300
I	-3.36647800	-0.95915200	0.35888700
C	0.87089100	-1.33256200	-2.16274700
H	1.49283800	-2.13282100	-2.58292100
H	1.46385300	-0.42227100	-2.20762800
C	-0.36856400	-1.13667500	-3.04693300
H	-0.06811300	-0.93211600	-4.07973800
H	-1.01325900	-2.02064500	-3.04793800
H	-0.96149400	-0.29051700	-2.68223100
N	-1.89620700	2.17325500	-0.59579200
C	-2.46570400	3.11987100	-0.93918000
C	-3.18467700	4.30472300	-1.36877800
H	-3.91837200	4.02940100	-2.13162600
H	-3.70041100	4.74967600	-0.51319600
H	-2.48025500	5.02955300	-1.78623300
C	0.91479500	1.41997000	-0.22927200
C	2.29445100	0.90509200	1.67885100
C	1.03037500	2.55497300	0.77949100
C	1.81458400	0.29741800	0.30870700
C	1.09323800	1.77541400	2.10934500
H	1.33926000	2.40840900	2.96709200
H	0.17685600	1.22176100	2.32443200
C	3.32863900	2.01994300	1.39173300
H	3.71141000	2.38742200	2.34801800
H	4.18689400	1.68925400	0.80505700
C	2.48112600	3.11191100	0.67383900
H	2.55298500	4.07853800	1.18178900
H	2.78513600	3.25312100	-0.36641900
H	2.64870500	0.14913100	2.37985500
H	0.25500700	3.31624100	0.69080600
C	3.03902800	-0.01236700	-0.54416100
O	3.47953800	0.70758700	-1.42125100
O	3.59911400	-1.17076500	-0.16773800
C	4.81468300	-1.57426500	-0.85738000
H	4.84595800	-2.65780400	-0.73022300
H	4.70799100	-1.33804800	-1.91819000
H	1.03774500	1.67900600	-1.28131400
C	6.03339100	-0.90431200	-0.25212200

H	6.93808400	-1.29591600	-0.72889200
H	6.00396900	0.17720600	-0.40753500
H	6.09499400	-1.10731700	0.82140400
7b			
Pd	0.82481200	0.36582700	-0.17972000
C	0.04827400	-1.39631200	0.21132100
C	-0.62070600	-2.06113700	-0.82068200
C	0.05861900	-1.90846400	1.51878100
C	-1.35935900	-3.21537600	-0.54502100
H	-0.59099700	-1.66741500	-1.83109800
C	-0.70447700	-3.06109600	1.77406800
C	-1.40771800	-3.71062900	0.76027000
H	-1.89123700	-3.72066000	-1.34578100
H	-0.73302200	-3.45355900	2.78820900
H	-1.98209500	-4.60478700	0.98526200
I	3.04925400	-0.90938800	-0.86897000
C	0.87191500	-1.29478500	2.64194700
H	0.23120300	-1.16011000	3.52200600
H	1.21722600	-0.29938900	2.34832400
C	2.08407000	-2.15701200	3.01984900
H	2.65089800	-1.69448400	3.83521200
H	1.77334000	-3.15490900	3.34686600
H	2.75445600	-2.27682400	2.16270800
N	1.66966600	2.35691600	-0.54410600
C	2.16275200	3.39136900	-0.70634800
C	2.77822600	4.68964700	-0.91076200
H	3.72810600	4.73384800	-0.37079200
H	2.96062500	4.84385400	-1.97804400
H	2.11224400	5.47351100	-0.53931700
C	-1.44431700	2.30007200	-0.14412400
C	-3.02040800	1.49119800	1.35627200
C	-1.41341000	3.07117500	1.16067200
C	-2.39680900	1.34665000	-0.02700000
C	-2.91997700	3.02668900	1.52943100
H	-3.12392600	3.36249100	2.55127300
H	-3.54863800	3.57920800	0.82537500
C	-1.94756000	1.02056800	2.38726900
H	-2.37435700	1.02468300	3.39443400
H	-1.59634600	0.01133500	2.17141400
C	-0.83428300	2.09944600	2.24581100
H	-0.67776300	2.63954500	3.18425000
H	0.12969100	1.68090600	1.93954300
H	-3.99928500	1.02947300	1.47549500

H	-0.92531000	4.04528900	1.12250700
C	-2.75486100	0.37086900	-1.07033200
O	-2.32088800	0.38102200	-2.21275500
O	-3.65427900	-0.52184300	-0.61401400
C	-4.16379300	-1.48792200	-1.56707400
H	-3.35798600	-1.77948300	-2.24147200
H	-4.45156600	-2.34685700	-0.95827200
H	-0.81708300	2.47928200	-1.00798900
C	-5.34745400	-0.91645500	-2.32621000
H	-5.76048900	-1.68121700	-2.99239500
H	-6.13571200	-0.59733800	-1.63737900
H	-5.04244500	-0.05969300	-2.93372500

TS2b

Pd	0.90144900	0.44044700	-0.31956100
C	-0.73768500	-0.84852400	-0.42914900
C	-0.93334300	-1.02893700	-1.80791900
C	-1.08588200	-1.86142900	0.49158500
C	-1.39850300	-2.24552200	-2.30854300
H	-0.73768900	-0.20987500	-2.49201900
C	-1.57694500	-3.06112700	-0.03843800
C	-1.72840100	-3.26091600	-1.41392000
H	-1.52088100	-2.38206200	-3.37869800
H	-1.84192700	-3.86731800	0.63615100
H	-2.11668900	-4.20744100	-1.77840900
I	2.69544000	-1.72916400	0.13485500
C	-0.90877300	-1.68765900	1.98328000
H	-1.55855100	-0.87182000	2.31594700
H	0.11779800	-1.35024500	2.15959000
C	-1.18098900	-2.91949200	2.84487600
H	-0.99220800	-2.68124000	3.89626200
H	-2.21989500	-3.25598800	2.76341900
H	-0.53098400	-3.75667000	2.56966500
N	2.54513600	1.71765700	-0.66499900
C	3.44419200	2.40284800	-0.91034300
C	4.57756100	3.25750500	-1.21019100
H	5.46002100	2.89321100	-0.67667500
H	4.77266300	3.24212800	-2.28621300
H	4.35828000	4.28158200	-0.89545700
C	-0.44745400	2.05356500	-0.48786100
C	-1.63934700	1.68952600	1.51573000
C	-0.26675400	3.20225700	0.52194100
C	-1.43070900	1.17828500	0.08070400
C	-1.69648500	3.20515200	1.14443800

H	-1.79249900	3.85490400	2.02042500
H	-2.48552500	3.44689700	0.42672200
C	-0.34134700	1.64630800	2.36524800
H	-0.58454100	1.83477000	3.41447600
H	0.14753700	0.67567200	2.30122100
C	0.54558200	2.77151500	1.76275300
H	0.62780900	3.62218300	2.44619600
H	1.55332900	2.43500500	1.52262300
H	-2.51610600	1.26962100	2.00308400
H	0.07707800	4.12717200	0.05745400
C	-2.67900400	0.84678800	-0.69627100
O	-2.90098400	1.25015300	-1.82307900
O	-3.53127100	0.11881000	0.03535800
C	-4.77959600	-0.26640000	-0.60080300
H	-4.57687300	-0.50683900	-1.64654900
H	-5.07699500	-1.17441700	-0.07328600
H	-0.48185800	2.28017600	-1.55056300
C	-5.81980000	0.82876100	-0.46478200
H	-6.76882100	0.48591600	-0.88992600
H	-5.98457000	1.07853400	0.58787500
H	-5.50868700	1.73095900	-0.99806400

8b

Pd	1.04572300	0.44557200	-0.36172900
C	-1.14129100	-0.84884300	-0.23959000
C	-0.44727200	-0.95104400	-1.47978700
C	-1.32312800	-2.02577500	0.54359800
C	0.15165300	-2.15705800	-1.89117200
H	-0.53878600	-0.15079400	-2.20975200
C	-0.69090700	-3.19328600	0.11184900
C	0.05810000	-3.26539200	-1.07200300
H	0.66690000	-2.19971100	-2.84466100
H	-0.80471900	-4.09804600	0.69691700
H	0.52432500	-4.20391300	-1.35448000
I	3.35368200	-1.27533600	0.00214100
C	-2.26889300	-2.07038000	1.73215600
H	-3.20362800	-1.59286800	1.42324800
H	-1.87664200	-1.46067900	2.54963500
C	-2.58509400	-3.46268100	2.28012600
H	-3.32434900	-3.37678300	3.08256600
H	-3.00225500	-4.11963300	1.50958100
H	-1.69977800	-3.95112600	2.69979100
N	2.24629500	2.13462800	-0.24948100
C	2.92657400	3.06936700	-0.21468900

C	3.78076200	4.24058200	-0.16458900
H	4.71022600	3.99366800	0.35618700
H	4.01054700	4.56892400	-1.18216900
H	3.26650900	5.04458200	0.36937700
C	-0.64256500	1.59519600	-0.32276600
C	-2.15599200	1.01957900	1.44482200
C	-0.69609200	2.63675800	0.80634800
C	-1.74589200	0.54854900	0.01365500
C	-2.18970000	2.54662900	1.20660000
H	-2.41467900	3.11427500	2.11478600
H	-2.88155000	2.85323400	0.41746500
C	-0.96422900	0.87794600	2.43102800
H	-1.32579100	0.90419900	3.46264300
H	-0.42207400	-0.05904200	2.29393700
C	-0.05474900	2.09281600	2.09952200
H	-0.11276200	2.85904400	2.87952500
H	0.99294700	1.81433500	1.98241300
H	-3.08420900	0.57658100	1.79693300
H	-0.32568400	3.61601600	0.49905900
C	-2.94992200	0.67552900	-0.92840700
O	-2.99749400	1.38452900	-1.91554800
O	-3.94492300	-0.13684300	-0.53733100
C	-5.16255500	-0.12736800	-1.33377100
H	-4.88969300	-0.06216500	-2.38899200
H	-5.61863900	-1.09915700	-1.13728300
H	-0.74068400	2.02179900	-1.32129700
C	-6.06981900	1.01354000	-0.91537100
H	-7.00811400	0.95958000	-1.47722200
H	-6.30298600	0.95230700	0.15206800
H	-5.60154200	1.98003800	-1.12013600

7c

Pd	0.40446800	0.27461600	-0.22557400
C	1.88074600	-0.97206900	0.20803200
C	2.61535300	-1.54474100	-0.83516000
C	2.10540700	-1.35680300	1.54091600
C	3.55356600	-2.54798200	-0.57009300
H	2.45828000	-1.21616700	-1.85759900
C	3.05507100	-2.36322300	1.78318600
C	3.77296500	-2.95907700	0.74565500
H	4.10990100	-2.99649100	-1.38870000
H	3.22315600	-2.68273100	2.80961600
H	4.50005800	-3.73613600	0.96369600
I	2.24745500	2.16321300	-0.56093900

C	1.37544700	-0.72387500	2.70871600
H	1.26170800	-1.47342500	3.50116800
H	0.36462300	-0.43097600	2.40740900
C	2.11622300	0.49664400	3.27391900
H	1.57258900	0.92179400	4.12500400
H	3.12068500	0.22253700	3.61487600
H	2.22033400	1.27534700	2.51216500
N	-1.23825200	1.63414900	-0.68675600
C	-2.14134700	2.32567000	-0.89845700
C	-3.28862900	3.17204800	-1.16533100
H	-3.55291100	3.72708800	-0.26117700
H	-3.04810700	3.87657400	-1.96621700
H	-4.13376100	2.54904100	-1.47070100
C	-1.01874100	-2.13078200	-0.00778300
C	-2.82464900	-1.69192500	-1.40556100
C	-0.97687300	-2.99023800	-1.25898200
C	-2.12284900	-1.34436200	-0.09709900
C	-2.50048700	-3.20774200	-1.47073300
H	-2.74220100	-3.66219600	-2.43678800
H	-2.96779800	-3.78010300	-0.66454100
C	-1.93789200	-1.17145100	-2.58052900
H	-2.45776900	-1.33794300	-3.52832500
H	-1.72324700	-0.10632200	-2.49180800
C	-0.66213500	-2.05573100	-2.47383600
H	-0.51544900	-2.65982500	-3.37378800
H	0.24251600	-1.46939000	-2.30633300
H	-3.87011500	-1.39343200	-1.45809600
H	-0.33948500	-3.87187100	-1.19258100
C	-2.61252600	-0.43028600	0.95616400
O	-2.05551200	-0.23375900	2.02558200
O	-3.77838600	0.14247300	0.60488400
C	-4.38351500	1.04022200	1.57398700
H	-3.59679500	1.64441900	2.03086000
H	-5.03164300	1.68257500	0.97564700
H	-0.34284000	-2.20526200	0.83302800
C	-5.17315800	0.26910200	2.61534700
H	-5.67675000	0.97380500	3.28526400
H	-5.93384900	-0.35731700	2.13955100
H	-4.51472300	-0.36537700	3.21399400

TS2c

Pd	0.12616800	0.28134300	-0.18721700
C	1.39370900	-1.39191600	0.16926000
C	2.34280800	-1.74197400	-0.80138000

C	1.66411500	-1.64614600	1.53549400
C	3.57719900	-2.28399700	-0.44210200
H	2.14245500	-1.58061000	-1.85014300
C	2.91900400	-2.17764100	1.86927500
C	3.87352100	-2.49415000	0.90344400
H	4.29750500	-2.53489800	-1.21525400
H	3.13790400	-2.35469500	2.91945100
H	4.83052300	-2.91340000	1.19995000
I	2.38295300	1.99021000	-0.16519700
C	0.69614900	-1.36361100	2.66149500
H	0.96392500	-2.00981100	3.50479500
H	-0.31669600	-1.63270600	2.35914400
C	0.69512800	0.09566700	3.14268300
H	0.04162400	0.20727800	4.01508300
H	1.70207000	0.42384000	3.42281600
H	0.33344900	0.76780900	2.35775300
N	-1.09477900	1.97257900	-0.33827200
C	-1.87218100	2.82760900	-0.34612600
C	-2.85917600	3.89024800	-0.35055300
H	-2.98753600	4.27205500	0.66625000
H	-2.52586200	4.70194000	-1.00309200
H	-3.81266200	3.49731900	-0.71451300
C	-0.54396300	-1.97972100	-0.50251100
C	-2.26483900	-0.98594900	-1.82175100
C	-0.54356000	-2.46133300	-1.95475100
C	-1.56908700	-0.97376700	-0.44072800
C	-2.09054200	-2.49817800	-2.14377900
H	-2.38935200	-2.76631100	-3.16244100
H	-2.59902200	-3.15264400	-1.42975000
C	-1.38349200	-0.36278500	-2.91924300
H	-1.93210200	-0.35668700	-3.86594600
H	-1.09134400	0.66363300	-2.69179800
C	-0.17307200	-1.33768300	-2.96845900
H	-0.04982600	-1.78058600	-3.96042400
H	0.75078800	-0.82064700	-2.71760100
H	-3.28155800	-0.59935900	-1.78379700
H	0.00073700	-3.39357300	-2.10220600
C	-2.43453700	-0.81700200	0.76544400
O	-2.36227100	-1.48860000	1.78234600
O	-3.34716100	0.15308400	0.58129800
C	-4.27374700	0.40455300	1.66962700
H	-3.74106800	0.29856000	2.61694900
H	-4.56797300	1.44734000	1.53559700
H	-0.46201400	-2.70846300	0.29266900

C	-5.46821300	-0.52738900	1.59130600
H	-6.18329700	-0.27285600	2.38051800
H	-5.97274700	-0.43069000	0.62498500
H	-5.16060800	-1.56768400	1.72732900

8c

Pd	0.27444000	0.34907100	-0.38917700
C	0.55784300	-2.00395300	0.09209800
C	1.30540700	-1.86009000	-1.11105900
C	1.29403000	-2.17878000	1.31005600
C	2.70106500	-1.97033600	-1.13690600
H	0.79813900	-1.72605900	-2.05264400
C	2.68261300	-2.30143900	1.24475800
C	3.38872700	-2.21852400	0.04080300
H	3.22616600	-1.86774100	-2.08070200
H	3.22957600	-2.46241000	2.16974500
H	4.46900500	-2.32642500	0.03788600
I	2.76276600	1.68700800	-0.05216300
C	0.67443600	-2.18593400	2.69064200
H	1.13428700	-2.99180900	3.27387300
H	-0.39633200	-2.38396700	2.65711000
C	0.90841000	-0.84682900	3.40974100
H	0.46144300	-0.86488000	4.40963800
H	1.97856400	-0.64259000	3.51825400
H	0.45321100	-0.02856700	2.84708100
N	-0.67712700	2.10910200	-0.80689500
C	-1.29898500	3.06140900	-1.01244200
C	-2.09398700	4.24781600	-1.26164800
H	-2.11228100	4.87028200	-0.36265300
H	-1.65828400	4.81650900	-2.08784500
H	-3.11431100	3.95191000	-1.52137900
C	-0.98002700	-2.06195100	0.07029000
C	-2.44324700	-0.90301200	-1.48863100
C	-1.76131800	-2.99798900	-0.91059900
C	-1.52684200	-0.66582400	-0.28399900
C	-3.09969400	-2.22168200	-0.98634400
H	-3.79803400	-2.65220800	-1.71101200
H	-3.60751800	-2.11353700	-0.02266900
C	-1.66228600	-1.40138500	-2.72986900
H	-2.29658000	-1.33987900	-3.61874400
H	-0.77859600	-0.78503700	-2.91798800
C	-1.32455700	-2.88416000	-2.38164700
H	-1.94589600	-3.56172200	-2.97604500
H	-0.29031400	-3.17162000	-2.56774700

H	-3.11309200	-0.07047800	-1.69280100
H	-1.81863000	-4.02600600	-0.54629000
C	-2.17686500	0.03928800	0.87408400
O	-1.91424700	-0.16705000	2.05007700
O	-3.09200500	0.94359700	0.47493600
C	-3.73558600	1.72959700	1.50964900
H	-2.99568600	1.98027100	2.27293800
H	-4.04959100	2.64222300	0.99888000
H	-1.31050900	-2.31398000	1.07503700
C	-4.92010400	0.98923700	2.10243100
H	-5.43208900	1.63400500	2.82450000
H	-5.63455800	0.71284300	1.32074400
H	-4.59322100	0.08333200	2.61933700

9

Pd	-0.68899700	-0.83811500	-0.24208500
C	0.48205100	0.89075400	2.25547600
C	0.82316200	2.23991100	2.52475200
C	-0.82556000	0.47120400	2.55428700
C	-0.15249200	3.10590700	3.04966300
C	-1.78957200	1.34086100	3.06934400
H	-1.11099900	-0.55497500	2.36155800
C	-1.45380100	2.67426100	3.32283400
H	0.12226200	4.13949900	3.24799700
H	-2.79235100	0.97562500	3.27288300
H	-2.18631400	3.36446400	3.73260100
C	0.08661700	1.46138000	-1.88327600
O	0.11205800	2.73994200	-2.03602000
O	-0.20097300	1.06657000	-0.63672800
O	0.37354000	0.62952900	-2.78963600
I	-3.39911400	-0.16215800	-1.07589500
C	2.18273800	2.82939500	2.20403900
H	2.34584100	3.70657100	2.83934700
H	2.98375700	2.12355200	2.44246600
C	2.28021800	3.24191100	0.72549400
H	3.29368800	3.58194000	0.47921200
H	2.01078100	2.39670900	0.09114900
H	1.58503800	4.06037400	0.50906200
K	-1.69101500	3.03896900	-0.08716000
K	2.63416600	2.18109000	-2.70070100
N	-1.28460800	-2.72667500	0.21378100
C	-1.69488100	-3.77888700	0.46393000
C	-2.20052400	-5.09992100	0.78719900
H	-2.16178800	-5.73620900	-0.10143400

H	-1.58704400	-5.54262500	1.57714100
H	-3.23572400	-5.02268400	1.13139200
C	1.53824600	-0.09460800	1.76878100
C	1.55362200	-2.46949600	1.16043700
C	1.93492700	-1.09218700	2.90744200
C	1.25403800	-1.06502600	0.56839800
C	1.06084300	-2.32687200	2.60783400
H	1.32457200	-3.18877600	3.23073900
H	-0.01172900	-2.15094700	2.69004300
C	3.08647500	-2.59396500	1.39339800
H	3.33280300	-3.62968200	1.65065600
H	3.67404400	-2.33492700	0.50969800
C	3.34444500	-1.63849500	2.59750500
H	3.74493600	-2.18463700	3.45776700
H	4.04975300	-0.83651400	2.35721600
H	1.14430300	-3.29114400	0.57810400
H	1.83562200	-0.65576400	3.90392200
C	2.07502000	-0.78475800	-0.64833600
O	2.71731400	0.23897200	-0.87686700
O	2.07561200	-1.83649200	-1.49554500
C	2.70614500	-1.66465200	-2.78497200
H	2.28914400	-2.47224000	-3.39134600
H	2.36412600	-0.71697900	-3.20375100
H	2.41409700	0.48755100	1.48871300
C	4.21962200	-1.77319100	-2.71481800
H	4.63554100	-1.70629300	-3.72632800
H	4.64783800	-0.97215600	-2.10804200
H	4.51866900	-2.73578100	-2.28759800

TS3

Pd	-0.17659200	0.13125300	-0.62903700
C	2.22473000	-1.51527700	-0.04330900
C	3.07449200	-2.63641900	-0.15364300
C	0.81635600	-1.70330400	-0.05782500
C	2.51075600	-3.88249600	-0.45641900
C	0.29162100	-2.97145200	-0.39164300
H	0.16888400	-1.21318200	0.82236800
C	1.13288800	-4.04919900	-0.62572600
H	3.16983700	-4.74131600	-0.55885600
H	-0.78290800	-3.09930200	-0.44865300
H	0.72755100	-5.02096600	-0.89222900
C	-1.46465000	-0.40146900	2.39281900
O	-2.72785700	-0.52129800	2.68731400
O	-0.94266400	0.75530800	2.20560000

O	-0.74636400	-1.48400100	2.21565300
I	-2.78628600	-0.99589200	-1.41266300
C	4.56018700	-2.58496400	0.15105500
H	5.11198400	-3.15379300	-0.60655400
H	4.93812100	-1.56352600	0.11815100
C	4.85766700	-3.16987200	1.54182000
H	5.93168200	-3.13682000	1.75451700
H	4.33869800	-2.60053000	2.32083100
H	4.52919400	-4.21189700	1.61416800
K	-3.08135400	1.60286400	1.14097200
K	-2.86162700	-2.85559700	1.62920700
N	-0.97180100	1.94097200	-1.38081000
C	-1.41090100	2.91288000	-1.82979200
C	-1.95705300	4.14036300	-2.37888900
H	-2.86189200	4.41624800	-1.82924500
H	-1.21782500	4.94127800	-2.28662300
H	-2.20562800	3.99255800	-3.43353100
C	2.76058400	-0.11021700	0.00401500
C	2.12166000	1.85074100	-1.31869200
C	3.66461000	0.21109500	-1.24340300
C	1.65218800	0.98944000	-0.12284900
C	2.66405400	0.77049700	-2.26626100
H	3.15533700	1.18251600	-3.15409600
H	1.90055300	0.04906800	-2.57193800
C	3.42739100	2.59530300	-0.91855100
H	3.66061500	3.35049400	-1.67594300
H	3.33744300	3.11463800	0.03900400
C	4.49508200	1.46281200	-0.89746000
H	5.26693800	1.63270000	-1.65483300
H	4.99364200	1.36779900	0.07200700
H	1.35745300	2.51699300	-1.70750000
H	4.25667900	-0.63646000	-1.58371400
C	1.45362500	1.78721600	1.13838400
O	2.04711700	1.58797700	2.18544100
O	0.63532500	2.83956900	0.93874500
C	0.33343800	3.65161800	2.09291400
H	-0.62297800	4.12445100	1.85170900
H	0.19953300	2.99244000	2.95122000
H	3.33745400	0.05012400	0.92011400
C	1.40582000	4.69995600	2.33548700
H	1.10611100	5.35129900	3.16406200
H	2.35716300	4.22866300	2.59422600
H	1.55024100	5.32233400	1.44625100

9'

Pd	0.12800700	0.95512800	0.90277000
C	-1.40107400	-0.08214400	-1.53366500
C	-2.54661800	-0.90040000	-1.41696600
C	-1.58470300	1.31235600	-1.58536000
C	-3.80807600	-0.29009400	-1.30211800
C	-2.84126800	1.90190200	-1.47162400
H	-0.72415100	1.95656600	-1.71043600
C	-3.96754500	1.09235000	-1.31336900
H	-4.68352500	-0.92829200	-1.20670000
H	-2.93713300	2.98345000	-1.50871900
H	-4.95717400	1.53063900	-1.21989700
C	-1.97024800	0.40152900	2.28545800
O	-1.26846600	-0.42744900	1.59252400
O	-1.58731900	1.59441400	2.43194300
C	-2.52382900	-2.41678700	-1.38008700
H	-3.36315500	-2.78261700	-1.98414900
H	-1.61856800	-2.81169100	-1.84647500
C	-2.64817300	-2.98155100	0.04325400
H	-2.64724800	-4.07773200	0.02317800
H	-1.82132700	-2.63484800	0.66316800
H	-3.58559600	-2.65451700	0.50722000
N	1.40458200	2.48305600	0.50213200
C	2.07888900	3.40644500	0.32578700
C	2.93567100	4.54978400	0.07699400
H	3.55276100	4.74637600	0.95822600
H	3.58147800	4.33683700	-0.77984900
H	2.32162700	5.42838400	-0.14006700
C	0.00210700	-0.66790200	-1.61536000
C	2.27385400	0.11174800	-1.13955000
C	0.83456700	-0.20644300	-2.85283100
C	0.98783300	-0.37134600	-0.43108400
C	1.70960500	0.93915300	-2.30515100
H	2.48563200	1.24799200	-3.01384900
H	1.15898900	1.82099300	-1.98280600
C	2.88648800	-1.09399400	-1.91005900
H	3.89160500	-0.83064500	-2.25399000
H	2.98357800	-1.99001900	-1.29147100
C	1.90798600	-1.28774500	-3.10996600
H	2.41586400	-1.10754100	-4.06280800
H	1.47864700	-2.29356700	-3.14657100
H	2.98214400	0.60330800	-0.47506600
H	0.21399400	0.02639700	-3.72087300
C	1.22963100	-1.56092900	0.46327800

O	0.66370300	-2.63775300	0.38811300
O	2.20227800	-1.30475600	1.36944100
C	2.55803200	-2.38354300	2.26879600
H	2.99741700	-1.88153400	3.13330600
H	1.64715500	-2.90090400	2.57856500
H	-0.10340100	-1.75035700	-1.65120900
C	3.54625600	-3.33795100	1.62270500
H	3.86127700	-4.09064100	2.35337400
H	3.09232500	-3.85306000	0.77223900
H	4.43548700	-2.80063700	1.27843500
C	-3.26985200	-0.09335100	2.86041000
H	-3.16939200	-1.12577400	3.20346200
H	-3.60084400	0.54800200	3.67931800
H	-4.02764200	-0.07402000	2.06896600

TS3'

Pd	0.54395900	0.98062400	-0.50519000
C	-2.12278900	-0.20723000	-0.04458000
C	-3.52919200	-0.33016200	-0.04283100
C	-1.53068500	1.07596400	-0.16701600
C	-4.30559200	0.80129800	-0.31996300
C	-2.34472400	2.18132800	-0.49561500
H	-0.71670200	1.61964500	0.75115700
C	-3.72359900	2.04150400	-0.59403900
H	-5.38852100	0.70297200	-0.32601800
H	-1.88810400	3.15681800	-0.62557600
H	-4.34701900	2.89523700	-0.84351200
C	0.33631700	3.51988000	0.80461200
O	0.74563700	3.19718400	-0.35395000
O	-0.29189000	2.73359600	1.58707800
C	-4.22640400	-1.61755100	0.34870200
H	-5.23668400	-1.62221300	-0.07457900
H	-3.71109900	-2.49069500	-0.05608900
C	-4.31646900	-1.75919700	1.87724800
H	-4.82847100	-2.68745200	2.15319600
H	-3.31904400	-1.77439300	2.32965100
H	-4.86941600	-0.92143400	2.31535000
N	2.55511400	0.79659500	-1.01271700
C	3.68050200	0.70357600	-1.25995700
C	5.09235300	0.56410300	-1.56304700
H	5.62667900	1.46662800	-1.25370000
H	5.49447500	-0.29941800	-1.02540300
H	5.22360100	0.41517700	-2.63858300
C	-1.22365000	-1.41158200	-0.05046900

C	0.78069100	-1.86996000	-1.38889400
C	-1.43533100	-2.29890800	-1.33078900
C	0.29518900	-1.05519600	-0.17655800
C	-0.42400600	-1.71629800	-2.33320800
H	-0.34097700	-2.31969900	-3.24344200
H	-0.62507700	-0.67558200	-2.60336800
C	0.71246600	-3.38357800	-1.04470900
H	1.22769800	-3.96539100	-1.81615500
H	1.19486900	-3.60947500	-0.09068400
C	-0.81735200	-3.68141700	-1.03913500
H	-1.08378800	-4.39307400	-1.82719400
H	-1.16622300	-4.09332400	-0.08702500
H	1.75025000	-1.55625900	-1.77148600
H	-2.46914300	-2.33387100	-1.67275000
C	1.03897800	-1.22554900	1.10726600
O	0.54058700	-1.13995600	2.22222500
O	2.35592900	-1.47783200	0.91374700
C	3.17849100	-1.60763700	2.09565600
H	4.18300200	-1.33525200	1.76326800
H	2.84125600	-0.88758400	2.84487500
H	-1.39751800	-2.02199300	0.84196300
C	3.14099900	-3.02574400	2.63688600
H	3.81088700	-3.11129000	3.49926200
H	2.12979300	-3.28979000	2.95769600
H	3.46865800	-3.74132700	1.87613600
C	0.56447700	4.93815600	1.27918000
H	-0.38172500	5.48669100	1.21043500
H	0.87172800	4.93896100	2.32799800
H	1.31259200	5.44377700	0.66709200

9''

Pd	0.07454700	0.66190500	0.93644100
C	0.57336700	-1.01285800	-1.52402100
C	1.65747100	-1.83543100	-1.13728300
C	0.86465600	0.14116800	-2.28445400
C	2.96322900	-1.45891800	-1.51428400
C	2.15551900	0.49362500	-2.66097400
H	0.03550100	0.78239900	-2.56118500
C	3.22686300	-0.32022300	-2.27303100
H	3.78801300	-2.10193400	-1.21498700
H	2.32570400	1.38956300	-3.25167300
H	4.24537500	-0.08747900	-2.57798900
C	1.40789800	2.68402400	0.26402800
O	1.75918800	1.97710400	1.32886800

O	2.16198100	3.53580600	-0.25023300
O	0.23597700	2.35039500	-0.23583800
C	1.55556400	-3.15462200	-0.39700900
H	2.38984600	-3.21553200	0.31227700
H	0.64691100	-3.21446500	0.19208600
C	1.63162000	-4.36036000	-1.34726200
H	1.55567900	-5.30106800	-0.79093000
H	0.82172500	-4.33498500	-2.08374700
H	2.57852700	-4.36716600	-1.89767900
K	4.06602600	1.65053300	0.17007200
N	0.27304300	-0.74284500	2.38924400
C	0.52700500	-1.42444400	3.28979200
C	0.83013700	-2.30625000	4.40139700
H	1.37706600	-1.75574300	5.17199700
H	-0.10048000	-2.69480600	4.82466000
H	1.44302600	-3.14034000	4.04739600
C	-0.92645200	-1.18522100	-1.23671500
C	-2.42494700	-1.19157200	0.70841300
C	-1.54806500	-2.56040700	-0.86778800
C	-1.49859300	-0.25121200	-0.10244600
C	-1.66451300	-2.52457900	0.66816000
H	-2.25601700	-3.35843800	1.06284700
H	-0.71567800	-2.48738800	1.19309100
C	-3.65625700	-1.54947100	-0.17020800
H	-4.40394400	-2.07505500	0.43343100
H	-4.14715000	-0.67035600	-0.59494300
C	-3.04709900	-2.49121400	-1.25710100
H	-3.49817800	-3.48758300	-1.20965800
H	-3.19108100	-2.11066500	-2.27319500
H	-2.68555800	-0.80880600	1.69598800
H	-1.03371500	-3.41787300	-1.30180600
C	-2.22050800	0.94418600	-0.64383300
O	-2.22208300	1.32818000	-1.80441900
O	-2.92258300	1.58142900	0.32943800
C	-3.65439600	2.76362500	-0.06395900
H	-3.75212600	3.34514800	0.85591600
H	-3.05645700	3.32910300	-0.78215200
H	-1.39771600	-0.85942600	-2.16811700
C	-5.01613400	2.41076000	-0.63695800
H	-5.57372000	3.32755500	-0.85777800
H	-4.91068400	1.84044500	-1.56345000
H	-5.59785900	1.82011800	0.07793300

TS3''

Pd	-0.69735500	-0.37333600	-0.36844500
C	2.16608300	-1.03404400	-0.01796400
C	3.36425500	-1.78073300	-0.07943500
C	0.92549600	-1.72055000	0.01849000
C	3.29041900	-3.16642900	-0.26479700
C	0.88960100	-3.11182400	-0.21126600
H	0.01842800	-1.55967300	0.87276800
C	2.06577600	-3.83041000	-0.37903700
H	4.21623500	-3.73423600	-0.32052600
H	-0.07191500	-3.61255600	-0.20001300
H	2.03929500	-4.90207800	-0.55446500
C	-2.16256300	-2.32712400	1.08480800
O	-2.11620700	-1.96205000	-0.20907100
O	-3.23311300	-2.85817800	1.50720100
O	-1.13126300	-2.10454600	1.82602800
C	4.72320000	-1.15338800	0.16228000
H	5.49361900	-1.76406400	-0.32111100
H	4.79019700	-0.15631000	-0.27598400
C	5.02614500	-1.05295800	1.66654600
H	6.01244200	-0.60780800	1.83720600
H	4.28079800	-0.43179100	2.17489500
H	5.01266900	-2.04248900	2.13586400
K	-4.65206700	-1.75179500	-0.36224400
N	-2.20514100	0.94832300	-0.89964100
C	-3.05864700	1.69277300	-1.13527200
C	-4.12816000	2.63081500	-1.42231900
H	-4.82641800	2.65632000	-0.58071700
H	-3.70578600	3.62846000	-1.57269700
H	-4.65840800	2.32016900	-2.32698800
C	2.17368900	0.46946700	-0.11986200
C	0.79071900	1.98979000	-1.46051400
C	2.79856800	0.96126400	-1.47699400
C	0.74904800	1.11431300	-0.19422500
C	1.58054300	1.07287700	-2.40921300
H	1.82674200	1.54578200	-3.36612600
H	1.08058700	0.11716200	-2.59277900
C	1.79537200	3.15517000	-1.24760800
H	1.69844200	3.88876200	-2.05515400
H	1.61762300	3.68282100	-0.30696100
C	3.18195400	2.44425800	-1.29389700
H	3.77648800	2.79352900	-2.14428300
H	3.77228000	2.60473100	-0.38627000
H	-0.18948200	2.31999900	-1.79999100
H	3.60995000	0.33168200	-1.84033400

C	0.33767500	1.77628900	1.07397400
O	0.74669500	1.48242600	2.19071600
O	-0.58287900	2.75355000	0.87278700
C	-1.10973500	3.40695800	2.04827500
H	-2.08769600	3.78347000	1.73827300
H	-1.24632400	2.66410900	2.83819500
H	2.74479000	0.90005300	0.71011500
C	-0.20371000	4.53639900	2.50601800
H	-0.65384700	5.04998100	3.36243500
H	0.77202000	4.14823300	2.80953000
H	-0.05937300	5.26793300	1.70451900

9'''

Pd	0.46419100	-0.01251700	-0.57505800
C	1.25219000	1.19098100	1.21250100
C	2.68481700	1.16297400	1.16602200
C	0.59284900	0.13256900	1.91597800
C	3.34729100	0.12123300	1.82094700
C	1.29296400	-0.89167600	2.56212200
H	-0.48261600	0.17894400	2.04320200
C	2.67932700	-0.88995700	2.51812400
H	4.43303000	0.10662600	1.78278400
H	0.72604600	-1.65446300	3.08454600
H	3.25001400	-1.67052800	3.01231200
C	-2.72606400	-2.02271700	2.38608600
O	-3.23466000	-2.25373100	1.24481400
O	-1.56168300	-2.36879800	2.74701600
I	2.25976100	-2.19738300	-1.08617800
C	3.56840000	2.21577300	0.53396800
H	4.46503500	1.71583400	0.15231400
H	3.08957100	2.68478600	-0.32168500
C	4.00061500	3.28489800	1.55109000
H	4.62894800	4.04214200	1.07059800
H	3.13642200	3.78986100	1.99423600
H	4.57408100	2.83254600	2.36674500
K	-0.91102400	-3.01036700	0.28280200
N	-0.71745900	-0.62841000	-2.16214200
C	-1.50457300	-0.90808200	-2.96214700
C	-2.50781700	-1.25034600	-3.95093600
H	-3.05297600	-2.13969600	-3.62155900
H	-3.20517000	-0.41471500	-4.05942400
H	-2.02631700	-1.45334300	-4.91156200
C	0.28430200	2.33300000	0.78254200
C	-0.63132900	2.58485600	-1.48136200

C	0.77678700	3.57022400	-0.00290200
C	-0.67202500	1.68251800	-0.24524700
C	0.83086000	3.06823800	-1.46150400
H	1.02139300	3.87049600	-2.18077900
H	1.54518900	2.25673700	-1.62956200
C	-1.38529300	3.88782500	-1.09834300
H	-1.51118200	4.51026300	-1.98971700
H	-2.38123900	3.69288100	-0.69215600
C	-0.42195300	4.55179100	-0.07003200
H	-0.08357700	5.53028600	-0.42239100
H	-0.88505700	4.69458800	0.91077200
H	-0.98793000	2.11229600	-2.39499300
H	1.67393700	4.03551800	0.39671800
C	-2.02215700	1.25780800	0.24499900
O	-2.34040800	1.19244700	1.42470800
O	-2.85178400	0.96761900	-0.76759700
C	-4.16415400	0.43698300	-0.42472000
H	-4.49589600	-0.03843800	-1.35097900
H	-4.03521500	-0.33186000	0.34180600
H	-0.24970800	2.64755600	1.68328700
C	-5.12114800	1.53715500	-0.00492200
H	-6.11544700	1.10812900	0.16052500
H	-4.79192100	2.01065000	0.92282300
H	-5.20539300	2.30207800	-0.78376700
C	-3.57853500	-1.22876100	3.37659300
H	-3.19888700	-1.32000800	4.39758200
H	-3.54490600	-0.17566400	3.07842300
H	-4.62254000	-1.55457100	3.33710400

TS3'''

Pd	-0.53025400	-0.32909500	-0.56177100
C	2.25779200	-1.16640300	-0.24509800
C	3.33910000	-2.06960300	-0.29741000
C	0.96896900	-1.62867500	0.13614600
C	3.08046100	-3.43255100	-0.10536600
C	0.75039000	-3.01327800	0.31440100
H	0.46060800	-1.03052200	1.12040200
C	1.79552300	-3.91355300	0.16690600
H	3.91298400	-4.13054000	-0.15380400
H	-0.23310100	-3.35868300	0.61238900
H	1.63073200	-4.97847000	0.30325800
C	-0.16998400	-0.00454900	3.25722200
O	-1.20312300	0.58089100	2.84457500
O	0.48106500	-0.89962600	2.62999000

I	-2.84159300	-2.06810900	-0.26679600
C	4.78045900	-1.61640800	-0.41250300
H	5.38156700	-2.43210000	-0.82878300
H	4.88413500	-0.76971800	-1.09246400
C	5.34559400	-1.22049600	0.96194500
H	6.38856800	-0.89694500	0.87601100
H	4.77033400	-0.39789800	1.40001300
H	5.30593000	-2.06451400	1.65874100
K	-2.88846100	1.22621700	1.16392200
N	-1.85568500	0.93356200	-1.61715500
C	-2.54216700	1.48462200	-2.36971200
C	-3.39933500	2.18406300	-3.30685700
H	-4.33182300	2.46437800	-2.80826600
H	-2.89015200	3.08372000	-3.66415300
H	-3.62333200	1.52899500	-4.15352200
C	2.40437200	0.28975500	-0.58366800
C	1.03977700	1.85188500	-1.87017800
C	2.88830800	0.57185500	-2.05363600
C	1.04421100	1.05836200	-0.55028600
C	1.58289500	0.78797500	-2.83774300
H	1.76278900	1.17220000	-3.84726700
H	0.94763700	-0.10098800	-2.89410300
C	2.20938400	2.87947200	-1.84183000
H	2.08366100	3.60148700	-2.65470700
H	2.24108200	3.44802500	-0.90763200
C	3.47648800	1.99648500	-2.05304400
H	3.95204800	2.21621000	-3.01420600
H	4.22626800	2.13364700	-1.26812500
H	0.08360300	2.30729200	-2.10950800
H	3.55307300	-0.19156700	-2.45481700
C	0.84915000	1.88769400	0.68039500
O	1.60217200	1.90968900	1.63814700
O	-0.25913900	2.67738600	0.60469500
C	-0.45747500	3.60276300	1.70756500
H	-1.50644800	3.90288800	1.62505200
H	-0.30960500	3.06183400	2.64334000
H	3.11200500	0.75501900	0.11117500
C	0.44349700	4.81807900	1.59072100
H	0.20023800	5.52787200	2.38864600
H	1.49446300	4.53734300	1.68785200
H	0.29511100	5.31862100	0.62872900
C	0.39176700	0.40235100	4.61589900
H	0.92720600	-0.42351300	5.09087600
H	1.10462500	1.21930200	4.45423400

H	-0.40042100	0.76590600	5.27542600
10(ANP)			
Pd	-0.64892900	1.00340200	0.10946500
C	2.12647600	0.15431800	-0.32250300
C	1.27205200	1.28330500	-0.34460900
C	3.48952800	0.28071800	-0.65986200
C	1.80081700	2.53359500	-0.69767100
C	3.98347900	1.54470800	-1.01558800
C	3.15250600	2.66307500	-1.03270100
H	1.16277800	3.41119300	-0.72307600
H	5.03194700	1.64486100	-1.28805800
H	3.55322300	3.63434400	-1.31385400
C	4.45170900	-0.89206300	-0.64644600
H	5.00789800	-0.90578400	-1.59257200
H	3.90440100	-1.83666200	-0.59538100
C	5.46032300	-0.82331100	0.51077400
H	6.14037900	-1.68211900	0.48937700
H	6.06552100	0.08743500	0.44992800
H	4.95155200	-0.81729400	1.48034500
N	-2.73849500	0.58724300	0.56835500
C	-3.83945300	0.26267000	0.71027400
C	-5.21300100	-0.17701300	0.87710500
H	-5.67964600	0.36349300	1.70519400
H	-5.77424000	0.01589300	-0.04156200
H	-5.22695300	-1.24943000	1.09142900
C	1.48102800	-1.15177000	0.04049500
C	-0.39812000	-1.59819900	1.54050000
C	1.85859900	-1.71993400	1.44356100
C	-0.07346600	-1.00101200	0.15204100
C	0.79919500	-1.08727800	2.36593300
H	0.82727400	-1.49237200	3.38385800
H	0.85291300	0.00439500	2.40793400
C	-0.11857500	-3.12575900	1.52075500
H	-0.51121800	-3.59409500	2.43004500
H	-0.59539200	-3.61886800	0.67035200
C	1.43885700	-3.20430500	1.47511600
H	1.83540900	-3.69956200	2.36778900
H	1.80902400	-3.75094800	0.60151400
H	-1.39072600	-1.34366900	1.91131900
H	2.90072000	-1.54721400	1.71628500
C	-0.79831100	-1.56611500	-1.01666800
O	-0.36277500	-1.64403300	-2.16035600
O	-2.04878100	-1.99584900	-0.69394700

C	-2.88119300	-2.46038000	-1.77578400
H	-3.90490800	-2.27956100	-1.43725800
H	-2.68618700	-1.85388100	-2.66362200
H	1.72528800	-1.90132700	-0.72140400
C	-2.64864800	-3.93449400	-2.05881400
H	-3.33105500	-4.27620300	-2.84476700
H	-1.62211600	-4.10407700	-2.39453000
H	-2.83050200	-4.53607100	-1.16238800
N	-1.20269600	3.10246400	0.11109800
C	-1.55560800	4.20390400	0.15118000
C	-1.98749300	5.58929600	0.19769900
H	-2.15501400	5.95505700	-0.81928200
H	-2.91719100	5.66610000	0.76817900
H	-1.21586300	6.19727500	0.67837700
TS1'			
Pd	1.10817500	-0.05175500	-0.11382700
N	3.07856400	0.61512600	-0.40623500
C	4.16677200	0.97953400	-0.57464800
C	5.52991200	1.43605900	-0.78153700
H	6.20802700	0.88062100	-0.12719300
H	5.82051200	1.27390300	-1.82347800
H	5.59989300	2.50280600	-0.54996000
C	-0.77265000	-0.78345600	-0.09293100
C	-0.71536100	-2.11041500	-0.61165000
C	-1.60383200	0.20268900	-0.70974900
C	-1.40656200	-2.37057600	-1.80048700
C	-2.31040500	-0.13410600	-1.87175000
C	-2.20204200	-1.40677400	-2.42429500
H	-1.33679100	-3.36823800	-2.22601100
H	-2.92599200	0.62195200	-2.34615400
H	-2.73761100	-1.65120800	-3.33588400
C	-1.70448800	1.58515300	-0.16659700
O	-0.81225600	2.20009100	0.39314700
O	-2.92702600	2.10824500	-0.38244800
C	-3.10050100	3.47730000	0.03075400
H	-4.12560200	3.73525800	-0.23474700
H	-2.95152900	3.57421800	1.10873500
H	-2.39646100	4.12901300	-0.49283600
C	-0.02544200	-3.24152900	0.11078500
H	0.91556800	-2.93735400	0.57005200
H	-0.66944000	-3.62532600	0.91197500
H	0.17306700	-4.06349600	-0.58203300
Br	-0.55193700	-0.66477800	2.01355000

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Pd	-0.32497000	-0.16298200	0.47559600
C	-1.72404500	1.17280700	-0.00497900
C	-1.47680800	2.04832300	-1.06662100
C	-2.91317900	1.24871200	0.73374100
C	-2.41644100	3.02681600	-1.40328400
H	-0.55260500	1.97123700	-1.63179800
C	-3.84120400	2.24442800	0.38036800
C	-3.60310500	3.12573600	-0.67289700
H	-2.21796000	3.70554500	-2.22819300
H	-4.76505500	2.32083900	0.94972600
H	-4.33768900	3.88639700	-0.92132500
I	-1.42509900	-1.84657100	-1.34396800
C	-3.25124800	0.28905300	1.85777400
H	-3.61086800	0.86042900	2.72254000
H	-2.34564100	-0.23597100	2.17963700
C	-4.31630600	-0.74057400	1.45558200
H	-4.54840200	-1.40653000	2.29393600
H	-5.24445600	-0.24728700	1.14828200
H	-3.96747500	-1.35384500	0.61864600
N	1.18684800	-1.66867100	1.00010900
C	2.06369900	-2.39045900	1.21707500
C	3.17989500	-3.27808600	1.48103100
H	2.81869300	-4.19865300	1.94758800
H	3.68197800	-3.51991800	0.54012800
H	3.88569700	-2.78171700	2.15274900
C	0.96094500	1.56309700	1.19928300
C	0.25866100	1.09422200	2.28425700
H	0.59257700	2.39843400	0.61446300
H	-0.66619100	1.57031700	2.58725500
H	0.71444700	0.38979200	2.97271500
C	2.37786900	1.14958800	0.93909800
O	3.09591300	0.62761800	1.77269300
O	2.70944600	1.45383700	-0.31981800
C	4.03245000	1.10117500	-0.88743000
C	3.90981400	1.57760500	-2.33167200
H	3.70504500	2.65170700	-2.36826000
H	4.84462400	1.38436800	-2.86517800
H	3.10109800	1.04918900	-2.84547900
C	5.12503700	1.86871500	-0.14602300
H	4.91557400	2.94273800	-0.16386200
H	5.20789800	1.53985300	0.89049900
H	6.08426500	1.69922200	-0.64478800

C	4.23012200	-0.41267400	-0.82677000
H	3.37449900	-0.92679700	-1.27502300
H	5.12620700	-0.67819400	-1.39591200
H	4.35483500	-0.75757800	0.19960200
TS2'			
Pd	0.28601000	0.16127600	-0.52396900
C	1.72917900	-1.34560000	-0.55864700
C	2.69644000	-1.19989800	-1.56349300
C	2.02848800	-2.01310200	0.64742200
C	4.00153900	-1.64098800	-1.35520700
H	2.42660700	-0.72836300	-2.50349100
C	3.35097000	-2.44680800	0.82995300
C	4.32998800	-2.26034400	-0.14652100
H	4.75034300	-1.50841800	-2.13051400
H	3.60757900	-2.94974000	1.75904100
H	5.34148200	-2.61531600	0.02811900
I	2.21387000	2.01069500	0.37438800
C	1.01382700	-2.26604300	1.74108600
H	1.38576200	-3.08716700	2.36348200
H	0.06553400	-2.59219300	1.30491400
C	0.73158200	-1.05006900	2.63649100
H	0.07486500	-1.33490700	3.46582400
H	1.65576200	-0.63663400	3.05416500
H	0.23801000	-0.25485000	2.06866200
N	-1.14372900	1.70108900	-0.42949700
C	-1.92981400	2.54119100	-0.31696800
C	-2.91066300	3.59818500	-0.15987700
H	-2.39863300	4.54502000	0.03402000
H	-3.50691800	3.68659100	-1.07195900
H	-3.56713900	3.36066800	0.68168400
C	-1.13343500	-1.16832700	-1.40215000
C	-0.05644800	-2.07313600	-1.48379100
H	-1.42089100	-0.61060200	-2.28946300
H	0.44430600	-2.18760900	-2.43580700
H	-0.05194400	-2.93498100	-0.82857700
C	-2.20860300	-1.38847000	-0.39017500
O	-2.12429700	-2.17070700	0.54451200
O	-3.26608000	-0.62025800	-0.67489600
C	-4.45313900	-0.57153200	0.20780400
C	-5.34795500	0.44567500	-0.49449600
H	-5.60212400	0.10537900	-1.50281400
H	-6.27473700	0.57574400	0.07130700
H	-4.84767600	1.41499600	-0.56953600

C	-5.12237300	-1.94439900	0.25172300
H	-5.33111200	-2.29771100	-0.76300600
H	-4.49529400	-2.67716900	0.76017000
H	-6.07351900	-1.86357400	0.78707200
C	-4.04157800	-0.07350700	1.59237400
H	-3.51365100	0.88143900	1.51463800
H	-4.93928500	0.08001900	2.19900100
H	-3.39781800	-0.79303200	2.09944900

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Pd	0.34678000	0.09074400	-0.50276900
C	1.22576100	-2.01114100	-0.80779500
C	2.12646500	-1.56575800	-1.81524300
C	1.71900500	-2.20384600	0.52026100
C	3.47418300	-1.35921000	-1.54569700
H	1.74925200	-1.45082700	-2.82719700
C	3.08410800	-1.99491900	0.75635400
C	3.95355200	-1.59204000	-0.25479500
H	4.14503800	-1.03642800	-2.33495700
H	3.46769700	-2.15875900	1.75925300
H	5.00721100	-1.45210800	-0.03305600
I	2.38343100	1.83382000	0.45936000
C	0.84523800	-2.62335400	1.67943600
H	1.38875800	-3.37629300	2.26151800
H	-0.08051400	-3.07807300	1.32787700
C	0.48663100	-1.44346300	2.59690900
H	-0.10367800	-1.78995200	3.45184700
H	1.38600900	-0.94803600	2.97650700
H	-0.10298000	-0.70177900	2.04858300
N	-0.94629600	1.68033700	-0.48993800
C	-1.62961900	2.61173200	-0.45253900
C	-2.47585500	3.78782200	-0.39015500
H	-3.20688400	3.66715200	0.41394900
H	-1.85919300	4.66916800	-0.19193600
H	-2.99954600	3.91628100	-1.34130800
C	-1.06375700	-1.22743400	-1.22551100
C	-0.17689600	-2.45653100	-1.26159900
H	-1.34598800	-0.81697200	-2.19434000
H	-0.10480500	-2.85481700	-2.27636700
H	-0.56426900	-3.23916500	-0.60974800
C	-2.20044600	-1.26671300	-0.26222100
O	-2.24280200	-1.99395900	0.72152500
O	-3.16935200	-0.41062400	-0.62756200
C	-4.36153600	-0.18748700	0.21477200

C	-5.13734900	0.86774900	-0.56973300
H	-5.40311500	0.49275900	-1.56273500
H	-6.05840800	1.12206600	-0.03751000
H	-4.54465800	1.77825700	-0.68929500
C	-5.17383000	-1.47814400	0.32347000
H	-5.39226700	-1.87311100	-0.67386900
H	-4.63988000	-2.23718600	0.89508700
H	-6.12491600	-1.26452500	0.82119200
C	-3.93644200	0.35264200	1.58010800
H	-3.31625800	1.24610900	1.46282700
H	-4.82797200	0.62782500	2.15193600
H	-3.37633400	-0.39337200	2.14478200

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Pd	0.01849700	-0.38815100	-0.80027700
C	3.53564600	-3.31064400	0.54948400
C	2.31410300	-3.86036300	0.15791900
C	1.26656300	-3.02345700	-0.23996600
C	1.44966800	-1.63402000	-0.26248700
C	2.69369800	-1.08404900	0.11917800
C	3.74166600	-1.92351000	0.54531600
H	4.34364300	-3.96314100	0.87294200
H	0.31267700	-3.45725900	-0.52790100
C	2.79269600	0.41284700	0.06486100
C	1.62431700	1.99906400	-1.38791900
C	3.63875900	1.00395700	-1.10800300
C	1.39083800	1.04220900	-0.20514100
C	2.60672300	1.17264600	-2.24026800
H	3.00756400	1.72768400	-3.09547300
H	2.17578400	0.22936800	-2.58701200
C	2.53924300	3.16171700	-0.90992800
H	2.56569000	3.95574100	-1.66347900
H	2.18071600	3.60926700	0.02108700
C	3.93530100	2.47803400	-0.75729200
H	4.65931700	2.90399900	-1.45958100
H	4.34852100	2.58347400	0.25098200
H	0.70616900	2.33080300	-1.87250900
H	4.52490200	0.41306500	-1.34872000
C	0.73316900	1.59349600	1.01261000
O	0.98256500	1.26943300	2.16619100
O	-0.21322200	2.52820300	0.71326100
C	-0.91263300	3.12475900	1.82998300
H	-1.84886200	3.48918000	1.40289500
H	-1.13310300	2.35009100	2.56758500

H	3.19248000	0.79036400	1.01226100
C	5.04402900	-1.36318900	1.07778200
H	5.84663300	-2.09033600	0.90865700
H	5.32320400	-0.45469700	0.53674400
C	4.95969600	-1.05010300	2.58084500
H	4.16610600	-0.32466800	2.78913900
H	4.73946500	-1.95729400	3.15387500
H	5.90413100	-0.63523400	2.95010500
H	2.17454700	-4.93872200	0.16840500
C	-0.11157700	4.26080700	2.44084600
H	-0.69131400	4.73308600	3.24134500
H	0.82502400	3.89048800	2.86541200
H	0.11657600	5.02224200	1.68827900
C	-2.95434900	-1.08246800	0.22007800
C	-3.36417100	-1.93682100	1.24895500
C	-3.10551200	0.31525400	0.28749900
C	-3.95020400	-1.34172900	2.37743500
C	-3.71515100	0.85783300	1.42877400
C	-4.13148300	0.03429900	2.46862000
H	-4.26749800	-1.98588600	3.19161300
H	-3.83642700	1.93132600	1.49636000
H	-4.59066600	0.46678400	3.35106500
C	-2.58356000	1.26140900	-0.73697200
O	-1.61623400	1.06014900	-1.47046900
O	-3.25767200	2.40364800	-0.76829600
C	-2.69867700	3.45187800	-1.59889400
H	-3.31949700	4.32598400	-1.40905900
H	-1.66294700	3.63605100	-1.31006200
H	-2.75116000	3.16485100	-2.65081200
C	-3.18949500	-3.42986700	1.18950400
H	-3.72954900	-3.86538500	0.34241000
H	-2.13394500	-3.69942300	1.07719100
H	-3.56464000	-3.88966900	2.10578400
Br	-2.19696300	-1.92310300	-1.35140600

TS4

Pd	-0.12570800	-0.51811100	-0.84088800
C	4.18507800	-2.26558000	0.24954600
C	3.18801200	-3.14701200	-0.17084400
C	1.91242000	-2.66580300	-0.47648200
C	1.64793900	-1.29390300	-0.38258400
C	2.67103700	-0.39748500	-0.01457200
C	3.94644200	-0.88833800	0.33508000
H	5.16809600	-2.64804300	0.51428000

H	1.13173300	-3.35744600	-0.77092200
C	2.33731700	1.06173000	-0.07180500
C	0.74025000	2.20134800	-1.53562000
C	2.95610900	1.80721200	-1.30025500
C	0.81087500	1.27921300	-0.30445900
C	1.88441400	1.62523900	-2.39202300
H	2.09128800	2.21644400	-3.29034800
H	1.72168400	0.58065900	-2.67611900
C	1.31963500	3.59198900	-1.15172000
H	1.10935800	4.31378600	-1.94780600
H	0.87768500	3.98394600	-0.23270200
C	2.85017900	3.32107500	-1.02207900
H	3.41581900	3.89061100	-1.76648400
H	3.24310000	3.58184500	-0.03424600
H	-0.24767400	2.24909100	-1.99149400
H	3.96164000	1.46497200	-1.55135300
C	0.07128500	1.70269200	0.91592800
O	0.41284000	1.47095700	2.06685200
O	-1.05763000	2.39564100	0.61419700
C	-1.81226000	2.93278400	1.72612200
H	-2.82847600	3.03803500	1.34118300
H	-1.81096600	2.20821700	2.54164900
H	2.65064800	1.56377700	0.84886700
C	5.02756600	0.02566600	0.87219100
H	6.00825700	-0.42029700	0.67195300
H	5.00930100	0.99046300	0.35784700
C	4.87886800	0.25709800	2.38509900
H	3.90988200	0.70902100	2.62251300
H	4.94692900	-0.69051600	2.93016500
H	5.66444900	0.92268700	2.75929800
H	3.39744300	-4.21088000	-0.24721200
C	-1.24634700	4.26959000	2.17028300
H	-1.86310200	4.68055500	2.97677200
H	-0.22534600	4.15329800	2.54395100
H	-1.24117800	4.98608300	1.34304900
C	-1.69906300	-1.30511600	0.62224800
C	-1.37175800	-1.96088200	1.81984800
C	-2.71710000	-0.32370900	0.56691900
C	-2.06695200	-1.55495200	2.96903200
C	-3.40964300	0.01283300	1.73780700
C	-3.08600000	-0.60227400	2.93957000
H	-1.80887700	-2.03501500	3.90873400
H	-4.16912400	0.78428000	1.68980400
H	-3.61458100	-0.34025300	3.84969500

C	-2.89960000	0.45906400	-0.66260400
O	-2.05230100	0.49647600	-1.56402300
O	-4.02816000	1.15247200	-0.71960500
C	-4.17455200	2.05443200	-1.84164800
H	-5.13022000	2.55255000	-1.68564400
H	-3.35809400	2.77918100	-1.84530300
H	-4.18232200	1.49447300	-2.77858300
C	-0.33619100	-3.04037900	1.92650800
H	-0.51263100	-3.83425900	1.19566400
H	0.66167900	-2.63873300	1.72882400
H	-0.34517700	-3.47806700	2.92686300
Br	-1.64841100	-2.64916900	-1.13966600

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Pd	-0.20682600	-0.76986900	-0.58924700
C	4.23092300	-1.85011400	0.71308500
C	3.28292800	-2.87486400	0.69004700
C	1.95942900	-2.59913400	0.34330600
C	1.61857100	-1.29117100	-0.00241300
C	2.56377200	-0.25473900	-0.01373000
C	3.89451500	-0.53684600	0.36625700
H	5.25277900	-2.06812300	1.01340600
H	1.20969500	-3.37963200	0.34087100
C	2.11198400	1.11408300	-0.43343400
C	0.32499100	1.68948300	-2.00433500
C	2.57727500	1.51294000	-1.87473300
C	0.56611100	1.20596700	-0.56089800
C	1.45214800	0.95910900	-2.76340200
H	1.53352800	1.27641100	-3.80752500
H	1.37423500	-0.13372300	-2.73774600
C	0.81440800	3.16406800	-2.09901400
H	0.49452500	3.58615900	-3.05675300
H	0.39775600	3.79396100	-1.30983200
C	2.36528600	3.03473500	-2.02295200
H	2.83737000	3.40006200	-2.93986500
H	2.79321700	3.58854000	-1.18199100
H	-0.69531500	1.54518800	-2.35512800
H	3.58630100	1.17099600	-2.10824100
C	-0.08950400	2.00147000	0.52223000
O	0.42681600	2.28315700	1.59180900
O	-1.33603600	2.38878300	0.17652600
C	-2.09655600	3.11713800	1.17269500
H	-3.13847600	2.91675000	0.91602200
H	-1.88236400	2.69551200	2.15665600

H	2.46388200	1.85770300	0.28560100
C	4.92959600	0.55872100	0.51052400
H	5.92661300	0.12614200	0.37343700
H	4.80669100	1.31720400	-0.26731800
C	4.85980500	1.23253100	1.89123600
H	3.87922000	1.68883100	2.06285500
H	5.03110000	0.50143400	2.68844300
H	5.61806300	2.01804600	1.98008600
H	3.56978500	-3.88867700	0.95603900
C	-1.78444200	4.60108600	1.11834700
H	-2.41733800	5.13649100	1.83403500
H	-0.73858900	4.78745800	1.37594000
H	-1.98049700	5.00263200	0.11931700
C	-1.14545100	-0.55549600	1.19075300
C	-0.64611500	-0.66571200	2.49254600
C	-2.51506800	-0.28853800	0.96584100
C	-1.58484500	-0.57691300	3.54205800
C	-3.41333900	-0.20008300	2.03683700
C	-2.94402000	-0.36370500	3.33253200
H	-1.21224000	-0.66650000	4.55842600
H	-4.45834700	0.00603700	1.83643300
H	-3.62318000	-0.30128900	4.17640400
C	-2.96274500	-0.02404600	-0.40826000
O	-2.19556100	-0.08693000	-1.37826800
O	-4.23773500	0.30461100	-0.54115700
C	-4.69486100	0.59744100	-1.88338200
H	-5.74919700	0.84773400	-1.77783200
H	-4.13726100	1.44225000	-2.29241200
H	-4.56931500	-0.27860900	-2.52266800
C	0.80083000	-0.82036200	2.87706100
H	1.18356200	-1.81222500	2.62779700
H	1.41943100	-0.08706800	2.36024400
H	0.91317600	-0.67135300	3.95378900
Br	-1.09395500	-3.15553200	-1.11820600

TS5

Pd	0.59289800	-0.23550000	-0.69762500
C	-1.97107800	3.83758900	-0.90094300
C	-0.59219100	3.98673800	-1.07024100
C	0.25239700	2.91200000	-0.82634000
C	-0.28664700	1.67095600	-0.44733600
C	-1.68668500	1.48390400	-0.38573100
C	-2.53509300	2.60420800	-0.56565700
H	-2.62548900	4.69548700	-1.03010100

H	1.32245300	3.05714200	-0.89475900
C	-2.27490800	0.09898000	-0.26175500
C	-1.63360600	-2.05201900	-1.22985200
C	-3.03679500	-0.32226600	-1.57397200
C	-1.20933100	-1.04236100	-0.12325400
C	-1.97142700	-1.08165000	-2.37526000
H	-2.38441900	-1.59038900	-3.25225700
H	-1.12790700	-0.45877000	-2.69026500
C	-3.03610500	-2.64614900	-0.92165700
H	-3.21832000	-3.46906800	-1.62019900
H	-3.11390800	-3.04192300	0.09085300
C	-4.00538300	-1.45739200	-1.18586500
H	-4.69043200	-1.67776600	-2.01051900
H	-4.60777300	-1.19869500	-0.30981900
H	-0.87454900	-2.80333400	-1.42310100
H	-3.50170400	0.51650400	-2.08959100
C	-1.15534400	-1.68747600	1.24177400
O	-2.15475500	-1.89785800	1.91549900
O	0.07641700	-2.02915100	1.62845700
C	0.20897400	-2.69033600	2.91301300
H	1.23092000	-2.46585500	3.22373800
H	-0.49095600	-2.23614500	3.61779900
H	-2.97544100	0.06060600	0.57695400
C	-4.02713100	2.54291200	-0.29939100
H	-4.51727800	3.34384000	-0.86281000
H	-4.46181300	1.60455200	-0.64705600
C	-4.34574200	2.71125500	1.19541300
H	-3.91509400	1.89787300	1.78737000
H	-3.94437300	3.65560400	1.57825100
H	-5.42871400	2.71038900	1.35929900
H	-0.17509700	4.94808500	-1.35482000
C	-0.02169300	-4.18361000	2.77786100
H	0.14724400	-4.67129000	3.74368200
H	-1.04762000	-4.39089100	2.46167700
H	0.66778000	-4.61648800	2.04682600
C	0.97567800	1.03520300	1.00269500
C	0.38590800	1.15749400	2.28081200
C	2.37996000	1.25596400	0.87708100
C	1.23742000	1.34966700	3.38407700
C	3.18495200	1.47461400	2.00345300
C	2.61650900	1.48952600	3.26762200
H	0.77965300	1.41920200	4.36634600
H	4.25132000	1.61020400	1.86892200
H	3.23108900	1.63665300	4.14934500

C	3.02488500	1.21980200	-0.45015500
O	2.46004000	0.79324500	-1.46450700
O	4.26241800	1.69534800	-0.48364400
C	4.93950100	1.64839300	-1.76219000
H	5.93018700	2.05987800	-1.57556700
H	5.01039800	0.61705400	-2.11288200
H	4.40323400	2.25574400	-2.49402300
C	-1.09047100	1.22766000	2.57139800
H	-1.52815300	2.09449900	2.07022600
H	-1.65611200	0.35490300	2.25940500
H	-1.24670700	1.34516700	3.64585900
Br	1.71920000	-2.40525900	-1.42766000

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Pd	0.14846300	0.95923100	-0.89518100
C	3.32095800	-0.12536900	-2.23125400
C	2.49531100	-0.97458900	-2.97435500
C	1.42137000	-1.57897500	-2.35586100
C	1.10789000	-1.29849100	-1.00634100
C	1.90711200	-0.35960000	-0.24942200
C	3.08231900	0.17640300	-0.89149800
H	4.20574200	0.29428200	-2.70105100
H	0.80425800	-2.29091500	-2.88921800
C	1.45357400	-0.09708300	1.21941500
C	0.29565900	1.96973100	1.91244400
C	2.25256500	0.85186100	2.14441500
C	0.10500500	0.66685900	1.10676300
C	1.78828700	2.25338900	1.68612900
H	2.16553900	3.05809500	2.32477500
H	2.01023500	2.48367300	0.64257400
C	0.30223900	1.59715500	3.41802500
H	0.35549200	2.51974100	4.00432400
H	-0.58849400	1.05486800	3.73982500
C	1.60867500	0.76236800	3.55336100
H	2.28078100	1.19478900	4.30006800
H	1.41227100	-0.27395200	3.84199500
H	-0.41102800	2.74902000	1.63617300
H	3.32121600	0.66204000	2.17224000
C	-1.11798000	-0.09655500	1.55822600
O	-1.06246500	-1.04257500	2.32535200
O	-2.25762900	0.45155400	1.12529800
C	-3.49184900	-0.11884200	1.63193800
H	-4.24007300	0.16474000	0.89175800
H	-3.39719600	-1.20583000	1.64867100

H	1.29705500	-1.05705100	1.71098500
C	4.20836400	0.93056900	-0.20922300
H	4.74169400	1.49851800	-0.97781200
H	3.85855900	1.65852600	0.51484300
C	5.20036200	-0.03946500	0.45509500
H	4.70993600	-0.66373800	1.20876600
H	5.64428000	-0.70820100	-0.28971400
H	6.00970500	0.51237600	0.94498700
H	2.72402800	-1.18656900	-4.01431700
C	-3.82453300	0.43860600	3.00375100
H	-4.80433800	0.06625600	3.32161500
H	-3.08293200	0.12794600	3.74409400
H	-3.86442800	1.53211400	2.97971800
C	0.14029800	-2.26627600	-0.38368300
C	0.69167300	-3.28795500	0.42293900
C	-1.24781500	-2.28188700	-0.65770700
C	-0.15737900	-4.24040200	0.99677600
C	-2.07159100	-3.24860000	-0.06255600
C	-1.53109800	-4.21924200	0.77042200
H	0.27571600	-5.01994700	1.61735200
H	-3.13359900	-3.23817500	-0.27395200
H	-2.17264100	-4.96914000	1.22266200
C	-1.89234700	-1.30972100	-1.59068100
O	-1.34831800	-0.75992600	-2.53682600
O	-3.18857800	-1.11657500	-1.29671500
C	-3.87192600	-0.13802900	-2.10463800
H	-4.89616300	-0.11978300	-1.73285900
H	-3.39745700	0.83882900	-1.98333400
H	-3.85789200	-0.43002800	-3.15750200
C	2.18124900	-3.40795500	0.64414300
H	2.73540000	-3.28271300	-0.29093300
H	2.56169900	-2.65891800	1.34677000
H	2.42189900	-4.39145000	1.05513500
Br	-1.30859900	2.95282000	-1.17591200

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Pd	0.15624900	-0.03868600	-0.82171300
C	-3.03406600	-3.57994700	-0.63139800
C	-1.87645100	-3.75511100	-1.39081900
C	-0.93239900	-2.72621000	-1.47476600
C	-1.14061500	-1.52582800	-0.78070300
C	-2.30360000	-1.36289300	0.00341900
C	-3.26892400	-2.38737400	0.06792400
H	-3.77375300	-4.37584800	-0.58092500

H	-0.03848200	-2.86718200	-2.07540800
C	-2.42394500	-0.05603400	0.73077200
C	-0.65988500	1.41048200	1.57926400
C	-2.17552300	-0.11850600	2.27274900
C	-1.31121700	0.93352000	0.26564200
C	-0.65500000	0.10446100	2.39662100
H	-0.33347900	0.24783700	3.43398600
H	-0.05290300	-0.68390300	1.93752900
C	-1.69858700	2.25942000	2.36513800
H	-1.20955100	2.77380400	3.19906400
H	-2.16049600	3.02613400	1.73719600
C	-2.71866300	1.19449000	2.87577800
H	-2.72058900	1.14546100	3.96963800
H	-3.74334900	1.40034600	2.55012600
H	0.29707600	1.91295700	1.44504700
H	-2.56822100	-1.02363200	2.74030800
C	-1.77541800	1.97423200	-0.69016100
O	-2.76641200	1.89694500	-1.40589700
O	-0.95407000	3.05633700	-0.69615500
C	-1.27411800	4.11442800	-1.62516700
H	-0.31976400	4.60942100	-1.82033200
H	-1.64625400	3.67471900	-2.55370900
H	-3.41043500	0.38373400	0.54839300
C	-4.58252400	-2.19775100	0.79729800
H	-4.96171100	-3.17446700	1.11919200
H	-4.43816000	-1.60180900	1.70285300
C	-5.63700600	-1.51779500	-0.09146000
H	-5.29316600	-0.53488500	-0.43068900
H	-5.84288900	-2.12310900	-0.98089600
H	-6.57865000	-1.37894300	0.45114700
H	-1.71059700	-4.68920900	-1.92216700
C	-2.28500200	5.08019300	-1.03166200
H	-2.46786100	5.90312100	-1.73114800
H	-3.23472300	4.57428800	-0.83818100
H	-1.91313700	5.50417500	-0.09337800
C	2.79385600	-1.05984200	0.27857100
C	2.86159400	-2.21645300	1.05997900
C	2.95158200	0.22884200	0.81345300
C	3.10472500	-2.03870900	2.43182200
C	3.21730000	0.35615800	2.18242600
C	3.28962700	-0.77651500	2.98845400
H	3.15005200	-2.92056200	3.06329400
H	3.33449300	1.34667100	2.60609200
H	3.48095100	-0.67332100	4.05122500

C	2.70057900	1.47045800	0.03120600
O	1.77549700	1.61311000	-0.76834300
O	3.54317200	2.44854200	0.32791300
C	3.27673600	3.73521400	-0.28646800
H	4.02752400	4.40804300	0.12437800
H	3.37901300	3.65959800	-1.37057800
H	2.27073400	4.07078100	-0.02825500
C	2.65687100	-3.59359300	0.49246200
H	1.66822600	-3.67984200	0.02818400
H	3.40050300	-3.82781100	-0.27633700
H	2.73314200	-4.34333000	1.28243600
Br	2.51725500	-1.27940400	-1.62661900

TS6

Pd	0.27165700	-0.30310900	-0.72345600
C	-3.92775300	-2.56220900	-0.75590000
C	-2.82556900	-3.17136300	-1.35718100
C	-1.57356600	-2.55305700	-1.31206100
C	-1.43155900	-1.32607300	-0.65260400
C	-2.54047400	-0.71660800	-0.03226700
C	-3.80756500	-1.33215300	-0.09682500
H	-4.90317700	-3.04053700	-0.80461600
H	-0.71800000	-3.02848900	-1.77756700
C	-2.29244600	0.59479300	0.64655400
C	-0.23341800	1.40413200	1.68218700
C	-2.25639400	0.53640200	2.20649200
C	-0.86870800	1.13589000	0.30707000
C	-0.77936800	0.21516900	2.49657100
H	-0.53010300	0.27648100	3.56120500
H	-0.46180200	-0.75252200	2.10828900
C	-0.97988800	2.59375500	2.35036400
H	-0.43234200	2.91799500	3.24136000
H	-1.06076300	3.45595700	1.68520000
C	-2.36512900	1.98378600	2.72867700
H	-2.51720100	1.99266100	3.81278500
H	-3.20146500	2.52238700	2.27173000
H	0.84853800	1.52920700	1.65828700
H	-2.99122200	-0.15172300	2.62890700
C	-0.86826600	2.24418900	-0.69229600
O	-1.69662500	2.38672400	-1.58363600
O	0.17549800	3.08723800	-0.52157300
C	0.33486500	4.13981200	-1.49919500
H	1.40102200	4.37593700	-1.47820000
H	0.07379400	3.75018500	-2.48598800

H	-3.04636300	1.32282600	0.33089300
C	-5.04915400	-0.65190300	0.44084400
H	-5.77919500	-1.41536400	0.73273000
H	-4.81678000	-0.07731000	1.34158100
C	-5.68632000	0.27853200	-0.60434200
H	-4.98417300	1.05699000	-0.92114600
H	-5.98218000	-0.28527300	-1.49555400
H	-6.57820300	0.76983700	-0.20030100
H	-2.93896400	-4.12676300	-1.86298100
C	-0.50656800	5.35301700	-1.14478800
H	-0.32387200	6.15440300	-1.86883000
H	-1.57097400	5.10498300	-1.16572600
H	-0.24985300	5.72653800	-0.14840900
C	1.82894700	-1.34121400	0.52818500
C	1.51736100	-2.35414400	1.44861000
C	2.75088900	-0.31406100	0.83513000
C	2.10764400	-2.24932400	2.71680900
C	3.33206100	-0.26945600	2.10949500
C	3.00773400	-1.23585100	3.05230600
H	1.85633700	-3.00776200	3.45284100
H	4.00622300	0.54569300	2.34767700
H	3.44790700	-1.20499400	4.04310700
C	2.94626600	0.77877500	-0.12777400
O	2.12860100	1.02795100	-1.02167100
O	4.04837300	1.49326100	0.05154600
C	4.21473000	2.64547700	-0.80924800
H	5.13138100	3.12593400	-0.47090000
H	4.31022900	2.32754600	-1.84941100
H	3.36223000	3.31860900	-0.70162300
C	0.58302900	-3.48947200	1.15263600
H	-0.43759200	-3.12150700	1.00869200
H	0.86797300	-4.00799100	0.23320500
H	0.58311500	-4.20761800	1.97543400
Br	2.00297800	-2.11102000	-1.57216300

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Pd	0.41357900	-0.29718800	-0.61710400
C	-3.70262400	-2.67068100	-0.62735200
C	-2.60743900	-3.23429600	-1.28221200
C	-1.36465900	-2.59947000	-1.24580900
C	-1.23657100	-1.41231800	-0.52575300
C	-2.32793400	-0.83055900	0.13919900
C	-3.58960700	-1.46193200	0.06884800
H	-4.67075600	-3.16349600	-0.66990700

H	-0.51175500	-3.01923900	-1.76305700
C	-2.12633100	0.48731200	0.82940900
C	-0.19831500	1.51142000	1.91089000
C	-2.16133500	0.48826800	2.39130900
C	-0.71928900	1.09504200	0.54122200
C	-0.68011800	0.32565000	2.77146500
H	-0.50035500	0.48163500	3.83968100
H	-0.25411000	-0.62851200	2.47090100
C	-1.09232400	2.65929600	2.47557400
H	-0.61060300	3.07476200	3.36617800
H	-1.22645400	3.47224300	1.76256900
C	-2.42818900	1.93929500	2.83895800
H	-2.61827500	1.98044100	3.91583900
H	-3.29347800	2.37555000	2.33022500
H	0.86600800	1.74407500	1.93652700
H	-2.84638500	-0.25230700	2.80611900
C	-0.67908300	2.00035900	-0.64142700
O	-0.83258200	1.50756400	-1.77180000
O	-0.39081600	3.27504500	-0.43068600
C	-0.21933300	4.13443000	-1.60125400
H	0.42636800	4.93705700	-1.24199700
H	0.30141600	3.56403100	-2.37199900
H	-2.89176000	1.18431600	0.46719600
C	-4.83721800	-0.82029500	0.63922600
H	-5.53334000	-1.60886800	0.94618900
H	-4.60542000	-0.24032100	1.53556600
C	-5.53042700	0.08918400	-0.38852100
H	-4.86561000	0.89551500	-0.71637000
H	-5.82462200	-0.48141000	-1.27570400
H	-6.43037400	0.54505800	0.03819900
H	-2.71821000	-4.16786900	-1.82737300
C	-1.55659100	4.65941500	-2.08312100
H	-1.39373500	5.35592700	-2.91201400
H	-2.19377500	3.84506200	-2.43808000
H	-2.07598300	5.19350000	-1.28168700
C	1.56079700	-1.09505800	0.84064400
C	1.41953900	-2.28811700	1.56458600
C	2.69427800	-0.27475400	1.06079400
C	2.41712800	-2.60063900	2.50698300
C	3.66759700	-0.61721100	2.01194800
C	3.52507200	-1.78790800	2.73939100
H	2.30491200	-3.51887700	3.07650500
H	4.51919000	0.03715400	2.15871100
H	4.26603500	-2.07215300	3.47928600

C	2.84632700	0.94572300	0.25953400
O	2.04803300	1.25327600	-0.63900800
O	3.89132000	1.70403400	0.55142600
C	4.04270600	2.92109400	-0.21836500
H	4.92242400	3.41217800	0.19437600
H	4.19437300	2.68267000	-1.27295300
H	3.15841500	3.55068300	-0.10147700
C	0.27256100	-3.25279500	1.42779600
H	-0.68764600	-2.75779800	1.58699300
H	0.24461600	-3.69487100	0.42972700
H	0.37310200	-4.05947000	2.15813500
Br	1.74548100	-1.62223000	-2.40979300

TS7

Pd	-0.51252200	-0.53440400	-0.20326700
C	0.78485600	3.60341900	-2.20466400
C	-0.48654500	3.14060700	-2.54511600
C	-1.02235800	2.04204000	-1.87749200
C	-0.28208000	1.42046200	-0.86491400
C	1.02205500	1.86270400	-0.52929000
C	1.55855800	2.96527300	-1.22712700
H	1.19833300	4.46825300	-2.71691600
H	-2.01326700	1.68458000	-2.13027700
C	1.89817900	1.05558800	0.40484300
C	1.57940900	-0.70219200	2.06176100
C	2.12643200	1.49100900	1.88918200
C	1.41377300	-0.40503800	0.57058000
C	1.11327800	0.62874800	2.67736200
H	1.28121200	0.67776800	3.75794300
H	0.06626700	0.84184100	2.47112900
C	3.09649000	-0.66706900	2.42179200
H	3.22542900	-1.04795000	3.43987300
H	3.69937900	-1.28756600	1.75993700
C	3.45651400	0.84685800	2.33655400
H	3.75823600	1.23910500	3.31255800
H	4.26767900	1.05021900	1.63068100
H	1.06559700	-1.60696800	2.37925300
H	2.09727600	2.56985200	2.04505500
C	2.03158200	-1.33211500	-0.45102600
O	2.05946600	-1.08047300	-1.65059800
O	2.54850500	-2.44691500	0.07814600
C	3.06218400	-3.43911400	-0.84664600
H	3.00324200	-4.37726700	-0.29168200
H	2.39455800	-3.48933900	-1.70921500

H	2.88041000	1.02208600	-0.07602000
C	2.97597500	3.44559000	-0.99434300
H	3.00204900	4.53335000	-1.12365700
H	3.28921700	3.24682000	0.03376300
C	3.97133900	2.80233200	-1.97419600
H	3.96139300	1.71032600	-1.89392200
H	3.71634500	3.06014700	-3.00740300
H	4.99139700	3.14868300	-1.77735200
H	-1.06184400	3.63773700	-3.32056200
C	4.48863400	-3.12498400	-1.25823800
H	4.86761600	-3.92415200	-1.90416500
H	4.53610400	-2.18284900	-1.81016000
H	5.14055100	-3.05538300	-0.38174300
C	-1.83824900	1.05964300	0.55429600
C	-1.82118300	2.15502600	1.44393700
C	-3.09503800	0.43435700	0.28994500
C	-2.97488100	2.40041800	2.21377700
C	-4.22832200	0.73119600	1.06259900
C	-4.15595500	1.68343800	2.06523800
H	-2.93840800	3.21994600	2.92520300
H	-5.15129100	0.20202900	0.85955300
H	-5.01864500	1.90498400	2.68447500
C	-3.25021400	-0.51414600	-0.83014800
O	-2.30486200	-0.87428900	-1.54130100
O	-4.49032000	-0.92648900	-1.05015100
C	-4.67876800	-1.85450200	-2.14526900
H	-5.74009600	-2.09724200	-2.13310300
H	-4.40476900	-1.38110600	-3.09027400
H	-4.07540000	-2.74992500	-1.98602200
C	-0.74933400	3.20983800	1.53700000
H	0.24534000	2.81758400	1.68731200
H	-0.73490400	3.79072900	0.60855800
H	-0.97205100	3.89383000	2.35890300
Br	-0.72803600	-2.96995800	0.49649700

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Pd	0.02450800	-0.76903000	-0.51458200
C	-0.12262500	2.65152100	-2.80298300
C	-1.43273200	2.19924900	-2.97342600
C	-2.08406900	1.61075400	-1.90942200
C	-1.43311700	1.39594000	-0.67301600
C	-0.05349900	1.76203200	-0.51674500
C	0.56854500	2.46786800	-1.60778200
H	0.35503000	3.17639700	-3.62074000

H	-3.12763200	1.32646500	-1.99830500
C	0.85513300	1.49065400	0.72287500
C	1.30638900	-0.44256700	2.15954900
C	0.32351700	1.59463600	2.18314100
C	1.43096000	0.03429100	0.70755900
C	-0.05337000	0.14932700	2.56374800
H	-0.26073400	0.04383000	3.63367500
H	-0.88630200	-0.26556000	1.99819200
C	2.27379400	0.41303000	3.02796500
H	2.35794800	-0.02841900	4.02635100
H	3.27874200	0.45949200	2.60517500
C	1.56933200	1.80184100	3.07776500
H	1.25864500	2.05174500	4.09698800
H	2.20682900	2.61522800	2.71728300
H	1.43256700	-1.51753900	2.26660400
H	-0.43514200	2.35581300	2.33090900
C	2.72242100	-0.23086000	-0.00111100
O	3.04768800	0.23176000	-1.08776700
O	3.50228200	-1.09134300	0.67948600
C	4.71982200	-1.52832800	0.03120100
H	4.94101200	-2.49238100	0.49408800
H	4.51946100	-1.67880200	-1.03186000
H	1.67917400	2.19393700	0.63315800
C	1.94065400	3.10959000	-1.45298600
H	1.90155800	3.78241400	-0.58521000
H	2.66897800	2.33508900	-1.21136000
C	2.45476800	3.90534500	-2.65298000
H	2.57876500	3.27204100	-3.53792900
H	1.79091000	4.73451600	-2.91948000
H	3.43455100	4.32973500	-2.41186300
H	-1.94733100	2.35257200	-3.91715000
C	5.84812500	-0.53623800	0.24918900
H	6.77155900	-0.92446000	-0.19374300
H	5.61621600	0.42308800	-0.22042000
H	6.02249600	-0.37423800	1.31765800
C	-2.36719300	0.95976800	0.42001300
C	-2.75884500	1.90673200	1.38946800
C	-3.01129500	-0.30596300	0.41043100
C	-3.59767800	1.50519200	2.43720200
C	-3.86769800	-0.67109600	1.45944300
C	-4.11843400	0.21562700	2.49992400
H	-3.85635500	2.22941400	3.20445300
H	-4.32838500	-1.65127000	1.45188100
H	-4.75306100	-0.08087000	3.32876200

C	-2.88560100	-1.26149400	-0.72919000
O	-1.92009700	-1.40336700	-1.48385200
O	-3.99249100	-1.98287600	-0.89464300
C	-3.96024000	-2.98690300	-1.93537000
H	-4.92572000	-3.48766300	-1.87874000
H	-3.83059600	-2.51448500	-2.91111900
H	-3.14784000	-3.69332800	-1.75405400
C	-2.39595200	3.36924200	1.27539300
H	-1.43690300	3.54225200	0.78875800
H	-3.15807400	3.88304900	0.67552600
H	-2.37950600	3.84515800	2.25945800
Br	0.80588600	-3.09646700	-0.22374600

TS4'

Pd	0.42677600	0.04363400	-0.59137400
C	-1.27261400	4.21955700	1.00579900
C	0.10923500	4.04138100	0.91653400
C	0.63184700	2.82993800	0.45364100
C	-0.24214800	1.80879500	0.07377400
C	-1.63414500	1.98598000	0.15738600
C	-2.16179200	3.20258400	0.63494300
H	-1.67269000	5.15981500	1.37789600
H	1.70749200	2.69481500	0.40564800
C	-2.47442000	0.82933900	-0.28464500
C	-1.90759100	-0.95344800	-1.86086900
C	-3.07820700	0.97893800	-1.71951200
C	-1.61450000	-0.46969100	-0.42254500
C	-1.98389000	0.38521600	-2.62528900
H	-2.31265600	0.26182600	-3.66237300
H	-1.04763000	0.95225900	-2.61581100
C	-3.39467400	-1.41427900	-1.93022100
H	-3.56565600	-1.93579800	-2.87734100
H	-3.65303000	-2.10682400	-1.12710400
C	-4.19270100	-0.07770900	-1.86381700
H	-4.76381200	0.08672700	-2.78289800
H	-4.89437200	-0.04814600	-1.02441400
H	-1.20774700	-1.70261800	-2.22999800
H	-3.39002000	2.00038100	-1.94568200
C	-1.85846500	-1.45378200	0.66827700
O	-2.30349400	-1.17190700	1.77329300
O	-1.56550700	-2.71608200	0.29249600
C	-1.88770600	-3.77832800	1.22189100
H	-1.19087000	-4.58141300	0.97357800
H	-1.69618200	-3.43844400	2.24058500

H	-3.28424600	0.65672400	0.42922700
C	-3.65041700	3.39731200	0.83064400
H	-3.88729500	4.46416500	0.74939000
H	-4.21102200	2.88957100	0.04002800
C	-4.12186900	2.88127600	2.20022400
H	-3.90385600	1.81476400	2.31882000
H	-3.61448000	3.41615000	3.01021600
H	-5.20132900	3.02271900	2.32212600
H	0.78110200	4.84316900	1.21220000
C	-3.33025800	-4.22171800	1.05427400
H	-3.53738700	-5.05999100	1.72804100
H	-4.01726100	-3.40682500	1.29941900
H	-3.52238700	-4.54978900	0.02822800
C	2.05142900	-0.58109100	0.81632900
C	1.84935900	-1.07963100	2.11062500
C	3.12921800	0.28921700	0.52503400
C	2.68432600	-0.57533000	3.11982100
C	3.95692000	0.73833800	1.56390400
C	3.72536700	0.31815900	2.86588900
H	2.51509700	-0.92798000	4.13356100
H	4.75571200	1.43298200	1.32936200
H	4.35447600	0.66862600	3.67703500
C	3.28878000	0.82344900	-0.83389900
O	2.35435800	0.87647100	-1.64096700
O	4.50733000	1.26513200	-1.11702800
C	4.68413700	1.88796100	-2.41148400
H	5.72319000	2.21275300	-2.43329100
H	4.49172700	1.16471800	-3.20619300
H	4.01169700	2.74239500	-2.51318300
C	0.80685300	-2.09762500	2.46664400
H	0.70172100	-2.83907000	1.67458900
H	1.07590100	-2.60599800	3.39571100
H	-0.16542600	-1.62156300	2.61371700
Br	1.78216000	-2.20528700	-0.80572400

12'

Pd	0.47652500	0.07648300	-0.67890900
C	-2.49141400	3.79577300	-0.32731400
C	-1.13661200	4.05051500	-0.54957800
C	-0.23148900	2.99087800	-0.64302100
C	-0.71556500	1.68689600	-0.54614800
C	-2.07592000	1.41569000	-0.35087200
C	-2.98256800	2.48849900	-0.22167200
H	-3.18531700	4.62615500	-0.22294400

H	0.82562200	3.18203500	-0.78834300
C	-2.49869600	-0.02553100	-0.32510000
C	-1.39969700	-1.86262400	-1.51759800
C	-3.17454300	-0.46832600	-1.66494200
C	-1.26303000	-0.98341300	-0.23798200
C	-1.96648200	-0.84639900	-2.53459900
H	-2.24602800	-1.32333000	-3.47882100
H	-1.30716000	-0.00052200	-2.75592700
C	-2.62600300	-2.80737100	-1.35972300
H	-2.62090800	-3.50057700	-2.20635900
H	-2.59864700	-3.39806000	-0.44419000
C	-3.84139700	-1.83980900	-1.42772700
H	-4.50598200	-2.09502100	-2.25850500
H	-4.43267700	-1.84713900	-0.50791000
H	-0.48262000	-2.38676200	-1.77525100
H	-3.83825800	0.29566300	-2.07187200
C	-1.21806700	-1.80384300	1.02914300
O	-2.22989900	-2.13925700	1.62565800
O	0.01268100	-2.15798700	1.38984600
C	0.15402800	-3.04564600	2.52574300
H	1.13520700	-2.80149200	2.93671800
H	-0.61629700	-2.81022000	3.26312200
H	-3.17029300	-0.22411800	0.51247400
C	-4.43659500	2.26052600	0.13055500
H	-5.02965600	3.10913400	-0.22719900
H	-4.82332400	1.37009300	-0.37278200
C	-4.63339600	2.11111200	1.64863600
H	-4.05990800	1.26466200	2.04111200
H	-4.29800200	3.01200700	2.17329200
H	-5.68870900	1.94709700	1.89169400
H	-0.78162800	5.07422300	-0.63225300
C	0.07823800	-4.49209200	2.07475500
H	0.27441500	-5.15539500	2.92358000
H	-0.91410200	-4.72520000	1.67801200
H	0.82325300	-4.68827800	1.29816700
C	1.24992200	0.73613300	1.07123200
C	0.70497400	0.78834100	2.35525800
C	2.59674200	1.11166400	0.84979100
C	1.58895700	1.08394700	3.41472600
C	3.44235500	1.40207900	1.92687800
C	2.93751600	1.36041000	3.22091600
H	1.17742200	1.10773800	4.42049400
H	4.47414800	1.67240900	1.73368800
H	3.57839600	1.57943300	4.06862300

C	3.06057200	1.28463600	-0.53655700
O	2.28066200	1.26029600	-1.49856800
O	4.35535200	1.51852200	-0.67877900
C	4.83236600	1.71638800	-2.03091700
H	5.90778100	1.85908800	-1.93667600
H	4.61060500	0.83564100	-2.63621200
H	4.36557300	2.60066300	-2.46985300
C	-0.74326100	0.60494900	2.72419400
H	-1.04497200	1.40710800	3.40483100
H	-1.39889100	0.64814400	1.86183600
H	-0.90870900	-0.33967200	3.24933200
Br	2.12124400	-1.94133200	-1.15245200

TS6'

Pd	-0.38557700	-0.08012300	-0.41748400
C	1.63128700	4.26493600	-0.33254600
C	0.26662100	4.15396800	-0.60448700
C	-0.34804700	2.89951600	-0.60213700
C	0.40659000	1.76154700	-0.29777600
C	1.77088700	1.87802800	0.02487200
C	2.40329000	3.13829900	-0.02502400
H	2.11065300	5.24057100	-0.36165600
H	-1.40294500	2.82849700	-0.84048500
C	2.47304300	0.61766200	0.41794900
C	1.62585800	-1.35682300	1.55970200
C	2.83221500	0.51917900	1.93535900
C	1.55841000	-0.63157800	0.21695800
C	1.58705600	-0.16147000	2.53178400
H	1.72391100	-0.45151100	3.57870200
H	0.67785700	0.43647500	2.43637400
C	3.07772000	-1.87969600	1.77250800
H	3.09314700	-2.57751600	2.61575900
H	3.45368100	-2.41836200	0.89949500
C	3.89188000	-0.58849300	2.08686800
H	4.28686600	-0.60947800	3.10764400
H	4.73603500	-0.44467600	1.40522700
H	0.87666500	-2.13227200	1.67605200
H	3.11035900	1.47723800	2.37713200
C	1.87911200	-1.42403200	-1.01583800
O	2.36666600	-0.95841600	-2.03854700
O	1.55336300	-2.72578800	-0.88129900
C	1.71236900	-3.56854300	-2.04646500
H	0.99157200	-4.37537200	-1.89758100
H	1.43416600	-2.99752700	-2.93548500

H	3.38392900	0.49626600	-0.17779200
C	3.89924800	3.28796900	0.15606800
H	4.11823800	4.30023000	0.51386800
H	4.27167700	2.59748200	0.91745100
C	4.65808100	3.04414100	-1.15909200
H	4.46801200	2.03652200	-1.54372900
H	4.34321200	3.75903800	-1.92677900
H	5.73838100	3.15337400	-1.01384200
H	-0.31771300	5.04221100	-0.83072000
C	3.13048500	-4.09996400	-2.15036200
H	3.20798400	-4.78076700	-3.00480000
H	3.84056200	-3.28149900	-2.29490600
H	3.40566600	-4.65163600	-1.24596300
C	-2.12893200	-0.26931700	0.94460500
C	-2.13527700	-0.58491700	2.30872700
C	-3.08124200	0.62149900	0.39345000
C	-2.98099000	0.18881700	3.12519300
C	-3.93213200	1.33738600	1.24591600
C	-3.85768800	1.14539200	2.61938700
H	-2.96618900	-0.01450600	4.19274300
H	-4.62656600	2.04809900	0.81247500
H	-4.50092800	1.70613600	3.28895300
C	-3.11333300	0.85406000	-1.05763400
O	-2.15763400	0.59587800	-1.79623500
O	-4.24979800	1.36865300	-1.50886800
C	-4.30370800	1.67465700	-2.92276100
H	-5.28539600	2.11795400	-3.08221400
H	-3.51444300	2.38182400	-3.18572900
H	-4.19635300	0.75998500	-3.50909500
C	-1.37987700	-1.71220800	2.95990200
H	-2.03796600	-2.21962600	3.67151200
H	-1.04539000	-2.44183700	2.22592700
H	-0.51448600	-1.34850300	3.51835500
Br	-1.84245600	-2.25296700	-0.36839500

15'

Pd	-0.56542800	-0.25854600	-0.32631700
C	2.19516000	3.19194800	-2.12017400
C	0.90306500	3.04851500	-2.62665800
C	0.05637400	2.06057400	-2.11414300
C	0.52503600	1.23679500	-1.09532500
C	1.81630100	1.38385700	-0.56082700
C	2.67624700	2.36337200	-1.09708100
H	2.85163900	3.95708400	-2.52683300

H	-0.95101600	1.94168300	-2.50063600
C	2.23774200	0.44548300	0.53836900
C	1.16925700	-0.94857900	2.22619300
C	2.37701100	0.95978700	2.01630900
C	1.22803600	-0.71807400	0.71965100
C	1.07265000	0.50400200	2.70804600
H	1.13667000	0.59280000	3.79707700
H	0.16426600	0.98375800	2.36491500
C	2.58927000	-1.33373700	2.75622900
H	2.48073000	-1.68352900	3.78716300
H	3.05521800	-2.13300700	2.18203900
C	3.38618300	0.00789800	2.69331400
H	3.63763400	0.36436500	3.69684300
H	4.31739200	-0.08090000	2.12587200
H	0.37470600	-1.62944500	2.52180100
H	2.62372400	2.01975600	2.08686900
C	1.45926800	-1.84269700	-0.23884600
O	0.81437900	-1.82924100	-1.29957500
O	2.34847400	-2.75965900	0.07041200
C	2.64956700	-3.78959500	-0.93333700
H	3.04093000	-4.61716900	-0.34151400
H	1.71527200	-4.08930300	-1.40988800
H	3.20289900	0.00906800	0.25078200
C	4.11389300	2.49517900	-0.64308400
H	4.44001100	3.53120700	-0.78616800
H	4.20249200	2.28335400	0.42622800
C	5.05023800	1.56071500	-1.42710000
H	4.75512000	0.51247200	-1.30933800
H	5.02493900	1.79535900	-2.49646400
H	6.08380000	1.66223800	-1.07924700
H	0.55278800	3.70523200	-3.41851700
C	3.66594100	-3.26689400	-1.92750600
H	3.93260400	-4.06961200	-2.62238100
H	3.26031800	-2.43233500	-2.50583500
H	4.57483600	-2.93694000	-1.41578300
C	-1.78215500	1.19764900	0.47288300
C	-1.58796300	2.35398800	1.24233100
C	-3.11291500	0.85896200	0.09947500
C	-2.72893000	2.97367500	1.80068100
C	-4.22357200	1.49974900	0.65484900
C	-4.02527800	2.54119700	1.55534500
H	-2.56862800	3.84707200	2.42813900
H	-5.22028800	1.19633300	0.35474000
H	-4.87014500	3.04654300	2.01192600

C	-3.28589600	-0.06718000	-1.03052100
O	-2.33512400	-0.36390600	-1.77236200
O	-4.51931700	-0.48680100	-1.25653800
C	-4.70794500	-1.36108800	-2.39374900
H	-5.76797300	-1.61031200	-2.39060900
H	-4.43913100	-0.84425400	-3.31738400
H	-4.10004800	-2.25994200	-2.27594700
C	-0.29127800	3.10020400	1.45546000
H	0.55597000	2.62075700	0.98433500
H	-0.39273300	4.09772100	1.01206100
H	-0.07673700	3.24223100	2.51908800
Br	-1.78876300	-2.29561600	0.87248700

TS8

Pd	1.05097700	-1.19656300	0.12078100
C	-1.88576200	-0.58714100	-0.44664700
C	-0.92600600	-0.99067000	0.50462900
C	-3.08699000	-1.27622800	-0.62002800
C	-1.22838200	-1.99793100	1.44088400
C	-3.30915900	-2.38097500	0.22365500
C	-2.41975700	-2.71374400	1.25001500
H	-0.56769600	-2.23860900	2.26774500
H	-4.22398900	-2.95728800	0.10868200
H	-2.65796400	-3.53982800	1.91524700
C	-4.14334900	-0.83045200	-1.60686100
H	-4.40475900	-1.67442400	-2.25805500
H	-3.73035900	-0.05156800	-2.25567200
C	-5.42051800	-0.31487900	-0.92685400
H	-6.15716900	0.00290500	-1.67250400
H	-5.87963700	-1.09459500	-0.31038600
H	-5.20431900	0.53886900	-0.27660900
C	-1.44401500	0.80754000	-0.78508500
C	-0.71010200	1.74148100	1.36731800
C	-2.37981500	1.88086900	-0.16272700
C	-0.23727500	0.82797500	0.21102600
C	-2.24515500	1.59081300	1.34824300
H	-2.73288200	2.35167200	1.96518500
H	-2.60912400	0.60830100	1.65053000
C	-0.59254900	3.19916900	0.83845500
H	-0.82826500	3.89304400	1.65142900
H	0.40633200	3.44955700	0.47958000
C	-1.67939600	3.25550600	-0.27970200
H	-2.38943300	4.06921700	-0.10450500
H	-1.24437700	3.40305400	-1.27318600

H	-0.20246300	1.56657900	2.31552900
H	-3.39038800	1.85579300	-0.57292400
C	1.09119500	1.20842300	-0.38468800
O	1.30516800	1.35838500	-1.58572300
O	2.00371400	1.55685700	0.57164700
C	3.32687900	1.89639300	0.10074400
H	3.98713600	1.65356100	0.93701900
H	3.57680400	1.25430600	-0.74704000
H	-1.17811900	1.02429700	-1.82166700
C	3.42966100	3.36497200	-0.27232300
H	4.45866100	3.60062900	-0.56568200
H	2.76919800	3.59658700	-1.11155800
H	3.16211900	4.00259800	0.57620100
N	3.05021200	-1.73227200	-0.20070400
C	4.16175900	-2.01442500	-0.37340300
C	5.55598900	-2.35672900	-0.59210700
H	5.63657800	-3.06771100	-1.41942300
H	6.12136300	-1.45275800	-0.83679200
H	5.97176500	-2.80811300	0.31322000

TS9

Pd	0.17791400	-0.26645300	0.64746800
C	-2.55432300	-0.91835100	-0.25154900
C	-1.30701300	-1.48971500	0.07500200
C	-3.63097400	-1.74505000	-0.63967400
C	-1.15285900	-2.88058700	0.06816700
C	-3.44333200	-3.13321700	-0.66371400
C	-2.22345900	-3.70019200	-0.29979900
H	-0.20125200	-3.33109900	0.32598800
H	-4.26657600	-3.77373100	-0.97120500
H	-2.09800200	-4.78004200	-0.31041900
C	-4.98935700	-1.19072200	-1.02618200
H	-5.27184600	-1.60283300	-2.00336900
H	-4.93967400	-0.10658400	-1.15073000
C	-6.09100000	-1.53837900	-0.01318000
H	-7.05425500	-1.12218400	-0.32778000
H	-6.20825700	-2.62266100	0.08387000
H	-5.85757800	-1.14068000	0.97989800
N	1.38069900	1.10991300	1.99978900
C	1.86301700	1.68840500	2.87882900
C	2.47330300	2.42292400	3.97195200
H	2.48209600	1.80209700	4.87216200
H	3.50043100	2.68821000	3.70575800
H	1.90173800	3.33491700	4.16590700

C	-2.65206700	0.57253600	-0.15815700
C	-1.52730100	2.11230600	1.36003900
C	-3.51955300	1.09656500	1.02964400
C	-1.26106400	1.20975800	0.13933500
C	-2.49175100	1.22725200	2.17024000
H	-2.90021600	1.72679700	3.05526600
H	-2.04283200	0.27338400	2.46572100
C	-2.46535000	3.27349300	0.92297800
H	-2.50227400	4.03608300	1.70795300
H	-2.11511000	3.76447200	0.01120000
C	-3.84806400	2.57509800	0.74400500
H	-4.57844500	2.95611000	1.46531500
H	-4.26615200	2.71511500	-0.25796300
H	-0.62937500	2.45684500	1.86404900
H	-4.39181700	0.47548700	1.23534600
C	-0.63514700	1.85840000	-1.04520500
O	-0.94312500	1.64900300	-2.21019400
O	0.33364200	2.74168400	-0.69353900
C	0.95971400	3.47414100	-1.77150600
H	1.92672400	3.78255500	-1.36913200
H	1.12026100	2.79859800	-2.61310700
H	-3.04432700	0.97833200	-1.09673900
C	0.12509200	4.67703100	-2.17560800
H	0.65136400	5.24926500	-2.94736400
H	-0.83996900	4.36116600	-2.58042100
H	-0.04914400	5.33612300	-1.31926200
C	1.62302500	-0.76383000	-1.15006000
C	1.00022500	-1.57356200	-2.09989200
C	2.53557600	0.24009300	-1.47928300
C	1.20162900	-1.29964000	-3.45212000
H	0.35065900	-2.38284500	-1.80122600
C	2.69549200	0.49277300	-2.85886500
C	2.04247000	-0.25097400	-3.83495400
H	0.69508400	-1.90840100	-4.19538200
H	3.38005700	1.28625000	-3.14764500
H	2.20221400	-0.02923500	-4.88565500
I	2.33575600	-2.07819900	0.95632800
C	3.41214100	0.99971800	-0.51235300
H	3.05444000	0.85276800	0.50255800
H	3.33613400	2.07069400	-0.72859500
C	4.88121000	0.56386900	-0.60875700
H	5.49290800	1.12147800	0.10873500
H	4.98658500	-0.50317600	-0.38745100
H	5.28661500	0.74237100	-1.60987200

TS4''

Pd	-0.43225200	-0.37956000	-0.82167700
C	3.88276100	-2.40858600	-0.31511300
C	2.83308200	-3.17135000	-0.82993200
C	1.56419600	-2.60787000	-0.97640200
C	1.35305900	-1.26560300	-0.63425700
C	2.43453700	-0.47270400	-0.20385000
C	3.70349300	-1.05737500	0.00214700
H	4.85961700	-2.86188600	-0.16352900
H	0.74205600	-3.22057000	-1.32493200
C	2.17845600	0.99493600	-0.06195900
C	0.62444600	2.37791300	-1.34421300
C	2.81595200	1.83914600	-1.21496200
C	0.66166500	1.32272000	-0.21903800
C	1.71250300	1.83701900	-2.28962700
H	1.93269100	2.51133100	-3.12424200
H	1.48226400	0.84105500	-2.68063000
C	1.29277300	3.68260600	-0.82689300
H	1.10826700	4.49821300	-1.53405600
H	0.89376600	3.99695200	0.14056300
C	2.80722300	3.31535200	-0.76944700
H	3.38992100	3.93219400	-1.46130800
H	3.23488800	3.44179900	0.23024000
H	-0.36294400	2.54049000	-1.76961500
H	3.79370500	1.47012800	-1.52971500
C	-0.00083400	1.69468300	1.06266700
O	0.41147800	1.41270400	2.17905500
O	-1.13617900	2.40689400	0.85928200
C	-1.82668200	2.88571300	2.03508000
H	-2.86938300	2.98107300	1.72427700
H	-1.75606700	2.13448900	2.82231200
H	2.54085300	1.36361100	0.90224300
C	4.84172400	-0.27866800	0.62795000
H	5.79341600	-0.74125200	0.34352300
H	4.86538800	0.74737600	0.25025100
C	4.73465300	-0.24828300	2.16159100
H	3.79521900	0.21409100	2.48223700
H	4.76348000	-1.26329900	2.57227500
H	5.56062000	0.32103500	2.60198600
H	2.99567200	-4.21275200	-1.09625000
C	-1.25955300	4.21916800	2.48979800
H	-1.83341400	4.59261300	3.34488700
H	-0.21595600	4.11094200	2.79843200

H	-1.31517300	4.96247000	1.68831200
C	-1.66120700	-1.25083800	0.91132400
C	-1.03946100	-1.91169300	1.97539800
C	-2.79298500	-0.45076500	1.06021700
C	-1.54101400	-1.60278600	3.25432900
C	-3.26268300	-0.18523100	2.34723600
C	-2.62861500	-0.75548600	3.45120600
H	-1.06003700	-2.07382800	4.10756400
H	-4.13000200	0.45622400	2.46980900
H	-2.99213700	-0.56325200	4.45583300
C	0.09087200	-2.88961600	1.84943400
H	-0.06174400	-3.55455500	0.99766500
H	1.04262400	-2.37420200	1.69226400
H	0.17021500	-3.49014000	2.75914700
Br	-1.92041700	-2.53519500	-1.07563500
H	-3.29142200	-0.02960900	0.20058400
N	-2.16050800	0.80053300	-1.69966600
C	-2.95878000	1.37030000	-2.31368100
C	-3.96157700	2.09481800	-3.07371100
H	-4.29919000	1.48324500	-3.91505300
H	-4.81429200	2.32569700	-2.42902100
H	-3.53159100	3.02626300	-3.45247400

11a1

Pd	0.22937300	-0.10913600	-0.94793100
C	-2.23617000	-1.39826100	-0.01978600
C	-3.28262900	-2.34214800	0.02651200
C	-1.15864200	-1.55397200	-0.92371800
C	-3.22642500	-3.45629100	-0.82106400
C	-1.14198200	-2.67590300	-1.76742000
C	-2.16639400	-3.62571900	-1.71071600
H	-4.02971900	-4.18897500	-0.78690800
H	-0.33880100	-2.82878400	-2.48149200
H	-2.13779400	-4.49399200	-2.36476500
C	-4.50682700	-2.13645200	0.89464100
H	-4.92666300	-3.11285200	1.16314000
H	-4.24063800	-1.64072100	1.83198100
C	-5.58494000	-1.30991600	0.17410100
H	-6.46096700	-1.16076400	0.81498000
H	-5.20178600	-0.32456200	-0.11162100
H	-5.91381300	-1.81628200	-0.73978100
N	1.62376900	1.54389700	-0.91644800
C	2.41818400	2.38084600	-0.85286900
C	3.42579700	3.41997300	-0.75456300

H	4.37344500	3.04772000	-1.15324900
H	3.11123800	4.29807900	-1.32544400
H	3.55895800	3.69976300	0.29433600
C	-2.20696700	-0.17947000	0.85153000
C	-0.32367200	1.13422600	1.68262300
C	-1.81547700	-0.43249200	2.34393400
C	-1.10275700	0.81944700	0.38839500
C	-0.28425700	-0.25912100	2.34108300
H	0.13967600	-0.24743000	3.35143100
H	0.24284400	-1.00051400	1.73509400
C	-1.25342800	1.90515600	2.66129000
H	-0.66990300	2.30810700	3.49599300
H	-1.74991600	2.74873600	2.17500000
C	-2.25278000	0.80972700	3.14781000
H	-2.14836700	0.63106400	4.22313400
H	-3.29742600	1.07472900	2.95485800
H	0.63432300	1.62452700	1.51726800
H	-2.19249100	-1.37864100	2.73807300
C	-1.62846100	1.96153400	-0.40133200
O	-2.64149700	1.94381300	-1.09208900
O	-0.84926900	3.06964000	-0.29097400
C	-1.22229500	4.21293700	-1.08813900
H	-0.29079300	4.76659100	-1.23096700
H	-1.58580300	3.86857000	-2.05954900
H	-3.18470500	0.31355400	0.82632200
C	-2.26454300	5.06291800	-0.38230000
H	-2.48493900	5.95505900	-0.97859300
H	-3.19194400	4.50039700	-0.24627300
H	-1.90136600	5.38703500	0.59825200
O	4.02316300	-0.37216400	-1.23746800
O	3.05578800	-1.66644900	0.37427600
C	3.85688100	0.21679700	1.73378900
C	5.40084000	-1.70847000	1.11760800
C	3.44025700	-2.08689000	2.64999800
C	3.97620500	-1.28362300	1.46834900
C	3.15068200	-1.12878300	-0.84899900
C	2.00882500	-1.59876700	-1.69365600
C	1.64114900	-0.93805200	-2.82096600
H	4.24913300	0.80201300	0.90168900
H	4.42473200	0.46675100	2.63521800
H	2.81127700	0.49102100	1.90051300
H	5.43009400	-2.77369000	0.86787100
H	6.04849600	-1.54292700	1.98420000
H	5.78990500	-1.13530500	0.27557500

H	2.40667300	-1.80537100	2.87073500
H	4.05069700	-1.89195800	3.53623300
H	3.47253700	-3.15928000	2.43529500
H	1.55860100	-2.54323200	-1.41034100
H	2.17061500	-0.04296600	-3.13114400
H	0.89053400	-1.33659800	-3.49387200

TS4a1

Pd	-0.18495400	-0.35089700	-0.66911400
C	2.52721500	-1.06878200	0.20601400
C	3.72500300	-1.81402600	0.16577000
C	1.29739500	-1.74975100	-0.09071400
C	3.73046800	-3.07900900	-0.43782800
C	1.36282400	-2.98343700	-0.78206400
C	2.57410200	-3.62472200	-0.99659800
H	4.66645100	-3.62878500	-0.49399200
H	0.44156500	-3.48493400	-1.05570700
H	2.60950000	-4.57492800	-1.52048700
C	5.01676400	-1.32452700	0.80105000
H	5.83417800	-1.35654800	0.07069800
H	4.92101500	-0.28830400	1.12630200
C	5.39147800	-2.18469700	2.01877700
H	6.32091800	-1.82327600	2.47173300
H	4.60367100	-2.14420600	2.77880700
H	5.53715100	-3.23375300	1.74242000
N	-1.60296300	0.94689800	-1.40822300
C	-2.35970300	1.77638600	-1.68591400
C	-3.30516100	2.82856200	-2.00886400
H	-4.03519200	2.91984700	-1.19975100
H	-2.77205400	3.77620900	-2.12687000
H	-3.82699700	2.58735500	-2.93913000
C	2.56874100	0.44613900	0.30973500
C	1.68059100	2.06457400	-1.33744300
C	3.59586700	1.04400300	-0.71952000
C	1.25971800	1.16476000	-0.16450500
C	2.75352800	1.18566500	-1.99967700
H	3.29573700	1.69281300	-2.80533200
H	2.36111500	0.23326900	-2.36873700
C	2.54092100	3.23796500	-0.80116400
H	2.74666900	3.96045900	-1.59946300
H	2.03972100	3.77576600	0.00679300
C	3.84684800	2.52145500	-0.34218300
H	4.71966300	2.90619700	-0.87949500
H	4.04118000	2.63969400	0.72877900

H	0.84819800	2.38163100	-1.96666000
H	4.50994500	0.46475600	-0.82755100
C	0.50559800	1.78034700	0.94032800
O	0.53583900	1.41441900	2.11507800
O	-0.28380700	2.81425900	0.53061300
C	-1.20117900	3.35433900	1.50261500
H	-2.01342100	3.78260100	0.90893900
H	-1.59733700	2.53695400	2.11020900
H	2.83678900	0.76339900	1.32388900
C	-0.54076200	4.41280000	2.36929700
H	-1.27693400	4.84869000	3.05370700
H	0.26622500	3.97396300	2.96133400
H	-0.12847100	5.21774900	1.75211700
O	-2.61033500	-0.55388900	1.58056100
O	-3.60176300	-1.88836200	0.00920000
C	-5.03022200	0.10704700	-0.11393000
C	-5.38753500	-1.65115000	1.68595000
C	-5.80183700	-2.20244700	-0.72809500
C	-4.95637000	-1.37912100	0.24309200
C	-2.52994600	-1.40755400	0.69876900
C	-1.30297500	-2.04301000	0.23429300
C	-0.05728300	-1.89394400	1.02714800
H	-4.39578800	0.69978600	0.54542800
H	-6.06354000	0.45601800	-0.01933200
H	-4.71230300	0.26066600	-1.14931900
H	-5.24921900	-2.71024900	1.92725300
H	-6.44947700	-1.41149400	1.80172800
H	-4.81021400	-1.05171800	2.38971100
H	-5.46593700	-2.04803600	-1.75821000
H	-6.85203100	-1.90406600	-0.65794100
H	-5.72843800	-3.26937600	-0.49553500
H	-1.44797800	-2.96449100	-0.31915900
H	-0.09145800	-1.07476700	1.74608800
H	0.30170300	-2.79451900	1.52391500

12a1

Pd	-1.08525600	-0.02899200	-0.43839600
C	2.73248100	-1.10270200	-0.08716600
C	4.11803000	-1.34231400	-0.34939500
C	1.99413800	-2.17843800	0.45831900
C	4.64068700	-2.63909200	-0.27952600
C	2.55557400	-3.46620200	0.51688300
C	3.85743300	-3.71918200	0.11218100
H	5.69153200	-2.78878100	-0.51426500

H	1.94356600	-4.27399700	0.90940300
H	4.26851200	-4.72404200	0.14860400
C	5.15309100	-0.24622100	-0.54654700
H	6.02479600	-0.68037500	-1.04757900
H	4.80757700	0.56013900	-1.18508200
C	5.60595100	0.34316100	0.80069400
H	6.36235200	1.12133500	0.64928700
H	4.76781500	0.79035400	1.34546300
H	6.03979800	-0.43368600	1.43932100
N	-2.42081800	1.70633100	-0.84288300
C	-3.26548100	2.49654900	-0.90211900
C	-4.32836900	3.48309700	-0.96961600
H	-5.24957400	3.05306100	-0.56619900
H	-4.05159900	4.36293600	-0.38201600
H	-4.49195800	3.77856900	-2.00968400
C	2.22842600	0.32688700	-0.36542700
C	0.69794200	1.96747400	-1.30461700
C	2.55896600	0.82736800	-1.83158600
C	0.78156900	0.93114500	-0.15737700
C	1.19089800	1.10050400	-2.47304100
H	1.27884600	1.64571500	-3.41926500
H	0.58222700	0.20446400	-2.62357200
C	1.82618100	3.03029000	-1.18848600
H	1.59424300	3.89779300	-1.81459600
H	1.93575700	3.39070800	-0.16165500
C	3.08698800	2.27407600	-1.69779000
H	3.41251700	2.65553700	-2.67157900
H	3.92918200	2.36098900	-1.00642700
H	-0.28382300	2.41897700	-1.40576200
H	3.20437500	0.14989700	-2.38938200
C	0.57522100	1.42896400	1.22458600
O	1.07672100	0.94005100	2.23314200
O	-0.24285000	2.51450700	1.27773600
C	-0.54599400	3.04019600	2.58771300
H	-1.50982100	3.54090800	2.46686400
H	-0.65916200	2.21020100	3.28936100
H	2.84296800	0.93937300	0.30681700
C	0.52562400	4.01083200	3.05253700
H	0.24143300	4.44551400	4.01700200
H	1.48372000	3.49845600	3.17357900
H	0.64978500	4.82560500	2.33201300
O	-2.14922800	-2.73700300	1.64230800
O	-2.74409000	-1.82302800	-0.38361900
C	-4.50019300	-0.87976500	1.05134000

C	-4.71120900	-3.21925200	0.07472200
C	-4.75721100	-1.20520900	-1.43102000
C	-4.20472200	-1.79347400	-0.13621400
C	-1.83796200	-2.24900300	0.57305700
C	-0.48210300	-1.89043100	0.07375400
C	0.62656500	-2.05108500	1.08224100
H	-4.10996300	-1.29745800	1.98027200
H	-5.58282400	-0.75537400	1.15096300
H	-4.05399700	0.10624800	0.89011600
H	-4.41655900	-3.85633700	-0.76510800
H	-5.80445000	-3.20715000	0.12637700
H	-4.32095900	-3.64657400	0.99864500
H	-4.35949900	-0.20085800	-1.60029400
H	-5.84756900	-1.14239600	-1.37092200
H	-4.49287500	-1.83606800	-2.28506000
H	-0.27796800	-2.37996400	-0.88522500
H	0.61713700	-1.21383600	1.78634400
H	0.44241500	-2.95584000	1.67454300

11a2

Pd	-0.07540700	-0.56084000	-0.92048500
C	2.61724700	-0.98457500	0.16704500
C	3.72910200	-1.68663700	0.67740900
C	1.47613100	-1.67531200	-0.30595100
C	3.70995200	-3.08690000	0.66269100
C	1.49718700	-3.07941600	-0.31290400
C	2.60988100	-3.78070500	0.16022300
H	4.56687400	-3.63289600	1.05108000
H	0.65549800	-3.65292900	-0.68690500
H	2.61287600	-4.86796300	0.14265100
C	4.90157700	-0.97010300	1.31543700
H	5.79658100	-1.59697000	1.22932400
H	5.12104100	-0.03680300	0.78939600
C	4.64605100	-0.66522600	2.80086100
H	5.49729000	-0.13911800	3.24702600
H	3.75611300	-0.04006000	2.92879000
H	4.48520200	-1.59099600	3.36383600
N	-1.63973100	0.76409900	-1.60929800
C	-2.51675300	1.45487600	-1.90857400
C	-3.62720600	2.32077100	-2.25697500
H	-4.49100000	1.71181000	-2.53711900
H	-3.88654200	2.94360400	-1.39633200
H	-3.34826300	2.96256200	-3.09729700
C	2.57606100	0.51090800	0.08921900

C	1.39553400	1.98722800	-1.45612400
C	3.45084300	1.13560000	-1.04674300
C	1.14903100	1.02243700	-0.27847700
C	2.47702700	1.21584100	-2.23809000
H	2.88865600	1.78322500	-3.08018300
H	2.13238300	0.23985300	-2.59144400
C	2.20626100	3.21371600	-0.95100000
H	2.22096900	3.99683400	-1.71662600
H	1.76989600	3.65023000	-0.04927100
C	3.63399800	2.63045200	-0.71257700
H	4.36530400	3.09072800	-1.38532300
H	3.98605700	2.77983000	0.31333400
H	0.49435200	2.25891400	-2.00364000
H	4.38384800	0.59612600	-1.22272500
C	0.39813800	1.54284400	0.89640300
O	0.55278300	1.17847200	2.05684500
O	-0.50318100	2.50287800	0.55832200
C	-1.27241700	3.08102800	1.63498400
H	-2.18002100	3.45660200	1.15669500
H	-1.54167100	2.29681000	2.34579500
H	2.88711700	0.94187400	1.04676100
C	-0.50759900	4.20156600	2.31836000
H	-1.13302600	4.65999600	3.09211700
H	0.39959000	3.81643100	2.79137100
H	-0.22909500	4.97773000	1.59855700
O	-3.87432700	-1.38135200	-1.18938500
O	-2.91948700	-1.52484500	0.87886300
C	-5.27473800	-1.63302600	1.55092800
C	-4.16153600	0.59657200	1.04851100
C	-3.43129800	-0.75979500	3.03298200
C	-3.98839000	-0.81273400	1.61324000
C	-2.96387200	-1.70436400	-0.44691500
C	-1.71018500	-2.38553500	-0.89528700
C	-1.27484300	-2.32107800	-2.17926700
H	-5.65619500	-1.69094600	0.53040400
H	-6.03494700	-1.16207000	2.18188700
H	-5.09994300	-2.64681400	1.92444000
H	-3.19306000	1.09690400	0.98320900
H	-4.80221000	1.17410800	1.72184900
H	-4.61871700	0.57845000	0.05949700
H	-3.25184600	-1.76872200	3.41626000
H	-4.14495700	-0.25885700	3.69306600
H	-2.48783900	-0.20561000	3.05398500
H	-1.22678800	-3.01344200	-0.15603300

H	-1.82857300	-1.75533000	-2.92197000
H	-0.43554500	-2.91498200	-2.52268700

TS4a2

Pd	0.95925200	-0.33071000	-1.46349400
C	-1.59372600	-1.01178900	-0.18244000
C	-2.83171600	-1.68914300	-0.11961800
C	-1.15924100	-0.56332800	-1.48508900
C	-3.37274400	-2.24963400	-1.28613700
C	-1.69220400	-1.21759500	-2.62574700
C	-2.74509100	-2.11350000	-2.52428500
H	-4.29093800	-2.82594900	-1.21274600
H	-1.34748300	-0.91346900	-3.60840700
H	-3.13907500	-2.61034300	-3.40507000
C	-3.64416800	-1.79721000	1.16424900
H	-3.75296200	-2.84396600	1.47291300
H	-3.13154500	-1.27688900	1.97511600
C	-5.04269300	-1.18284400	0.99527900
H	-5.57810200	-1.19523200	1.95064100
H	-4.97680600	-0.14503700	0.65522900
H	-5.64590800	-1.73564200	0.26884000
N	2.98926000	-0.09987800	-1.66416500
C	4.13484700	0.06378800	-1.66721300
C	5.57141200	0.27195700	-1.65046300
H	5.79308500	1.23319400	-1.17816500
H	6.05188400	-0.52865100	-1.08100900
H	5.96025200	0.27397600	-2.67253800
C	-0.64437500	-1.01168700	1.01963100
C	1.45030300	-2.36095900	1.00672500
C	-0.68545500	-2.40692600	1.73206500
C	0.88519700	-0.96881600	0.63510600
C	0.21662000	-3.25408400	0.81300400
H	0.36190600	-4.27533900	1.18258900
H	-0.14107100	-3.29361900	-0.22030200
C	1.61904300	-2.45329700	2.54255000
H	2.04753700	-3.42327600	2.82434700
H	2.27266100	-1.67550500	2.93917000
C	0.14764900	-2.33095400	3.03513900
H	-0.12092900	-3.15110400	3.70885300
H	-0.03649000	-1.39449600	3.57269500
H	2.34582400	-2.64145400	0.44787500
H	-1.67760000	-2.81118800	1.90073600
C	1.59889600	0.18197200	1.17970900
O	1.11555600	1.27790800	1.47128500

O	2.94963900	-0.04122400	1.30643600
C	3.75537900	1.08823700	1.68269000
H	4.75683100	0.85412100	1.31066300
H	3.38785100	1.98161100	1.17050100
H	-0.88860300	-0.20172900	1.71518100
C	3.77295100	1.29698300	3.18857900
H	4.43960800	2.12816500	3.44474200
H	2.76970700	1.53197600	3.55260500
H	4.13402300	0.39948900	3.70154900
O	-0.13483400	3.11134700	-0.95799700
O	-1.83423800	1.93073900	-0.01523100
C	-2.84134700	4.15012500	0.11900100
C	-1.13975200	3.41704500	1.85270300
C	-3.37443200	2.28055700	1.71620400
C	-2.27344400	2.98428400	0.92758500
C	-0.85895900	2.13555600	-0.90342000
C	-0.88602300	1.06321600	-1.98873000
C	0.28700700	1.03434100	-2.90875800
H	-2.06264300	4.63769900	-0.47039800
H	-3.27365400	4.88983600	0.79999500
H	-3.63126900	3.80215300	-0.55433800
H	-0.67255100	2.54790300	2.31636000
H	-1.55337900	4.06819100	2.63009800
H	-0.37009500	3.96026500	1.30548800
H	-4.17381500	1.94472400	1.05020400
H	-3.80254000	2.96884500	2.45065000
H	-2.97367700	1.41228500	2.24762900
H	-1.84208200	1.22430400	-2.49383800
H	0.07340600	0.73039700	-3.93217500
H	0.94565000	1.89761300	-2.84163700

12a2

Pd	1.38453200	-0.70699200	-0.78701800
C	-2.22733000	0.76560400	-0.60338400
C	-3.53812500	1.12267800	-0.14952600
C	-1.44809800	1.78802900	-1.20073500
C	-4.05249800	2.40547300	-0.34954200
C	-2.01674100	3.06590700	-1.38857000
C	-3.30201200	3.38628900	-0.98717100
H	-5.05468400	2.63010500	0.00635300
H	-1.40493500	3.83272900	-1.85638400
H	-3.70488300	4.38087500	-1.15552400
C	-4.43163300	0.18784400	0.65316500
H	-5.46657200	0.52645000	0.53679400

H	-4.40730900	-0.83502800	0.27871000
C	-4.08451200	0.19836000	2.15286100
H	-4.76249100	-0.45600600	2.71221600
H	-3.06039600	-0.14200000	2.33532700
H	-4.17715400	1.21088300	2.56032100
N	3.43824400	-0.23559900	-1.11108500
C	4.54876500	0.05196300	-1.26826400
C	5.93952500	0.42081100	-1.46177700
H	6.15459600	1.34028000	-0.90981800
H	6.58710400	-0.38114000	-1.09638400
H	6.13126700	0.58416600	-2.52605800
C	-1.91215900	-0.72368600	-0.38753200
C	-0.68853000	-2.68100700	-1.21386500
C	-2.68820800	-1.65646800	-1.38821700
C	-0.51161700	-1.39585200	-0.33622300
C	-1.58901700	-2.15132300	-2.34055400
H	-1.93769800	-2.94523500	-3.01068900
H	-1.13479300	-1.36003400	-2.93624600
C	-1.64965000	-3.66842300	-0.50304000
H	-1.64144400	-4.63755000	-1.01315200
H	-1.36819700	-3.84941000	0.53885400
C	-3.03577100	-2.96732900	-0.64204900
H	-3.72632400	-3.57433500	-1.23673200
H	-3.50827900	-2.78265300	0.32722900
H	0.25230400	-3.14189400	-1.51797400
H	-3.54577100	-1.16922000	-1.85534600
C	-0.08923700	-1.67861200	1.06510100
O	-0.63253600	-1.40038300	2.11987500
O	1.16182500	-2.28521000	1.03198500
C	1.81735100	-2.53685600	2.30413900
H	2.88054000	-2.56714100	2.05920200
H	1.62376800	-1.69366400	2.97014700
H	-2.32222100	-0.92258400	0.60072200
C	1.34265700	-3.84606000	2.90482400
H	1.90108800	-4.05097400	3.82452800
H	0.27894000	-3.79793900	3.15147900
H	1.50867400	-4.67489200	2.20962500
O	1.97865600	2.89144800	-0.67995200
O	0.40320000	2.07836100	0.74151400
C	1.36692400	3.87334600	2.11326600
C	2.43650100	1.56925700	2.02322000
C	0.16554000	1.87392500	3.06033700
C	1.13427600	2.36826900	1.98888200
C	0.92041200	2.32439900	-0.46586500

C	0.02861500	1.79682500	-1.59785400
C	0.69956000	0.56377100	-2.19814800
H	2.05940900	4.23079200	1.35069900
H	1.78281900	4.09593300	3.10104000
H	0.41927000	4.41208500	2.01280100
H	2.23417900	0.50524600	1.86808900
H	2.90841300	1.68986700	3.00350500
H	3.13091800	1.91043300	1.25475700
H	-0.78286900	2.41686000	2.99888700
H	0.59422000	2.03666500	4.05371100
H	-0.03620800	0.80757900	2.93065500
H	0.11601600	2.57872800	-2.36317400
H	1.59561300	0.88106100	-2.73895900
H	0.02780500	0.06527600	-2.89701300

11a3

Pd	0.03696800	-0.57094200	-1.16935900
C	-0.61876900	2.19045500	-0.40449700
C	-0.43424400	3.57859600	-0.23856300
C	0.34354700	1.40728000	-1.08447500
C	0.69357800	4.18317000	-0.80785900
C	1.45838600	2.04648700	-1.64664000
C	1.62739500	3.42799900	-1.51709800
H	0.83905300	5.25436800	-0.68628300
H	2.22602000	1.47822300	-2.15626500
H	2.49623500	3.91105100	-1.95803500
C	-1.37196000	4.40988900	0.61249800
H	-1.34954900	5.44932200	0.26542500
H	-2.40408400	4.06494700	0.50382800
C	-0.97852000	4.36993600	2.09864400
H	-1.67091600	4.96309700	2.70633600
H	-0.98403000	3.34398600	2.48150900
H	0.03036800	4.77171900	2.24230600
N	-0.49597700	-2.70047200	-1.30747800
C	-0.80247500	-3.81536700	-1.34305500
C	-1.19699500	-5.21213400	-1.37267800
H	-0.66470900	-5.73055000	-2.17484700
H	-0.95411600	-5.68110000	-0.41487400
H	-2.27417600	-5.28437200	-1.54754100
C	-1.81377700	1.46286300	0.12849600
C	-2.91615900	-0.56845800	-0.65505600
C	-3.14379600	1.68264700	-0.66373700
C	-1.62156700	-0.07918500	0.02256000
C	-3.12946300	0.54336500	-1.70100000

H	-4.07907100	0.45371200	-2.24026700
H	-2.30836000	0.61188200	-2.42050800
C	-4.11319700	-0.31799600	0.30447900
H	-5.00539200	-0.83641600	-0.06245400
H	-3.91364700	-0.69063200	1.31280300
C	-4.29854900	1.23108300	0.25493900
H	-5.26711400	1.49730800	-0.18114400
H	-4.24002500	1.69609900	1.24433100
H	-2.86500300	-1.58989600	-1.02847600
H	-3.25279900	2.69440300	-1.05990300
C	-1.22992800	-0.71227700	1.31274600
O	-0.64897900	-0.14926800	2.23542100
O	-1.58884700	-2.01942700	1.37565100
C	-1.17806000	-2.75873600	2.54568800
H	-1.15088300	-3.80022100	2.21574300
H	-0.16902000	-2.44963000	2.82925000
H	-1.98027000	1.74093000	1.17465100
C	-2.15451400	-2.57110200	3.69347900
H	-1.85470800	-3.19531700	4.54225000
H	-2.16999700	-1.52799700	4.01935500
H	-3.16610900	-2.86318500	3.39379800
O	3.97212100	0.14498100	-1.12938800
O	2.98271000	-1.00697800	0.57583200
C	3.06496600	1.24532000	1.56635600
C	5.05459500	-0.33398700	1.70797700
C	2.90048100	-0.86508100	2.91279300
C	3.53342300	-0.20408600	1.69102400
C	3.19938200	-0.69803500	-0.70818900
C	2.33421300	-1.55951200	-1.57077200
C	1.96767100	-1.21745600	-2.82615500
H	3.47963200	1.72848400	0.68169300
H	3.39261900	1.79857600	2.45205100
H	1.97370000	1.29033000	1.51861200
H	5.34780500	-1.38821500	1.73795300
H	5.44883300	0.15604000	2.60363200
H	5.50095500	0.13266900	0.82877600
H	1.81031000	-0.78655800	2.86217000
H	3.24576100	-0.36601100	3.82291400
H	3.17963700	-1.92173600	2.97040600
H	2.04601500	-2.51425500	-1.14454700
H	2.30171000	-0.29360900	-3.28508600
H	1.38657200	-1.89930500	-3.43824400

TS4a3

Pd	-1.10781300	-0.85939200	-1.09656800
C	0.93474800	1.17321400	-0.47625800
C	2.02147600	1.99531000	-0.83129900
C	0.85587200	-0.13616200	-1.07475900
C	2.80368400	1.65501600	-1.94950100
C	1.61866500	-0.40333900	-2.23645800
C	2.54951300	0.51401900	-2.70684700
H	3.60779300	2.32222200	-2.24732500
H	1.54440600	-1.37767700	-2.70348500
H	3.12759500	0.30453600	-3.60132500
C	2.39709800	3.25179700	-0.05792300
H	2.27218300	4.13757900	-0.69307100
H	1.73159100	3.38023600	0.79682900
C	3.84337500	3.21025300	0.45717200
H	4.07456000	4.13047800	1.00434300
H	3.99103600	2.36633800	1.13737200
H	4.56810800	3.11735800	-0.35728700
N	-3.01775200	-1.62706600	-1.25489700
C	-4.11797000	-1.98054000	-1.18862400
C	-5.49908800	-2.41623700	-1.09095600
H	-5.56697700	-3.26580000	-0.40539600
H	-6.11616600	-1.59599400	-0.71323400
H	-5.86301700	-2.71887400	-2.07689800
C	-0.24599900	1.72210700	0.31330100
C	-2.59736300	1.90696000	-0.44388900
C	-0.70657800	3.11971900	-0.23349200
C	-1.57813900	0.91503700	0.13775100
C	-1.68854100	2.74341900	-1.35800000
H	-2.18730800	3.61920800	-1.78833800
H	-1.22727700	2.15868500	-2.15998500
C	-2.98122800	2.95156400	0.63404100
H	-3.79037500	3.60159800	0.27937000
H	-3.32193200	2.47614400	1.55665100
C	-1.65533200	3.75331400	0.81119200
H	-1.80258700	4.81636600	0.59406700
H	-1.24777400	3.67913000	1.82484000
H	-3.45677400	1.42764600	-0.91661100
H	0.10180400	3.78117300	-0.53127200
C	-1.95995200	0.13210500	1.30425800
O	-1.18604000	-0.35688400	2.13735800
O	-3.31231400	-0.07699300	1.38923000
C	-3.76513000	-0.98921300	2.40525000
H	-4.71100400	-1.38649200	2.02580100
H	-3.04805700	-1.80897000	2.49942600

H	0.01663800	1.81179900	1.37511000
C	-3.96426600	-0.28629900	3.73776100
H	-4.36426400	-0.98798100	4.47820300
H	-3.01288600	0.10457700	4.10780000
H	-4.67079600	0.54406800	3.63624900
O	2.99699600	-2.61849400	-0.73167300
O	2.82115000	-1.23290300	1.06603100
C	5.08664100	-0.67002100	0.29961100
C	4.66902800	-2.70184300	1.76914000
C	4.30209200	-0.38761400	2.67739300
C	4.25687600	-1.26963300	1.43334900
C	2.35242900	-1.90030800	0.00907500
C	0.85450100	-1.66051000	-0.12522400
C	0.08423200	-2.63607500	-0.91547800
H	5.03536700	-1.28818600	-0.59727200
H	6.13137100	-0.59987000	0.61804500
H	4.73264800	0.33498900	0.05743700
H	3.99436700	-3.12602700	2.51945900
H	5.68090500	-2.69426400	2.18611400
H	4.65996400	-3.33814300	0.88396500
H	3.93057000	0.61589600	2.45279800
H	5.33183900	-0.30543800	3.03618100
H	3.68839200	-0.81458200	3.47637700
H	0.43707200	-1.43134600	0.85530200
H	0.61727000	-3.13802200	-1.71930900
H	-0.58682400	-3.28488300	-0.35558900

12a3

Pd	-1.88974400	-1.06304900	-0.42901300
C	0.72016600	1.23603700	-1.11290700
C	1.38746500	2.09424200	-2.02662400
C	1.20424000	-0.08954000	-1.00734700
C	2.23332500	1.54733800	-3.00303300
C	2.04747500	-0.61315900	-1.99582500
C	2.51335700	0.18528200	-3.03704400
H	2.69091000	2.21064300	-3.73228700
H	2.37192000	-1.64689800	-1.91944900
H	3.14530900	-0.23265600	-3.81544700
C	1.36108400	3.61470100	-1.91533200
H	0.96227100	4.06480000	-2.83348200
H	0.71232100	3.93481500	-1.10098500
C	2.76414700	4.18218700	-1.64345100
H	2.71842200	5.27076300	-1.52823700
H	3.17962200	3.76077500	-0.72126400

H	3.46226500	3.96052000	-2.45586600
N	-2.59214800	-2.85496200	-1.32719800
C	-2.95610200	-3.83052200	-1.83462400
C	-3.41057600	-5.05351500	-2.47104000
H	-3.31432300	-5.88864200	-1.77137100
H	-4.45856300	-4.94648200	-2.76497600
H	-2.80375000	-5.25261700	-3.35888000
C	-0.45973900	1.78831400	-0.29303400
C	-2.88094700	1.37454900	-0.05472100
C	-1.42637100	2.67423800	-1.16707900
C	-1.49746800	0.81877000	0.38334900
C	-2.58662500	1.73565700	-1.51874500
H	-3.41551300	2.25480900	-2.01219500
H	-2.28179600	0.88005700	-2.13206400
C	-3.11816800	2.77374300	0.57338900
H	-4.15631100	3.08802300	0.42325700
H	-2.92795400	2.77561800	1.64918300
C	-2.12830800	3.67615700	-0.22421900
H	-2.66694500	4.43222300	-0.80426800
H	-1.41732000	4.19795900	0.42372100
H	-3.71003500	0.68184200	0.12709700
H	-0.95853100	3.13945500	-2.02863600
C	-1.33243100	0.67236700	1.84601300
O	-0.29941900	0.87410400	2.47885000
O	-2.47637700	0.26534500	2.46364200
C	-2.41561100	0.09071800	3.89633800
H	-3.20932900	-0.62612100	4.12025800
H	-1.45150800	-0.34861800	4.16276900
H	-0.03739600	2.42087800	0.49819100
C	-2.64081100	1.40487400	4.62387200
H	-2.64869800	1.23378200	5.70587300
H	-1.84296300	2.11570700	4.39316200
H	-3.60104000	1.84662200	4.33946700
O	2.52568900	-2.79602800	0.49190700
O	3.16309100	-0.69407200	1.08547500
C	5.25432900	-1.51464600	0.09563000
C	4.65146800	-2.04101400	2.50905700
C	5.14664900	0.32381800	1.80685300
C	4.57314200	-1.02286500	1.37248000
C	2.29707100	-1.60511600	0.61477500
C	0.97601100	-0.92328700	0.25175800
C	-0.15482600	-1.92174700	0.15317400
H	4.85532000	-2.47885300	-0.22182300
H	6.32810100	-1.62371800	0.27704900

H	5.11509400	-0.79002700	-0.71264100
H	4.09057400	-1.68339900	3.37841600
H	5.69643900	-2.17216000	2.80754900
H	4.24903200	-3.00660600	2.20182400
H	5.04266800	1.06287000	1.00652400
H	6.20862500	0.21717900	2.04609200
H	4.62596800	0.69676200	2.69405300
H	0.78849300	-0.23247400	1.07268000
H	0.05201100	-2.69123000	-0.59578800
H	-0.35569500	-2.40091800	1.11848000

11b1

Pd	-0.24458600	0.27711300	-0.86190800
C	2.08145300	1.55157500	0.40239500
C	2.99519400	2.57909700	0.71265000
C	0.99508800	1.79672200	-0.46236900
C	2.79568000	3.85031800	0.15879500
C	0.82767900	3.07372600	-1.01743800
C	1.72471700	4.09827400	-0.69977300
H	3.49653900	4.64742800	0.39688900
H	0.00510800	3.28081600	-1.69244900
H	1.58678500	5.08930300	-1.12564700
C	4.23084600	2.31953000	1.54958000
H	4.51129100	3.24068700	2.07353600
H	4.02688100	1.56996000	2.31919400
C	5.41654600	1.85240700	0.68925800
H	6.30005300	1.65893100	1.30762300
H	5.17322600	0.93211000	0.14776400
H	5.67994700	2.61426100	-0.05229800
N	-1.79836000	1.61196000	-1.60252600
C	-2.72701200	2.28328600	-1.76427500
C	-3.89790500	3.11693600	-1.96346600
H	-3.89685800	3.93155800	-1.23371300
H	-3.88540600	3.53594700	-2.97349400
H	-4.79949500	2.51275600	-1.83146200
C	2.21144500	0.15390600	0.91476800
C	0.57420300	-1.61009300	1.28950000
C	1.80331000	-0.07170500	2.40615200
C	1.24833100	-0.81754100	0.14886500
C	0.32215000	-0.47919800	2.30792600
H	-0.08210000	-0.83732300	3.26144300
H	-0.32638600	0.30694400	1.91265300
C	1.63918900	-2.45980200	2.04022100
H	1.14621100	-3.17757000	2.70467000

H	2.26443500	-3.03212300	1.35125500
C	2.44579500	-1.40010500	2.85357800
H	2.31826000	-1.54878900	3.93118200
H	3.51911300	-1.42931700	2.63851000
H	-0.30465600	-2.17804100	0.99154800
H	2.03064200	0.77952700	3.05191000
C	1.97194500	-1.57494300	-0.90692300
O	2.89937300	-1.14319500	-1.58130300
O	1.50740800	-2.84525300	-1.06479300
C	2.09997300	-3.63313400	-2.12122800
H	1.32840400	-4.35854700	-2.39078100
H	2.29939500	-2.98614400	-2.97862400
H	3.24701200	-0.18073300	0.78803500
C	3.36614500	-4.32538100	-1.64834500
H	3.76402900	-4.95894200	-2.44851200
H	4.12852100	-3.59019600	-1.37780900
H	3.16157700	-4.95912200	-0.77956200
O	-2.66684900	-2.22205900	0.71670300
O	-3.82416200	-0.37451800	0.04362400
C	-3.48751700	0.13824800	2.42032100
C	-5.41960800	-1.32833200	1.65276900
C	-5.34459900	1.11088100	1.03430400
C	-4.51843500	-0.13875900	1.32704500
C	-2.93048000	-1.36111500	-0.10729200
C	-2.29562800	-1.25556400	-1.45200800
C	-1.21260400	-1.98115500	-1.79361500
H	-2.89447300	-0.74835800	2.64493500
H	-4.00559900	0.45341100	3.33119900
H	-2.81626600	0.94538300	2.11109300
H	-6.09687000	-1.53305900	0.81761200
H	-6.02496300	-1.09102400	2.53308000
H	-4.83327700	-2.22372400	1.86150600
H	-4.69403600	1.95073800	0.77367000
H	-5.92643300	1.38479800	1.91890800
H	-6.03704800	0.93177400	0.20628100
H	-2.77623300	-0.59380900	-2.16109900
H	-0.76877600	-2.69131400	-1.10968400
H	-0.80065500	-1.92738200	-2.79615300
TS4b1			
Pd	-0.64834400	0.83434000	-0.49498900
C	1.93563900	1.65632100	0.30629700
C	3.09812400	2.45088100	0.45636700
C	0.73071500	2.25425400	-0.11184600

C	3.02043300	3.82030000	0.16132200
C	0.68089300	3.62337900	-0.39110700
C	1.82862300	4.41005200	-0.25875100
H	3.91417700	4.42968400	0.27399000
H	-0.25148900	4.08101300	-0.71491100
H	1.79505400	5.47550300	-0.47479500
C	4.43546700	1.88937500	0.90228700
H	5.02216500	2.70129500	1.34658300
H	4.29844000	1.14431500	1.69221800
C	5.23684000	1.27175700	-0.25490000
H	6.19228400	0.87027700	0.10125900
H	4.67962400	0.46312200	-0.73704100
H	5.45132600	2.02805800	-1.01833500
N	-2.24715600	2.05229500	-0.56184000
C	-3.21936800	2.67917900	-0.55257200
C	-4.44217900	3.46007200	-0.53795500
H	-4.19939900	4.52628400	-0.55299800
H	-5.04542300	3.21177600	-1.41566000
H	-5.00903300	3.22969600	0.36853000
C	1.94943400	0.20519400	0.72985600
C	0.77368900	-1.86862600	1.20406200
C	1.49679200	0.01020900	2.22218400
C	1.19175000	-1.03065500	-0.03477300
C	0.18416100	-0.77589500	2.11097600
H	-0.16778600	-1.16183200	3.07345300
H	-0.63560700	-0.22277600	1.63885000
C	2.00575900	-2.32650100	2.03837100
H	1.70099500	-3.13477500	2.71007400
H	2.81098400	-2.71618100	1.41383400
C	2.42301700	-1.05447600	2.83491800
H	2.22634900	-1.17190600	3.90595300
H	3.48195300	-0.80650200	2.71453400
H	0.09113100	-2.67754200	0.96091500
H	1.45671600	0.95400300	2.76917900
C	2.23833000	-1.61762100	-0.96474900
O	2.95913800	-0.95029200	-1.68745900
O	2.25185900	-2.96207400	-0.94941000
C	3.20222500	-3.62224900	-1.82885000
H	2.77005500	-4.61038500	-1.99761200
H	3.24126800	-3.07751800	-2.77432000
H	2.98806900	-0.11675700	0.67221500
C	4.57027400	-3.71469600	-1.17973400
H	5.25211800	-4.25927900	-1.84141100
H	4.98606300	-2.71945700	-1.00178500

H	4.51503500	-4.25140100	-0.22771400
O	-2.28727000	-2.30471200	0.57896200
O	-3.76648700	-1.03120200	-0.61084400
C	-4.50449600	-0.58559900	1.68245400
C	-5.27862900	-2.66398000	0.44096200
C	-5.99655300	-0.38098900	-0.32740700
C	-4.87895100	-1.19181700	0.32797200
C	-2.52353200	-1.51342200	-0.33197100
C	-1.54728100	-0.92627000	-1.23906600
C	-0.16030700	-1.42416300	-1.29129500
H	-3.71427900	-1.16010100	2.16711900
H	-5.38223000	-0.57266900	2.33638500
H	-4.15948600	0.44535900	1.55121800
H	-5.47985300	-3.07831800	-0.55239500
H	-6.19171700	-2.75267600	1.03879100
H	-4.48756300	-3.24778500	0.91164300
H	-5.69781100	0.66582200	-0.43963500
H	-6.90085800	-0.42037600	0.28699600
H	-6.23313700	-0.78125900	-1.31822700
H	-1.96121600	-0.57060400	-2.18020100
H	-0.06547000	-2.48141100	-1.06140500
H	0.29935600	-1.19825100	-2.25122100

12b1

Pd	-0.74185900	1.31279700	-0.07408400
C	1.71568000	1.89504200	0.14163700
C	2.80082600	2.47317200	-0.58586100
C	0.58320500	2.73830000	0.38460300
C	2.76004300	3.83530100	-0.91866500
C	0.59085500	4.09947300	0.08658100
C	1.69092700	4.65750100	-0.56714400
H	3.60782000	4.26031200	-1.44987600
H	-0.28104200	4.71097700	0.30906900
H	1.70023400	5.71118400	-0.83525000
C	4.02439100	1.70115500	-1.03575700
H	4.86232300	2.40071100	-1.12745100
H	4.31624000	0.94220300	-0.30954200
C	3.79989600	1.01320300	-2.39141400
H	4.69727900	0.46815200	-2.70354100
H	2.97485200	0.29813400	-2.33903200
H	3.55891200	1.74813800	-3.16747500
N	-2.67607600	1.80161900	0.36350200
C	-3.77220800	2.05861200	0.63273600
C	-5.14355100	2.38278900	0.98165800

H	-5.32772400	3.44575000	0.80127900
H	-5.83096000	1.78566100	0.37663500
H	-5.30916300	2.16194700	2.04009100
C	1.90258400	0.50156900	0.80073000
C	0.86439000	-1.64669300	1.41618600
C	1.36396300	0.38764200	2.26593100
C	1.44022400	-0.90426800	0.15262500
C	0.12872800	-0.52074100	2.15414200
H	-0.25316600	-0.83706400	3.13119800
H	-0.71284900	-0.10654300	1.58989000
C	1.98264400	-1.95285800	2.44439900
H	1.57772800	-2.61362400	3.21693700
H	2.85214900	-2.45850700	2.02009700
C	2.32649500	-0.54872900	3.03449800
H	2.12072800	-0.51259900	4.10916700
H	3.37546800	-0.27510300	2.88790000
H	0.25935900	-2.50250800	1.13071800
H	1.21495800	1.35827900	2.74054000
C	2.69801400	-1.68674300	-0.27363600
O	3.85400400	-1.33621400	-0.11451600
O	2.37983100	-2.88686700	-0.79242900
C	3.47695100	-3.76150900	-1.16689100
H	3.04325800	-4.42700900	-1.91590400
H	4.26278800	-3.16121900	-1.63005700
H	2.98215300	0.40577400	0.86760200
C	3.99722900	-4.53683800	0.02878800
H	4.75212300	-5.25656100	-0.30534200
H	4.45933900	-3.86820000	0.75925800
H	3.18759800	-5.08908000	0.51565600
O	-1.82010000	-2.34972400	0.15764900
O	-3.24152800	-1.06714300	-1.07856400
C	-4.63879800	-1.63970000	0.86655100
C	-4.40265100	-3.23206800	-1.09589100
C	-5.55976300	-1.02250300	-1.38838100
C	-4.45176100	-1.76975500	-0.64669900
C	-2.00980600	-1.40514900	-0.60622000
C	-0.99205100	-0.48910100	-1.12882200
C	0.48413100	-0.93789400	-1.10737500
H	-3.85222100	-2.16675600	1.40684900
H	-5.60764800	-2.06227400	1.15166500
H	-4.62556200	-0.58710700	1.16407200
H	-4.20959300	-3.29015300	-2.17214500
H	-5.36649000	-3.71176300	-0.89646900
H	-3.62017500	-3.77792500	-0.56845400

H	-5.55875400	0.03702500	-1.11573000
H	-6.53600700	-1.44635200	-1.13516300
H	-5.41865100	-1.09930100	-2.47099600
H	-1.27312800	-0.15849700	-2.13105300
H	0.50186900	-1.97945700	-1.44109600
H	0.99280200	-0.36231200	-1.88765700

11b2

Pd	0.20492900	-0.49037700	-0.76744000
C	-2.38849600	-1.27671400	0.37105400
C	-3.48859900	-2.11912200	0.63390600
C	-1.24029200	-1.78327200	-0.27401900
C	-3.40407400	-3.47070100	0.27523900
C	-1.18126300	-3.14066700	-0.62278900
C	-2.26103600	-3.98224000	-0.34034300
H	-4.24922000	-4.12476200	0.47789500
H	-0.30461600	-3.54492400	-1.11740800
H	-2.21208200	-5.03523800	-0.60728300
C	-4.78300900	-1.58265000	1.20922200
H	-5.30030500	-2.38758700	1.74383900
H	-4.58394600	-0.79579700	1.94190900
C	-5.71110100	-1.03031300	0.11468700
H	-6.64101300	-0.64336000	0.54587900
H	-5.22970900	-0.21647700	-0.43780100
H	-5.97013000	-1.81390800	-0.60553300
N	1.63798000	-1.99997700	-1.38599400
C	2.59836200	-2.62952500	-1.52853300
C	3.81819600	-3.39551200	-1.69719000
H	3.72280300	-4.06677900	-2.55502400
H	4.64785600	-2.70343600	-1.86368000
H	4.00988400	-3.98382400	-0.79554800
C	-2.35126400	0.17126100	0.74923400
C	-0.41175700	1.54103500	1.33081800
C	-2.13829700	0.42732700	2.27480900
C	-1.11155700	0.88924300	0.11207900
C	-0.60495600	0.45329000	2.40405100
H	-0.26804400	0.76747000	3.39818300
H	-0.12665100	-0.49402700	2.14228900
C	-1.31163600	2.67624300	1.89179200
H	-0.75684700	3.26102800	2.63345900
H	-1.63850500	3.36791300	1.11210800
C	-2.49333400	1.90252100	2.55458200
H	-2.53606400	2.09366900	3.63192400
H	-3.46584900	2.17338000	2.13058400

H	0.61723600	1.84810500	1.15737300
H	-2.66337400	-0.28831800	2.91077200
C	-1.48963600	1.77962800	-1.01622900
O	-2.45837500	1.63441300	-1.75144700
O	-0.61291100	2.81137100	-1.18038800
C	-0.86715400	3.72154300	-2.27449300
H	0.11178200	4.14138400	-2.51732400
H	-1.23765800	3.15426500	-3.13139200
H	-3.27327100	0.66797900	0.43057600
C	-1.84800300	4.80698800	-1.86750700
H	-1.98360200	5.51375800	-2.69331800
H	-2.82097300	4.37438900	-1.61985300
H	-1.47607100	5.36074400	-0.99972200
O	4.04888100	-0.02418700	-1.03273200
O	3.12993900	0.90632700	0.83754000
C	5.46340300	0.70442100	1.58001700
C	3.86580000	-1.27085100	1.70538400
C	3.49269100	0.75452800	3.14800100
C	4.02493000	0.24595600	1.81110400
C	3.19486000	0.64629000	-0.47646000
C	2.04455200	1.29647600	-1.16437000
C	1.63247500	0.91088200	-2.39174500
H	5.84080600	0.35241800	0.61919000
H	6.10126300	0.30626100	2.37525700
H	5.52434800	1.79688200	1.60760800
H	2.80763700	-1.54626400	1.75764400
H	4.38555800	-1.74437400	2.54379900
H	4.28542400	-1.65336300	0.77496900
H	3.54222800	1.84658100	3.19256100
H	4.09309800	0.34568700	3.96554800
H	2.45309300	0.44583100	3.29174600
H	1.56354600	2.12316200	-0.65833500
H	2.14708100	0.12480800	-2.93389400
H	0.83257300	1.43409900	-2.90240000

TS4b2

Pd	-0.65470700	0.59995500	0.17325400
C	1.96729900	1.63933900	-0.12927700
C	3.03932900	2.47413400	-0.52398300
C	0.64008100	2.05376000	-0.34382900
C	2.74610900	3.69969300	-1.13989900
C	0.37599400	3.28274400	-0.95632600
C	1.43041700	4.10733000	-1.35929800
H	3.56924500	4.34138300	-1.44598500

H	-0.65033700	3.60149600	-1.12286200
H	1.22967300	5.06375200	-1.83668500
C	4.49442400	2.08451300	-0.34641800
H	5.09908000	2.99739000	-0.30408200
H	4.64454100	1.57220600	0.60894100
C	5.01032400	1.19874900	-1.49255900
H	6.05640100	0.91621300	-1.32985100
H	4.41610900	0.28481100	-1.58739900
H	4.94761000	1.73306500	-2.44700400
N	-2.22732600	1.85065100	0.36667800
C	-3.10771500	2.58895600	0.49962800
C	-4.21216800	3.51484300	0.66707200
H	-4.68688400	3.69498700	-0.30154100
H	-4.94618900	3.08956900	1.35712800
H	-3.83900900	4.46076700	1.06966000
C	2.23527000	0.35089100	0.60618400
C	1.42059100	-1.55766000	1.86122300
C	2.28744700	0.50315900	2.16861900
C	1.36284500	-1.01063500	0.40776100
C	1.06973400	-0.28990700	2.66352400
H	1.07892900	-0.45414100	3.74582300
H	0.10546800	0.15125900	2.38385400
C	2.88199000	-1.81683800	2.33260200
H	2.86264000	-2.45354600	3.22197000
H	3.47310500	-2.33586300	1.57718400
C	3.43388900	-0.39723900	2.66232500
H	3.59194600	-0.27170900	3.73859700
H	4.38046600	-0.18305600	2.15724700
H	0.77171300	-2.41788300	2.02358100
H	2.35021400	1.54601800	2.48483800
C	2.07932600	-1.76830000	-0.69471500
O	2.41306000	-1.26548200	-1.75354800
O	2.27053300	-3.06644100	-0.39932700
C	2.93127900	-3.88186100	-1.40598900
H	2.59562900	-4.89790600	-1.19035200
H	2.56929700	-3.58207400	-2.39146500
H	3.22678900	0.02047400	0.29611000
C	4.43940800	-3.75756900	-1.30166800
H	4.91122800	-4.41936900	-2.03560100
H	4.76212900	-2.73325200	-1.50565800
H	4.78711100	-4.04733200	-0.30538500
O	-2.74040400	-1.20552000	-1.64930600
O	-3.88984900	-1.24171000	0.32728500
C	-5.44741700	-2.40925300	-1.17385200

C	-5.38983300	0.12708600	-1.06694800
C	-6.15609500	-1.20831200	0.91534500
C	-5.21915200	-1.18018800	-0.29139200
C	-2.75467100	-1.25714600	-0.41916600
C	-1.57532600	-1.31532200	0.44087400
C	-0.30553200	-1.71066100	-0.18381000
H	-4.79961700	-2.39164000	-2.05051500
H	-6.49061800	-2.43370200	-1.50498800
H	-5.24877400	-3.32411900	-0.60597800
H	-5.24597500	0.98371300	-0.40279700
H	-6.40575600	0.18072400	-1.47164800
H	-4.67877600	0.19170500	-1.89076500
H	-6.02183500	-2.13117700	1.48793900
H	-7.19698900	-1.15420700	0.58322000
H	-5.95799000	-0.35811200	1.57547700
H	-1.75669300	-1.62265300	1.46661800
H	-0.33682700	-1.62796400	-1.26972300
H	0.04694200	-2.69491800	0.10870100

12b2

Pd	1.58519300	-0.40247600	0.66125900
C	-0.87414800	-1.60456800	-0.69987300
C	-1.38122600	-2.54715000	-1.64241000
C	0.51791400	-1.37156400	-0.70508000
C	-0.52947700	-3.12114100	-2.59575900
C	1.34806600	-1.94698100	-1.67831300
C	0.82488600	-2.81058900	-2.63865600
H	-0.94635900	-3.82800700	-3.30906800
H	2.41322400	-1.73739200	-1.67343100
H	1.47251600	-3.25287500	-3.39139700
C	-2.83346700	-2.99499800	-1.70909700
H	-2.84034600	-4.05068700	-2.00403900
H	-3.31375600	-2.95550600	-0.72823500
C	-3.66012800	-2.19389000	-2.72615200
H	-4.68707400	-2.57394900	-2.77781100
H	-3.70174100	-1.13848200	-2.44807500
H	-3.22069200	-2.27375200	-3.72663200
N	2.72148100	-2.12972800	1.27699600
C	3.28101700	-3.09570200	1.58483600
C	3.97954200	-4.30905000	1.96770700
H	4.92334900	-4.37810600	1.41967600
H	4.18400300	-4.29174200	3.04187100
H	3.35868000	-5.17775900	1.73080300
C	-1.86887600	-0.95112700	0.25597600

C	-1.95859400	0.82330300	1.94390900
C	-1.84281600	-1.42557000	1.74515300
C	-1.90470400	0.62231900	0.38619000
C	-1.07425300	-0.31549800	2.47840800
H	-1.13706400	-0.40808700	3.56898300
H	-0.02509200	-0.24736100	2.18941600
C	-3.33695500	0.34759000	2.47542300
H	-3.43627600	0.63145900	3.52753900
H	-4.18708200	0.78604100	1.94877300
C	-3.26365700	-1.20642300	2.31893900
H	-3.37169500	-1.70423300	3.28789100
H	-4.04246700	-1.59696800	1.65650200
H	-1.69454200	1.83777000	2.24825400
H	-1.46379800	-2.44350900	1.86388900
C	-3.20315500	1.17052200	-0.22265000
O	-4.00695200	0.55291100	-0.89783400
O	-3.36372300	2.47421300	0.07901900
C	-4.54661800	3.13485900	-0.44017300
H	-4.27367800	4.19177300	-0.46809000
H	-4.72794400	2.78391800	-1.45838800
H	-2.84600900	-1.21413800	-0.13354900
C	-5.75079300	2.89729700	0.45223800
H	-6.60332300	3.47194000	0.07469000
H	-6.02686200	1.83980400	0.46294600
H	-5.54567200	3.22116700	1.47719800
O	1.55431900	2.12446300	-1.86479600
O	2.73905800	2.31384400	0.08296200
C	3.90417600	3.94112200	-1.34666400
C	4.47238000	1.46547000	-1.43267000
C	4.96255700	2.80881900	0.63261900
C	4.02054900	2.63599700	-0.55753600
C	1.64008100	1.96591600	-0.65338400
C	0.61593100	1.35400200	0.22530500
C	-0.78132000	1.39827900	-0.35335400
H	3.23672400	3.82212000	-2.20010500
H	4.89358200	4.24222900	-1.70617600
H	3.51784600	4.73874700	-0.70378900
H	4.49283900	0.54088200	-0.84582800
H	5.48289400	1.65634700	-1.80736900
H	3.80349200	1.32765800	-2.28284400
H	4.61501600	3.61406100	1.28728100
H	5.96860000	3.05791300	0.28228400
H	5.01777000	1.88496900	1.21729000
H	0.66188600	1.80239400	1.22505200

H	-0.75398700	1.04312300	-1.38721900
H	-1.08929300	2.44931700	-0.39956300

11b3

Pd	0.20486900	0.49065700	0.76725200
C	-2.38867600	1.27659900	-0.37104100
C	-3.48888900	2.11886800	-0.63394200
C	-1.24061000	1.78333500	0.27410000
C	-3.40460800	3.47043100	-0.27517600
C	-1.18180100	3.14071700	0.62296500
C	-2.26169700	3.98212600	0.34053100
H	-4.24983800	4.12437600	-0.47785400
H	-0.30521900	3.54505600	1.11763800
H	-2.21295200	5.03511600	0.60754200
C	-4.78317000	1.58224100	-1.20940500
H	-5.30047800	2.38710000	-1.74412800
H	-4.58392800	0.79537500	-1.94202700
C	-5.71134200	1.02987100	-0.11495800
H	-6.64115700	0.64278600	-0.54624100
H	-5.22993000	0.21613200	0.43765400
H	-5.97054600	1.81349300	0.60517100
N	1.63792000	2.00014900	1.38519200
C	2.59829900	2.62964700	1.52799000
C	3.81811900	3.39561500	1.69676200
H	3.72287300	4.06652700	2.55488000
H	4.64781900	2.70346900	1.86277000
H	4.00965300	3.98428700	0.79531500
C	-2.35123200	-0.17138300	-0.74920700
C	-0.41150500	-1.54094700	-1.33064900
C	-2.13811400	-0.42744500	-2.27475200
C	-1.11148900	-0.88927300	-0.11196700
C	-0.60474500	-0.45321100	-2.40389400
H	-0.26772100	-0.76734400	-3.39800300
H	-0.12659500	0.49417100	-2.14208800
C	-1.31112400	-2.67626200	-1.89181600
H	-0.75616100	-3.26077600	-2.63356700
H	-1.63786400	-3.36812800	-1.11225500
C	-2.49296100	-1.90269500	-2.55452800
H	-2.53577200	-2.09384400	-3.63186400
H	-3.46540700	-2.17366500	-2.13043900
H	0.61748000	-1.84791500	-1.15699200
H	-2.66323600	0.28811300	-2.91077700
C	-1.48956900	-1.77977000	1.01623800
O	-2.45833600	-1.63461300	1.75144200

O	-0.61287900	-2.81155100	1.18026600
C	-0.86707700	-3.72178900	2.27435500
H	0.11186000	-4.14170600	2.51704100
H	-1.23744700	-3.15451900	3.13131700
H	-3.27321900	-0.66817300	-0.43061200
C	-1.84806200	-4.80713100	1.86743600
H	-1.98362400	-5.51389600	2.69325600
H	-2.82101000	-4.37442900	1.61989500
H	-1.47627900	-5.36092000	0.99960600
O	4.04873000	0.02457600	1.03303700
O	3.13032400	-0.90653400	-0.83718300
C	5.46372500	-0.70442400	-1.57963000
C	3.86601600	1.27077800	-1.70509900
C	3.49303000	-0.75462300	-3.14766000
C	4.02525800	-0.24601100	-1.81077800
C	3.19493300	-0.64619900	0.47675000
C	2.04460700	-1.29635200	1.16464500
C	1.63232700	-0.91043600	2.39184400
H	5.84091900	-0.35266700	-0.61862700
H	6.10171000	-0.30595800	-2.37461700
H	5.52476700	-1.79687100	-1.60753400
H	2.80781100	1.54609100	-1.75703900
H	4.38544600	1.74425000	-2.54374900
H	4.28590400	1.65344300	-0.77486700
H	3.54231600	-1.84669200	-3.19207700
H	4.09362500	-0.34602100	-3.96519000
H	2.45352100	-0.44569500	-3.29154600
H	1.56357700	-2.12299100	0.65855900
H	2.14682800	-0.12412500	2.93374000
H	0.83231000	-1.43340700	2.90257400

TS4b3

Pd	-0.53538700	1.50993200	0.47420900
C	-2.05403500	-0.31214100	-1.13781700
C	-3.18532100	-0.83187400	-1.82906000
C	-1.97478900	1.07846500	-0.90336600
C	-4.12357500	0.05953100	-2.36869400
C	-2.94235300	1.93467900	-1.44877500
C	-4.00139000	1.43858000	-2.20736200
H	-4.97381800	-0.34837700	-2.91075400
H	-2.87345500	3.00571000	-1.26509800
H	-4.73894400	2.10872700	-2.64376800
C	-3.51675300	-2.30985700	-1.93367800
H	-4.20714900	-2.45282900	-2.77236100

H	-2.63718100	-2.91128200	-2.15969100
C	-4.18350900	-2.84711900	-0.65582700
H	-4.41546900	-3.91337400	-0.75510500
H	-3.53871000	-2.72459400	0.22060400
H	-5.11841700	-2.31307400	-0.45432700
N	-1.21276600	3.33337800	1.01256700
C	-1.62705000	4.37578200	1.29815900
C	-2.14769500	5.68186100	1.65857600
H	-3.21156800	5.59777600	1.89828600
H	-1.60866600	6.06720100	2.52871900
H	-2.02055300	6.37085400	0.81873700
C	-0.99692300	-1.30547000	-0.64882200
C	1.28041000	-2.06580800	-0.24425100
C	-0.32326300	-2.10769800	-1.82086600
C	0.26884300	-1.05708800	0.38915800
C	1.15049400	-1.70906800	-1.73533100
H	1.79783400	-2.31758500	-2.37461100
H	1.31579600	-0.65581600	-1.95864500
C	0.74888300	-3.52320600	-0.21101400
H	1.58660600	-4.21229900	-0.35305800
H	0.28775500	-3.77447100	0.74633200
C	-0.25448400	-3.58709800	-1.39595300
H	0.13108500	-4.20614900	-2.21283800
H	-1.22436000	-3.99276600	-1.09753800
H	2.27944600	-1.98910400	0.17705400
H	-0.80356100	-1.92374800	-2.78211200
C	-0.22944200	-1.38454500	1.78615000
O	-1.33554700	-1.09127600	2.20744000
O	0.70416500	-2.00074100	2.53261200
C	0.34912900	-2.32314300	3.90513800
H	1.30711000	-2.36828100	4.42638300
H	-0.24656600	-1.50409900	4.31290500
H	-1.56076500	-2.03456300	-0.06166100
C	-0.39023800	-3.64532500	3.97853500
H	-0.60276100	-3.88599000	5.02548300
H	-1.33934900	-3.59272700	3.43845000
H	0.21399600	-4.45409200	3.55651300
O	1.98245800	1.54002900	-1.06388600
O	3.58020500	0.14792800	-0.23613200
C	4.97431600	2.02557200	-0.98760800
C	4.22844800	0.22264900	-2.61674200
C	5.81856300	-0.33353800	-0.74987200
C	4.65091700	0.54627000	-1.18576000
C	2.36873100	0.70692800	-0.25722900

C	1.53835300	0.22688600	0.90810800
C	1.10575600	1.38668400	1.74554700
H	4.14440600	2.66037700	-1.30007000
H	5.85511400	2.28326400	-1.58349800
H	5.20164100	2.22809000	0.06367200
H	3.95357200	-0.83209500	-2.70694700
H	5.07316800	0.41305800	-3.28609900
H	3.38715700	0.83894000	-2.93445300
H	6.08867600	-0.13112700	0.29074500
H	6.68873100	-0.13065800	-1.38041200
H	5.56033300	-1.39250000	-0.84487600
H	2.06979000	-0.52082100	1.48680100
H	1.73643800	2.27131400	1.64646000
H	0.91743200	1.13360600	2.79085000
12b3			
Pd	-0.02588600	-1.37926100	-1.28110100
C	-1.24698500	-1.04161400	1.24731100
C	-2.22993300	-1.30049800	2.25376000
C	-0.89309900	-2.12066700	0.40078900
C	-2.65754300	-2.61661100	2.48872100
C	-1.35776100	-3.41758500	0.64983900
C	-2.20641500	-3.68685100	1.72200700
H	-3.38487100	-2.78821900	3.27880300
H	-1.06849800	-4.22667400	-0.01902800
H	-2.54729800	-4.69862200	1.93052200
C	-2.98367500	-0.22975700	3.02543500
H	-3.44205400	-0.69712400	3.90374900
H	-2.33208400	0.55143700	3.40810200
C	-4.09955500	0.40773000	2.17863900
H	-4.64346900	1.16377400	2.75611400
H	-3.70354900	0.89268400	1.28047500
H	-4.81778200	-0.35306600	1.85410200
N	-1.76062200	-1.46106000	-2.25223300
C	-2.80097100	-1.45627900	-2.75884000
C	-4.10643900	-1.44566200	-3.39323800
H	-4.07497800	-0.83051500	-4.29701800
H	-4.39468400	-2.46664500	-3.65909100
H	-4.84422700	-1.03253000	-2.69927500
C	-0.72588200	0.43767600	1.19635900
C	1.01828600	2.18872600	1.13971100
C	-0.07190600	0.84443300	2.57273600
C	0.19698200	1.31002600	0.12509800
C	1.38076500	1.15468900	2.21675800
H	1.94592200	1.59180100	3.04691000

H	1.92146200	0.28133600	1.85693000
C	0.12518000	3.16643500	1.93427400
H	0.75249200	3.91786600	2.42319300
H	-0.57975900	3.70575600	1.29723000
C	-0.58036300	2.24939000	2.97163500
H	-0.27019100	2.49224400	3.99339200
H	-1.66781300	2.34130100	2.92462100
H	1.85426200	2.68850000	0.65162800
H	-0.20751300	0.08199700	3.33930000
C	-0.76637900	2.14555300	-0.72072200
O	-1.93945500	1.89170600	-0.92343900
O	-0.14166400	3.21004300	-1.25852600
C	-0.93028400	4.07499500	-2.11749000
H	-0.19129200	4.57223800	-2.74868800
H	-1.57787900	3.45521700	-2.74138500
H	-1.65197100	1.00432900	1.12460700
C	-1.73075200	5.07570400	-1.30489500
H	-2.26339600	5.75190100	-1.98200100
H	-2.46688500	4.56800100	-0.67647300
H	-1.07302700	5.67571800	-0.66866100
O	1.88989300	-1.33864100	-0.35554000
O	3.47261300	0.26312100	-0.14514000
C	4.82844300	-1.63768200	-0.92311200
C	4.24693800	-1.37770200	1.53985400
C	5.75843400	0.28759800	0.40958700
C	4.58776500	-0.67140900	0.23221800
C	2.26580700	-0.15095800	-0.43315100
C	1.30524200	0.86660700	-0.97230900
C	0.82302400	0.24064000	-2.31705500
H	4.00031900	-2.33713500	-1.04418000
H	5.73829200	-2.20948000	-0.71815300
H	4.97288900	-1.08782400	-1.85793000
H	4.04843600	-0.65111200	2.33241400
H	5.10729000	-1.98266800	1.84148900
H	3.38340200	-2.03460300	1.43007800
H	5.96928900	0.82010400	-0.52224600
H	6.64974600	-0.27657000	0.69703800
H	5.54282400	1.01950900	1.19325600
H	1.84168200	1.79992400	-1.15632200
H	1.69851500	0.06006700	-2.95392900
H	0.14686600	0.91911600	-2.84564400

11b4

Pd	-0.13590300	-0.70779700	-0.74371600
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C	2.52767900	-1.06562000	0.42991100
C	3.57392800	-1.71689700	1.11464600
C	1.28970300	-1.71407800	0.23436400
C	3.36990800	-3.02546500	1.57149400
C	1.10828800	-3.02070800	0.70999500
C	2.15164800	-3.67558800	1.37111900
H	4.17552600	-3.53328700	2.09718400
H	0.16238200	-3.53227900	0.56844200
H	2.01143300	-4.69153300	1.73266900
C	4.87192700	-1.00865900	1.44308800
H	5.67877800	-1.74737200	1.51255000
H	5.14715400	-0.31647800	0.64252500
C	4.78266800	-0.23771300	2.77054400
H	5.72289000	0.28058800	2.98899700
H	3.98236700	0.50921800	2.74005600
H	4.56898000	-0.91970800	3.60062400
N	-1.54116200	-2.35985000	-0.82931800
C	-2.47298400	-3.04554400	-0.83898100
C	-3.66059800	-3.87760000	-0.84773700
H	-3.88800400	-4.20361800	0.17095000
H	-4.49702800	-3.29182200	-1.23817600
H	-3.49870800	-4.75370100	-1.48161900
C	2.63283700	0.33224500	-0.09421500
C	1.51729100	1.49914200	-1.91781900
C	3.48764100	0.52294800	-1.38969100
C	1.23291500	0.87456200	-0.53643300
C	2.44798000	0.42944800	-2.52336100
H	2.86175800	0.71433600	-3.49713000
H	1.96971300	-0.55092800	-2.60341000
C	2.49279700	2.69989100	-1.75741700
H	2.53083100	3.28294300	-2.68369000
H	2.17592900	3.37790300	-0.96095800
C	3.86443900	2.01690100	-1.46200400
H	4.57693300	2.19731700	-2.27387900
H	4.32199500	2.37070700	-0.53247000
H	0.62462500	1.75068600	-2.48913700
H	4.33732000	-0.16005500	-1.45724100
C	0.61492400	1.74315800	0.50184400
O	0.78053500	1.63900000	1.71085400
O	-0.18188100	2.71230600	-0.03098900
C	-0.87094500	3.57873500	0.89893100
H	-1.77401400	3.89254900	0.37048100
H	-1.15424700	3.00068600	1.77858000
H	3.04755500	0.97885300	0.68683700

C	-0.00468100	4.76780800	1.27417800
H	-0.56118600	5.43809300	1.93833000
H	0.89749200	4.43657500	1.79581800
H	0.28992600	5.33345000	0.38451200
O	-4.01528200	-0.45909000	-1.13733500
O	-3.07678200	0.91639100	0.42273000
C	-3.85081200	-0.94001400	1.83467400
C	-5.41805700	0.95038000	1.17084400
C	-3.45907100	1.38946600	2.68951500
C	-3.98788800	0.55136700	1.52902700
C	-3.15751800	0.33210900	-0.78084800
C	-2.02332800	0.78810900	-1.63548600
C	-1.63037200	0.08207200	-2.71850200
H	-4.26310700	-1.55199700	1.03271800
H	-4.38959800	-1.16711300	2.75964200
H	-2.79792200	-1.20194600	1.97771300
H	-5.46052000	2.00952000	0.89811000
H	-6.06412500	0.79518200	2.04054000
H	-5.79927700	0.35434700	0.34100700
H	-2.41834700	1.13211000	2.90638800
H	-4.05841300	1.19956200	3.58445900
H	-3.51477000	2.45613900	2.45473900
H	-1.54950400	1.72318800	-1.36160500
H	-2.14011100	-0.83245900	-3.00356700
H	-0.84969500	0.44637200	-3.37697500

TS4b4

Pd	1.57670900	0.90891600	0.54079300
C	1.42355500	-1.55759900	-0.87768100
C	1.59809800	-2.55242600	-1.87043400
C	2.21858800	-0.39028500	-0.89351600
C	2.55006500	-2.33736300	-2.87895500
C	3.16393600	-0.21637900	-1.91081400
C	3.32960600	-1.18184000	-2.90822500
H	2.68197100	-3.09900500	-3.64442500
H	3.77973200	0.68174300	-1.93145800
H	4.06397200	-1.04119300	-3.69860900
C	0.79626500	-3.84067500	-1.91360500
H	1.37981600	-4.59403400	-2.45500500
H	0.64717000	-4.23860600	-0.90480700
C	-0.56546700	-3.67607600	-2.60745500
H	-1.11401400	-4.62476100	-2.62285300
H	-1.18256300	-2.92839500	-2.10075100
H	-0.42978700	-3.34740700	-3.64401500

N	3.23431200	2.07670500	0.59686000
C	4.19377800	2.72428600	0.58382800
C	5.39694400	3.53627000	0.56837400
H	5.19857300	4.47256800	0.03879400
H	5.70264400	3.75948900	1.59448600
H	6.19991400	2.99563100	0.05955500
C	0.48345200	-1.81553100	0.28042200
C	-0.36796200	-1.14912000	2.46782400
C	1.20421400	-2.45951200	1.51865800
C	-0.49190400	-0.71235900	0.98207300
C	1.14942800	-1.36831400	2.59603400
H	1.44544200	-1.72889800	3.58649000
H	1.74343800	-0.47581800	2.35693200
C	-0.89493700	-2.59935400	2.68079200
H	-1.04159100	-2.76889400	3.75159000
H	-1.85531900	-2.77111800	2.19391700
C	0.24115100	-3.50230600	2.11428900
H	0.73001900	-4.07271400	2.91095200
H	-0.11757300	-4.21381500	1.36469400
H	-0.80974400	-0.43927200	3.16636800
H	2.19498700	-2.84130600	1.26632700
C	-1.84806300	-0.88047000	0.32305400
O	-2.00746300	-1.02593400	-0.87718100
O	-2.86338500	-0.81095000	1.19985500
C	-4.20853500	-0.92367900	0.66278100
H	-4.83322400	-0.40149300	1.38967500
H	-4.24829600	-0.39814600	-0.29135600
H	-0.24329500	-2.54509100	-0.07369400
C	-4.61268700	-2.37862500	0.51784000
H	-5.64474300	-2.43590800	0.15612700
H	-3.96792000	-2.89159900	-0.20089700
H	-4.55678300	-2.89879100	1.47890600
O	-0.49196200	2.11975000	-1.01450400
O	-2.54877100	2.04410300	-0.04546800
C	-3.14108800	1.89009500	-2.43263800
C	-2.72456000	4.13946900	-1.31982500
C	-4.70730100	2.74546800	-0.65766500
C	-3.26551900	2.72027200	-1.15677300
C	-1.23382200	1.82068100	-0.09174200
C	-0.75288200	1.18815700	1.19466600
C	0.33056500	1.98116500	1.82280700
H	-2.12150600	1.90380700	-2.81867600
H	-3.81049800	2.30440500	-3.19297400
H	-3.42883400	0.85315300	-2.24168800

H	-2.77451700	4.67821100	-0.36831700
H	-3.34084200	4.67543300	-2.04810800
H	-1.69287800	4.13539800	-1.67301900
H	-5.09236300	1.73120600	-0.52317000
H	-5.33840200	3.26129200	-1.38683900
H	-4.77599600	3.27572800	0.29684500
H	-1.58574800	0.96892800	1.85495700
H	0.34783200	3.03254100	1.53369600
H	0.42526700	1.84024000	2.89958900

12b4

Pd	1.83638900	-0.66426600	-1.06398200
C	0.87183700	-0.29480000	1.56844700
C	0.61188600	-0.55668000	2.94499600
C	1.87169700	-1.07735900	0.92634600
C	1.29892200	-1.59627500	3.59708100
C	2.54792900	-2.08761200	1.61169900
C	2.25792300	-2.36532800	2.94974700
H	1.07638200	-1.78336300	4.64515500
H	3.30650100	-2.67451700	1.09643400
H	2.77826700	-3.15901600	3.48143900
C	-0.37286100	0.20649100	3.82087700
H	0.01966700	0.19835200	4.84414500
H	-0.43885000	1.25947100	3.53799500
C	-1.77848900	-0.41305600	3.83006700
H	-2.42748600	0.10776300	4.54393400
H	-2.23778900	-0.34626200	2.84225600
H	-1.73312900	-1.46781700	4.12340800
N	3.63267900	0.19996500	-1.13618000
C	4.67847000	0.69682000	-1.14890400
C	5.98689000	1.32472400	-1.17104100
H	6.55614400	0.95645200	-2.02943200
H	5.86932600	2.40901500	-1.25571800
H	6.52756400	1.08982200	-0.24973100
C	0.16911200	0.95646500	0.96172900
C	-0.15827300	2.67415200	-0.77519800
C	1.08766100	2.23070100	1.04917800
C	-0.62610100	1.21480500	-0.44674000
C	1.33210200	2.62908700	-0.41226100
H	1.81396600	3.60882300	-0.50857700
H	1.89742200	1.89645500	-0.97965400
C	-0.68898600	3.67867700	0.28087300
H	-0.56074000	4.69847000	-0.09415800
H	-1.75201800	3.55408300	0.49878500

C	0.21614600	3.41375700	1.52352500
H	0.83923900	4.28552000	1.74963900
H	-0.36228200	3.17855500	2.42133000
H	-0.40278900	2.95367000	-1.80095000
H	1.97744200	2.05788200	1.65711800
C	-2.13737700	1.20735000	-0.13560700
O	-2.66453800	0.71961300	0.84696800
O	-2.84162300	1.80831500	-1.11091800
C	-4.28741500	1.81616500	-0.97518000
H	-4.65029500	1.93367500	-1.99808400
H	-4.60708000	0.84585900	-0.58968000
H	-0.64464600	1.12329300	1.65616700
C	-4.75413700	2.95305400	-0.08570400
H	-5.84899600	2.97337700	-0.06651900
H	-4.39449800	2.82166200	0.93784300
H	-4.40013600	3.91587000	-0.46655300
O	0.05570200	-1.84128600	-1.08040400
O	-2.13306300	-1.40737700	-1.42525900
C	-2.20452700	-2.84363200	0.57969800
C	-2.12964700	-3.84478400	-1.76342100
C	-4.14533500	-2.53983000	-0.99123700
C	-2.63551900	-2.71149900	-0.87830000
C	-0.86791200	-1.07586400	-1.41638300
C	-0.54200600	0.34130000	-1.79466200
C	0.77075300	0.28373500	-2.63394800
H	-1.13006800	-3.00100300	0.67608400
H	-2.72280300	-3.70114400	1.01919400
H	-2.48291000	-1.94653300	1.13727200
H	-2.40205700	-3.66695600	-2.80810500
H	-2.59792000	-4.78004700	-1.44229100
H	-1.04695600	-3.95663200	-1.69007200
H	-4.48173400	-1.69704300	-0.38082000
H	-4.64250800	-3.44698100	-0.63718400
H	-4.43991300	-2.36436800	-2.02990300
H	-1.36159200	0.73906000	-2.39866800
H	0.55418200	-0.30054900	-3.53785600
H	1.08217800	1.28409100	-2.94497900

TS10

Pd	0.11197500	0.39136200	-0.82699600
C	3.03297600	2.72169800	1.38387000
C	3.60741800	1.72707200	2.16649400
C	2.99881800	0.47690800	2.21954400
C	1.78621700	0.24912800	1.55884500

C	1.15093900	1.29088200	0.83698600
C	1.82366700	2.53272300	0.69211700
H	3.53766400	3.67824100	1.28036700
H	3.46459300	-0.34323400	2.75759400
C	-0.85862200	1.34274100	1.12714900
C	-2.66436700	1.73257600	-0.39994300
C	-1.36711700	2.77738600	1.13715800
C	-1.69032000	0.67597600	0.12472400
C	-1.80928800	3.00212100	-0.32765600
H	-2.39188400	3.91987700	-0.44920100
H	-0.99752600	2.98647000	-1.05257400
C	-3.65925800	1.98499000	0.77006500
H	-4.45658900	2.65533500	0.43557600
H	-4.12930000	1.06641400	1.13000800
C	-2.75855200	2.66856800	1.84160200
H	-3.11575800	3.67272800	2.08592800
H	-2.70078200	2.10003600	2.77410500
H	-3.12330500	1.48705500	-1.35511900
H	-0.70348200	3.50705100	1.59694300
C	-2.25270500	-0.67641700	0.43766000
O	-1.92888300	-1.36733100	1.38929500
O	-3.21049500	-1.01950700	-0.43829700
C	-3.83340800	-2.31204200	-0.24806500
H	-4.18933600	-2.59074800	-1.24194000
H	-3.07262700	-3.02636600	0.07476400
H	-0.72487700	0.84453800	2.07750500
C	1.43824200	3.65016500	-0.25867900
H	0.40675000	3.96360500	-0.12690700
H	2.05293700	4.52146800	-0.01210900
C	1.67531900	3.28537400	-1.73232500
H	2.71619600	2.98823200	-1.89989400
H	1.03656400	2.44935200	-2.04013900
H	1.45310200	4.14091700	-2.37954300
H	4.53724500	1.91093100	2.69623700
C	-4.97585100	-2.22891200	0.74830400
H	-5.46923600	-3.20370100	0.82539700
H	-4.60793000	-1.94961000	1.73916800
H	-5.71916500	-1.49294700	0.42612300
C	1.32655200	-1.17834800	1.53254500
C	0.68028000	-1.76698500	2.63173500
C	1.71484600	-1.99685800	0.44360600
C	0.39870400	-3.13969700	2.60051000
C	1.43813800	-3.36865900	0.44232200
C	0.76082900	-3.93594700	1.51869400

H	-0.11536900	-3.58557900	3.44772200
H	1.75177900	-3.97869200	-0.39737600
H	0.53205900	-4.99711600	1.51867700
C	2.46764200	-1.44036300	-0.71783400
O	2.21567400	-0.39258800	-1.31778200
O	3.47882100	-2.22313400	-1.08379100
C	4.22159900	-1.81477700	-2.25700100
H	4.96938800	-2.59218700	-2.40719400
H	3.55641200	-1.74739100	-3.12021800
H	4.70216700	-0.85017700	-2.08150900
C	0.23635700	-0.95872700	3.82281300
H	0.38390000	-1.51677400	4.75235800
H	0.77143200	-0.01051100	3.90194700
H	-0.83381700	-0.73997100	3.73517700
Br	-0.81278100	-0.65865300	-2.90334000

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Pd	0.11829600	0.56497500	-0.57376400
C	2.97042400	2.43766600	2.07916500
C	3.46122500	1.35021200	2.80129400
C	2.98950300	0.07030300	2.52117700
C	1.98518900	-0.12051700	1.55630000
C	1.44719500	0.99328600	0.89683400
C	1.97356300	2.27713100	1.10375500
H	3.37397200	3.43232400	2.25517800
H	3.40891300	-0.79311400	3.02921100
C	-1.18247000	1.30334400	1.17469100
C	-2.90963400	1.67282300	-0.36454500
C	-1.60457800	2.75645000	1.13782600
C	-1.97985500	0.63500100	0.24576600
C	-2.02591600	2.93241500	-0.33679100
H	-2.59463600	3.85138500	-0.50427600
H	-1.19430300	2.87983100	-1.04401800
C	-3.90854400	2.00350100	0.79193800
H	-4.69676400	2.66089700	0.41425000
H	-4.38514000	1.10566900	1.19256700
C	-3.01018000	2.73655600	1.83292200
H	-3.34549200	3.76370200	2.00174300
H	-2.97963600	2.23038100	2.80162100
H	-3.36089600	1.38980000	-1.31102800
H	-0.90325700	3.47115100	1.56427900
C	-2.35720700	-0.79831700	0.41369200
O	-1.75506300	-1.59566300	1.11099300
O	-3.48378000	-1.08157300	-0.25582600

C	-3.96983900	-2.44492000	-0.15778900
H	-4.57858500	-2.57826400	-1.05404700
H	-3.11499600	-3.12375900	-0.19819300
H	-0.77219600	0.83019000	2.05637200
C	1.61379200	3.44891700	0.21929900
H	0.57866800	3.36805500	-0.10866300
H	1.71048400	4.38353600	0.78351500
C	2.51763100	3.50436500	-1.02348400
H	3.56958000	3.62046200	-0.74042500
H	2.42692600	2.58188900	-1.60587300
H	2.24311600	4.34678500	-1.66818600
H	4.23054200	1.49517300	3.55411600
C	-4.78556100	-2.64811500	1.10554300
H	-5.19168800	-3.66503600	1.11936900
H	-4.16527000	-2.51223900	1.99516500
H	-5.62223200	-1.94355800	1.14551100
C	1.60383600	-1.51810500	1.18968600
C	1.03515200	-2.38490900	2.14243600
C	1.90167500	-2.02424900	-0.09717500
C	0.79656300	-3.71970300	1.79512300
C	1.68231700	-3.37118400	-0.41496400
C	1.12080800	-4.21801800	0.53471600
H	0.33925700	-4.37661200	2.52984100
H	1.93337400	-3.73691900	-1.40445800
H	0.92960500	-5.25837400	0.29125900
C	2.44040600	-1.15433800	-1.17324200
O	1.99023900	-0.04634900	-1.50147200
O	3.46324300	-1.68688700	-1.82107100
C	3.97853900	-0.94458700	-2.95587200
H	4.78974700	-1.55465700	-3.34954300
H	3.19377100	-0.81370700	-3.70324900
H	4.35077600	0.02780800	-2.62858300
C	0.64215500	-1.89090600	3.51139800
H	-0.08808500	-2.56738300	3.96312500
H	1.50260000	-1.83098800	4.18695400
H	0.20181700	-0.89194000	3.45841800
Br	-1.07159500	-0.16577600	-2.74480100

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Pd	-0.04363400	-0.01363100	-0.10712800
C	2.01298900	3.66011100	-1.01069900
C	3.31050100	3.38075600	-0.58127200
C	3.58443000	2.16926400	0.04816900
C	2.55620700	1.23565100	0.25763600

C	1.25843500	1.54207400	-0.16754100
C	0.96128000	2.75019300	-0.81470200
H	1.80031600	4.60117600	-1.51234200
H	4.59330800	1.93049900	0.37185600
C	-0.41804100	3.07478200	-1.34325100
H	-1.17398400	2.85773000	-0.58398300
H	-0.46622600	4.14823000	-1.55727900
C	-0.77619900	2.29055000	-2.61533000
H	-0.03605200	2.45488600	-3.40644300
H	-0.81999200	1.21491200	-2.41300900
H	-1.75651800	2.59981300	-2.99434000
H	4.10599900	4.10211200	-0.74323500
C	2.88383300	-0.07622800	0.89485100
C	3.29918000	-0.12739500	2.24034400
C	2.84691100	-1.27563100	0.14712500
C	3.65592300	-1.36399200	2.79592900
C	3.24611200	-2.49421100	0.70965100
C	3.63928900	-2.53724700	2.04344000
H	3.95502400	-1.40031500	3.83971200
H	3.21987200	-3.39691600	0.10954800
H	3.92721500	-3.48079400	2.49589800
C	2.34960800	-1.28857100	-1.25050200
O	1.32756600	-0.71028700	-1.64920500
O	3.08441000	-2.01658300	-2.07246900
C	2.59302100	-2.16851200	-3.42961000
H	3.29911700	-2.84119600	-3.91346100
H	1.59041500	-2.59931100	-3.41597000
H	2.57866200	-1.19925900	-3.93118000
C	3.35600700	1.11727800	3.09132200
H	4.26081400	1.70048700	2.88670400
H	2.50344900	1.77436600	2.90023200
H	3.36400800	0.85417100	4.15228700
Br	-1.38972100	-2.16178100	-0.56428900
O	-2.95280200	1.83538800	0.39792400
O	-3.71343200	-0.16468900	1.17287000
C	-4.86000400	-0.04500000	-0.99076700
C	-5.83019800	1.08665200	1.07467700
C	-5.67479800	-1.42408200	0.94666800
C	-5.04253400	-0.10070300	0.52545500
C	-2.78288500	0.76284900	0.95672500
C	-1.47949300	0.31487800	1.54275900
C	-0.44232300	1.20421100	1.75546800
H	-4.45126400	0.91484600	-1.30953700
H	-5.83073900	-0.18889900	-1.47513000

H	-4.18135300	-0.84135500	-1.31013800
H	-5.88525400	1.03621100	2.16676000
H	-6.85070100	1.05624400	0.67990400
H	-5.37071600	2.03270600	0.78645200
H	-5.07190500	-2.26391500	0.58964300
H	-6.68001100	-1.50753100	0.52389400
H	-5.75093600	-1.48673900	2.03651600
H	-1.49067900	-0.65015500	2.03496500
H	-0.55861800	2.24984300	1.50073500
H	0.37471300	0.94080400	2.41670300

TS11

Pd	-0.09667700	-0.08486300	-0.30276400
C	2.01310200	3.51998900	-1.22506500
C	3.30728700	3.18281200	-0.83549800
C	3.52201700	2.04275100	-0.06196100
C	2.44124700	1.24878200	0.33873600
C	1.13418900	1.61060800	-0.04447300
C	0.90422800	2.74970800	-0.84186600
H	1.84519400	4.39916500	-1.84179000
H	4.52797900	1.75180100	0.22537000
C	-0.46181700	3.13757000	-1.35841400
H	-1.23198900	2.93494900	-0.61190100
H	-0.46516000	4.21506800	-1.55646500
C	-0.83840400	2.38869700	-2.64706700
H	-0.09006700	2.54278700	-3.43232200
H	-0.91365800	1.31176900	-2.45847100
H	-1.80697400	2.73531800	-3.02374700
H	4.14728300	3.80024900	-1.13932700
C	2.72300100	-0.01089500	1.09369100
C	3.03567900	0.03580600	2.46559000
C	2.76168500	-1.25276600	0.41984900
C	3.31116700	-1.16251000	3.13944500
C	3.08106200	-2.43147200	1.10462400
C	3.32922200	-2.38630200	2.47337300
H	3.52604900	-1.12651300	4.20379600
H	3.11536400	-3.37219800	0.56676800
H	3.54976200	-3.29995600	3.01618500
C	2.49326100	-1.34154600	-1.04287200
O	1.57976100	-0.77196200	-1.64780700
O	3.35125700	-2.13430400	-1.67157800
C	3.11744300	-2.35204900	-3.08495000
H	3.88934000	-3.05369200	-3.39712500
H	2.12322600	-2.77529700	-3.23966500

H	3.21124200	-1.41065300	-3.62962100
C	3.11798400	1.34605700	3.20972000
H	4.10286800	1.80777800	3.07007900
H	2.37765500	2.06970100	2.86096700
H	2.97564000	1.19047100	4.28231200
Br	-1.43415000	-2.12868200	-0.90851700
O	-2.95313500	1.86182500	0.34683500
O	-3.52185000	-0.17272400	1.19397300
C	-4.94003500	-0.07301100	-0.81128700
C	-5.68398600	0.97902700	1.38367000
C	-5.43695400	-1.51914500	1.18220000
C	-4.91884400	-0.16155500	0.71463400
C	-2.66357200	0.80173400	0.88397800
C	-1.28787500	0.42097400	1.31980000
C	-0.28394900	1.42144400	1.48205300
H	-4.61671400	0.90877300	-1.15947100
H	-5.95999100	-0.25142500	-1.16620000
H	-4.27899500	-0.83376800	-1.23643200
H	-5.59566600	0.91062500	2.47267300
H	-6.74446900	0.90742000	1.12204600
H	-5.30725700	1.94949600	1.05866400
H	-4.84910000	-2.32468300	0.73303400
H	-6.48330200	-1.64014400	0.88767300
H	-5.37122000	-1.60409400	2.27131000
H	-1.23682200	-0.46467800	1.94656100
H	-0.57134700	2.45497600	1.33734900
H	0.46242500	1.24342600	2.24414300
19			
Pd	-0.02946900	-0.13411100	-0.54253000
C	1.53499500	3.15269800	-1.80641100
C	2.83230700	2.67023800	-1.67648000
C	3.13082100	1.76832100	-0.66045500
C	2.15134800	1.36835500	0.25364800
C	0.82655200	1.91121600	0.17683100
C	0.52433200	2.79251500	-0.90710500
H	1.29148400	3.83782400	-2.61337000
H	4.12822900	1.34837600	-0.57635200
C	-0.85296800	3.35568000	-1.17179600
H	-1.48133300	3.31987900	-0.28472000
H	-0.74307800	4.40499300	-1.46821400
C	-1.57073500	2.58931200	-2.29530600
H	-0.98984900	2.61148200	-3.22370200
H	-1.71399600	1.54316900	-2.00650700
H	-2.55324900	3.02968700	-2.49464800

H	3.60451500	2.98000900	-2.37419500
C	2.54352500	0.28386300	1.20906100
C	2.73879200	0.52847900	2.57974200
C	2.83018000	-1.00642500	0.68803100
C	3.10869500	-0.53721800	3.41477200
C	3.22587100	-2.04237900	1.54117300
C	3.33274000	-1.81391800	2.91121200
H	3.24014800	-0.34533100	4.47633800
H	3.43740300	-3.02236700	1.12980100
H	3.61705300	-2.62307500	3.57623600
C	2.75190700	-1.31173800	-0.77560800
O	1.91098000	-0.90466300	-1.57910800
O	3.73262600	-2.12869500	-1.15687900
C	3.71009800	-2.56320200	-2.53641000
H	4.55948200	-3.23724800	-2.63796800
H	2.77582100	-3.08535400	-2.75274800
H	3.81908200	-1.70595200	-3.20376300
C	2.62050300	1.90861300	3.17979900
H	3.53647200	2.15553800	3.72702200
H	2.46546400	2.67755000	2.42123300
H	1.79533900	1.96263400	3.89856800
Br	-1.33624800	-2.18050400	-1.00963800
O	-3.01920100	1.77428900	0.45796000
O	-3.22877700	-0.37461400	1.16595800
C	-4.83181300	-0.31902100	-0.69467500
C	-5.49617600	0.44227700	1.64069500
C	-4.93567300	-1.97228600	1.19137300
C	-4.64955700	-0.52161600	0.81006600
C	-2.52838500	0.72228900	0.84715100
C	-1.07233800	0.49176100	1.07513100
C	-0.20004900	1.71085000	1.32853900
H	-4.66920200	0.72071600	-0.98158900
H	-5.85067300	-0.60336200	-0.97647300
H	-4.12413500	-0.95155800	-1.23829200
H	-5.30556100	0.29401300	2.70860900
H	-6.55768500	0.24984400	1.45385000
H	-5.27584900	1.47895600	1.38344300
H	-4.28559300	-2.64373600	0.62366800
H	-5.97929800	-2.21877200	0.97486000
H	-4.75599200	-2.13293200	2.25901900
H	-0.91362100	-0.33064300	1.77308200
H	-0.80446900	2.61380400	1.41836500
H	0.34248600	1.57606800	2.26079800

21

Pd	0.19276400	-0.83487300	-0.05527300
C	3.94452400	-1.44329200	-2.03949600
C	4.57792500	-0.21146700	-1.87140100
C	3.89655400	0.84205500	-1.26591300
C	2.57184500	0.66967200	-0.83307300
C	1.95407900	-0.57141000	-1.01801600
C	2.62206700	-1.64889700	-1.61644200
H	4.47813200	-2.26830600	-2.50535600
H	4.38422200	1.80087100	-1.11668500
C	1.99111800	-3.01684600	-1.75689400
H	0.95229600	-2.92163000	-2.09198100
H	2.52755200	-3.57713000	-2.53022600
C	2.01130700	-3.81393200	-0.44346900
H	3.03522200	-3.93416000	-0.07309900
H	1.42991000	-3.30047300	0.32963600
H	1.57978400	-4.81042600	-0.58783500
H	5.60172400	-0.07507200	-2.20688100
C	1.85922800	1.79949400	-0.16419800
C	1.53586700	2.96183800	-0.89265300
C	1.54170100	1.74745700	1.21210800
C	0.90330700	4.02440000	-0.23320300
C	0.94487900	2.83616100	1.86016200
C	0.61343000	3.97213000	1.12914200
H	0.63539400	4.90845800	-0.80498600
H	0.72353600	2.77430200	2.91977300
H	0.12772600	4.81096100	1.61730800
C	1.80094900	0.52609200	2.01409700
O	1.54181400	-0.63323000	1.65987000
O	2.32100300	0.77355700	3.20433400
C	2.48722000	-0.36131700	4.09310000
H	2.85073600	0.06097300	5.02838500
H	1.52929200	-0.86393000	4.23766300
H	3.21681000	-1.05805000	3.67621800
C	1.84139800	3.07500600	-2.36582600
H	2.89969600	3.29871000	-2.54036900
H	1.62086400	2.14367300	-2.89460700
H	1.25344400	3.87883500	-2.81636800
Br	-1.63530500	-1.42795800	1.65917600
O	-2.18741400	1.38152100	-0.91479100
O	-3.63167900	-0.37897800	-1.01567300
C	-5.16628000	1.43436000	-1.62850800
C	-4.60752100	0.96479400	0.80696000
C	-5.90366100	-0.71384100	-0.54369600

C	-4.83135000	0.37152200	-0.58316500
C	-2.43438700	0.20096200	-1.09627800
C	-1.41480000	-0.80140700	-1.55553500
C	-0.28205600	-0.34305400	-2.20687300
H	-4.39004300	2.19936600	-1.67486500
H	-6.11468200	1.91371200	-1.36635300
H	-5.27602000	0.97763600	-2.61722600
H	-4.22337300	0.19811300	1.48445400
H	-5.56180200	1.33808300	1.19210300
H	-3.89376400	1.78832600	0.77710200
H	-6.01789700	-1.18146400	-1.52637100
H	-6.86325100	-0.27578300	-0.25474500
H	-5.64140900	-1.48835700	0.18306600
H	-1.75043000	-1.82599900	-1.67116300
H	-0.11776900	0.72345300	-2.31173400
H	0.27879100	-0.99783500	-2.85898300

TS14

Pd	0.07075500	-0.83993100	0.12627700
C	3.66870000	-1.93789900	-1.86263400
C	4.46628800	-0.81498700	-1.64625100
C	3.89073400	0.36535100	-1.17743300
C	2.51342000	0.43129000	-0.93169200
C	1.71990900	-0.70768900	-1.15942100
C	2.28640200	-1.90841900	-1.62947000
H	4.11723700	-2.86059400	-2.22182500
H	4.50455100	1.24064300	-0.98698800
C	1.47817700	-3.16970800	-1.83681600
H	0.47541900	-2.92608100	-2.20145500
H	1.96346000	-3.77365800	-2.61093900
C	1.34541600	-4.00489100	-0.55376900
H	2.32972000	-4.26759000	-0.15147900
H	0.80296800	-3.44347900	0.21515000
H	0.79681000	-4.93207700	-0.75197000
H	5.53378900	-0.85924500	-1.83991800
C	1.93720500	1.69229500	-0.37315800
C	1.72882200	2.80428000	-1.21149300
C	1.65829800	1.80767500	1.00666800
C	1.19624000	3.97792600	-0.66148600
C	1.16258800	3.00393500	1.54116900
C	0.90938300	4.08143100	0.69850100
H	1.01130100	4.82504200	-1.31594800
H	0.96325800	3.07462300	2.60446400
H	0.49931700	5.00200900	1.10139900

C	1.89785100	0.67144100	1.93791900
O	1.61816200	-0.51258100	1.72417900
O	2.44957500	1.05517800	3.08187400
C	2.62324100	0.03303900	4.09399800
H	3.01674400	0.55681800	4.96381400
H	1.66364500	-0.43406200	4.32292700
H	3.33217600	-0.72134900	3.74742100
C	2.08782600	2.75770900	-2.67632200
H	3.16942400	2.86720600	-2.81722500
H	1.80235700	1.80947400	-3.13911800
H	1.59777800	3.57049000	-3.21827900
Br	-1.65878300	-1.27126700	1.91008800
O	-2.05771800	1.47735100	-1.00019100
O	-3.50740100	-0.28087800	-0.99851600
C	-5.02459200	1.50103400	-1.73405200
C	-4.48246400	1.18127500	0.73013500
C	-5.78388700	-0.56821800	-0.52067600
C	-4.70153200	0.50362400	-0.62203500
C	-2.30272000	0.28532400	-1.10697000
C	-1.27800100	-0.74954600	-1.45620900
C	-0.10107500	-0.30395800	-2.12633900
H	-4.24315400	2.25668500	-1.82500300
H	-5.97152300	2.00166800	-1.50854500
H	-5.13171200	0.98349800	-2.69278700
H	-4.10119500	0.45593800	1.45357400
H	-5.43715400	1.57903700	1.08905600
H	-3.76686900	2.00018800	0.65298000
H	-5.89622000	-1.09606300	-1.47262700
H	-6.74155900	-0.10536700	-0.26582600
H	-5.53188900	-1.29731300	0.25495300
H	-1.66344500	-1.74154500	-1.67279000
H	0.02235500	0.76712800	-2.23143900
H	0.28675300	-0.90727800	-2.93514800

22

Pd	0.05929400	-0.65744500	0.56697600
C	2.64771300	-3.10858600	-0.89796600
C	3.68453200	-2.23601300	-0.57388700
C	3.47898800	-0.86379000	-0.64488400
C	2.24586600	-0.34225000	-1.06161300
C	1.18717300	-1.22762600	-1.43212400
C	1.40349800	-2.63431100	-1.31996200
H	2.80487000	-4.18162200	-0.83431100
H	4.27399900	-0.17633100	-0.37361900

C	0.33189900	-3.65684200	-1.62999000
H	-0.46196600	-3.22580700	-2.24205700
H	0.78474900	-4.45931400	-2.22325400
C	-0.27590500	-4.26745300	-0.35578400
H	0.49370500	-4.76424500	0.24383500
H	-0.73481500	-3.49201100	0.26556700
H	-1.04085100	-5.00834700	-0.61074400
H	4.64799200	-2.62585500	-0.25960300
C	2.10034600	1.14705500	-1.03269400
C	1.99172700	1.90034800	-2.21640800
C	2.17948500	1.82322000	0.21183900
C	1.87727600	3.29561700	-2.12601300
C	2.08837000	3.21832600	0.26974900
C	1.90767200	3.95210300	-0.90004500
H	1.77909000	3.87027600	-3.04300900
H	2.14716000	3.71916000	1.22908100
H	1.81576900	5.03254300	-0.85500700
C	2.37619000	1.09391200	1.50196400
O	1.84140500	0.03836300	1.84854600
O	3.22070500	1.73568400	2.30553200
C	3.42651900	1.16214600	3.61798700
H	4.12092600	1.83531300	4.11863400
H	2.48038600	1.11123400	4.16063600
H	3.85768700	0.16311000	3.52848500
C	2.02637900	1.26287700	-3.58435200
H	2.37131300	0.22824600	-3.54763500
H	1.03559400	1.27088800	-4.05236900
H	2.69713100	1.82357900	-4.24266300
Br	-1.64474100	-0.43575000	2.34123800
O	-1.87903600	1.47248600	-1.25038100
O	-3.42437600	-0.08795300	-0.65242200
C	-4.88539700	1.47970000	-1.84048500
C	-4.19445300	1.91768100	0.56561900
C	-5.66978500	-0.03690100	0.01013200
C	-4.53995700	0.86255500	-0.48554100
C	-2.18970700	0.32201500	-0.97006600
C	-1.23188900	-0.82807900	-0.98502700
C	-0.13435000	-0.70836000	-2.03385500
H	-4.06633600	2.09957400	-2.20801000
H	-5.77985900	2.10290300	-1.74072900
H	-5.09509300	0.69598400	-2.57561200
H	-3.81591500	1.43395700	1.46975800
H	-5.09861200	2.48252600	0.81514600
H	-3.43664700	2.61111600	0.20037900

H	-5.87879600	-0.82992400	-0.71440500
H	-6.58059500	0.55189800	0.15230800
H	-5.39920700	-0.49876800	0.96426700
H	-1.73961400	-1.78868100	-0.93652100
H	-0.03350900	0.34187000	-2.29408800
H	-0.37285900	-1.26228300	-2.94844000

18'

Pd	-0.85661700	-0.92325000	-0.30778100
C	1.76792600	0.01288800	2.92213500
C	1.78336800	1.40771100	2.91781500
C	1.07781100	2.10783400	1.94000200
C	0.36682300	1.41271900	0.94882200
C	0.40468600	0.01430400	0.95011400
C	1.07789800	-0.71220900	1.93740100
H	2.29650500	-0.53391900	3.69932900
H	1.05296100	3.19342500	1.95107900
C	0.99829300	-2.22009100	2.02128900
H	0.97073100	-2.64398500	1.01449700
H	1.90282100	-2.60187100	2.50764900
C	-0.24003200	-2.68356700	2.80408600
H	-0.22629500	-2.29713900	3.82914300
H	-1.15675800	-2.32758500	2.32318400
H	-0.28260500	-3.77728000	2.85263300
H	2.32904500	1.94884500	3.68502700
C	-0.47078500	2.16820300	-0.03160700
C	0.12279600	3.04157000	-0.96587000
C	-1.88151900	2.06824400	0.00410800
C	-0.70003900	3.76970000	-1.83614500
C	-2.68564700	2.83459100	-0.84941300
C	-2.08952400	3.67617000	-1.78246800
H	-0.23424900	4.42420800	-2.56746100
H	-3.76485900	2.74843000	-0.79049500
H	-2.70386500	4.25561300	-2.46417700
C	-2.56844500	1.13576600	0.93342600
O	-2.26043000	-0.05057400	1.12093200
O	-3.60465200	1.67408400	1.55262700
C	-4.39577600	0.79315700	2.39192500
H	-5.21194500	1.41106800	2.76226900
H	-4.77640400	-0.04146100	1.80058400
H	-3.78858300	0.42077900	3.21889100
C	1.62072200	3.19102600	-1.05687300
H	2.01157700	3.81125400	-0.24265000
H	2.12108400	2.22323300	-0.99429400

H	1.89887200	3.67007100	-1.99947800
Br	-2.89499200	-2.10524100	-1.37616200
O	2.67655700	-2.20117300	-0.68547000
O	3.07712500	0.03429700	-0.85160500
C	5.26827500	-0.79594500	-1.55273700
C	4.68069900	-0.64059800	0.91361000
C	4.91433100	1.44589900	-0.45953500
C	4.51096900	-0.02561000	-0.47305800
C	2.32921300	-1.06691200	-0.96603000
C	1.01223400	-0.73674700	-1.60290700
C	0.20664400	-1.76530900	-2.05169000
H	4.97318500	-1.84623900	-1.57195100
H	6.34181100	-0.74044700	-1.34882200
H	5.08264900	-0.35527700	-2.53715900
H	4.08810800	-0.09226400	1.64883600
H	5.73476500	-0.57125300	1.20023200
H	4.38161800	-1.68834500	0.92680300
H	4.75041500	1.90515900	-1.43871600
H	5.97554100	1.53234200	-0.20943500
H	4.33588800	1.99553000	0.28845800
H	0.90195100	0.27142000	-1.98722300
H	0.47660500	-2.79340900	-1.83312500
H	-0.52576600	-1.59782200	-2.83029800

TS11'

Pd	-1.08789100	-0.99091900	-0.29820900
C	1.68982900	-0.23173300	2.78669100
C	1.61150200	1.15050700	2.93668200
C	0.94958600	1.91946500	1.97701700
C	0.40191000	1.31422300	0.84254900
C	0.53425400	-0.08208900	0.67474900
C	1.15763200	-0.87649600	1.65996400
H	2.16827900	-0.83432200	3.55421400
H	0.83658000	2.99063500	2.11349000
C	1.18643300	-2.38842500	1.61321800
H	1.15267400	-2.74327900	0.58288600
H	2.13041100	-2.73747100	2.04593600
C	0.01168700	-3.00161500	2.39186500
H	0.00707200	-2.66796900	3.43501800
H	-0.94048600	-2.70757400	1.93701700
H	0.07357700	-4.09525200	2.38206100
H	2.04432200	1.62897700	3.80992600
C	-0.40164900	2.15210200	-0.10171900
C	0.23353000	3.02945400	-1.00366400

C	-1.81374700	2.14165900	-0.03320800
C	-0.55452700	3.80614200	-1.86400000
C	-2.57924400	2.95745800	-0.87656700
C	-1.94646000	3.76727300	-1.81384900
H	-0.06006700	4.46072200	-2.57609000
H	-3.66054100	2.94180500	-0.79944300
H	-2.53502400	4.38037700	-2.48894800
C	-2.54394800	1.31220000	0.96973800
O	-2.33691900	0.12509000	1.23066600
O	-3.50375800	1.99886000	1.58029400
C	-4.33178500	1.26413000	2.51398400
H	-5.06136200	1.98594700	2.87794200
H	-4.82836700	0.43568300	2.00490000
H	-3.72419700	0.88431600	3.33760800
C	1.73497900	3.17019500	-1.03509300
H	2.08668000	3.75545300	-0.17734900
H	2.24042500	2.20473200	-0.98814100
H	2.05245600	3.68895300	-1.94334900
Br	-3.07195000	-2.19526900	-1.28123300
O	2.86407900	-2.11174700	-1.01310700
O	3.21110900	0.11382700	-0.68877400
C	5.41410300	-0.51036300	-1.57001600
C	4.84484500	-0.85577700	0.88377200
C	5.02255300	1.46704000	-0.05877400
C	4.65413100	0.01617700	-0.35505100
C	2.47094200	-0.96071300	-0.96258200
C	1.05088600	-0.55623600	-1.28678300
C	0.16517100	-1.53409100	-1.83507700
H	5.15293000	-1.54763600	-1.78405700
H	6.48905200	-0.45505700	-1.37297500
H	5.19565900	0.10158700	-2.45065600
H	4.23481800	-0.48261400	1.71040800
H	5.89589900	-0.81325600	1.18559000
H	4.58126600	-1.89511700	0.68658500
H	4.85457600	2.09865300	-0.93592500
H	6.07957500	1.52807700	0.21485100
H	4.42453300	1.85323300	0.77169300
H	0.96412800	0.45382300	-1.67027400
H	0.46981000	-2.57627200	-1.78846000
H	-0.41521100	-1.25164800	-2.70940000
19'			
Pd	-1.15543900	-1.07170200	-0.14939000
C	0.91693100	-0.49713200	2.99191300

C	0.23617500	0.67650500	3.30038300
C	-0.22192300	1.49800900	2.27631200
C	0.02456900	1.17916100	0.93531300
C	0.77659700	0.00746800	0.60868800
C	1.19310100	-0.85372100	1.66833300
H	1.25830100	-1.14998200	3.79001100
H	-0.78852300	2.39485400	2.50583600
C	1.93359600	-2.15645300	1.44856500
H	2.33480700	-2.23572200	0.43932900
H	2.79630100	-2.17566400	2.12408300
C	1.04740000	-3.38027300	1.72796800
H	0.67134200	-3.36892100	2.75588900
H	0.18393000	-3.38873700	1.05434200
H	1.61366100	-4.30594600	1.58183700
H	0.04872800	0.94280900	4.33614600
C	-0.61535900	2.06184000	-0.09040700
C	0.13645400	2.91405800	-0.92061900
C	-2.03245500	2.11726600	-0.14645500
C	-0.53598900	3.73331100	-1.84083200
C	-2.67589300	2.96511700	-1.05379000
C	-1.92383900	3.75323400	-1.92236800
H	0.05135500	4.37834600	-2.48876500
H	-3.75900100	2.99356300	-1.08358400
H	-2.42111800	4.39625600	-2.64148800
C	-2.90053700	1.29535400	0.75370900
O	-2.75183600	0.10920800	1.04939400
O	-3.93007800	2.00194500	1.21678100
C	-4.88430800	1.28946500	2.03805700
H	-5.64226600	2.02608300	2.30066500
H	-5.32752700	0.46551300	1.47498700
H	-4.39544200	0.90476700	2.93532400
C	1.64073700	3.00693700	-0.83407600
H	1.94796900	4.05607800	-0.77707800
H	2.03955300	2.48411800	0.03441500
H	2.11470800	2.58194900	-1.72601000
Br	-2.67844200	-2.51754600	-1.45326500
O	3.22119300	-1.04278600	-1.95209800
O	3.39543300	0.28546900	-0.11084400
C	5.34707100	1.07755900	-1.37330500
C	5.47946200	-1.00908500	0.07416100
C	5.13561800	1.24765400	1.12964500
C	4.87357600	0.38198300	-0.09905600
C	2.72962200	-0.41226000	-1.03413200
C	1.21954100	-0.28617500	-0.84144800

C	0.41126100	-1.47988700	-1.33205000
H	5.15188400	0.46638900	-2.25533700
H	6.42402200	1.25984900	-1.30515400
H	4.84467100	2.04284900	-1.49009300
H	5.07757600	-1.49188800	0.96998800
H	6.56296800	-0.91414000	0.19500100
H	5.27831700	-1.64123200	-0.79112800
H	4.67119900	2.23173300	1.01637600
H	6.21238200	1.38519400	1.26325500
H	4.73093400	0.77209000	2.02806900
H	0.93751700	0.57255200	-1.45446500
H	0.83210200	-2.45676200	-1.09595600
H	0.09915200	-1.42391200	-2.37316500

21'

Pd	-0.95010500	-0.83518600	0.27572600
C	-1.24285800	1.93052800	3.54448800
C	-0.87413900	3.13413000	2.94580500
C	-0.42009800	3.13684100	1.63097000
C	-0.33868200	1.93709900	0.90268200
C	-0.74004600	0.74032300	1.51342700
C	-1.18376600	0.71369700	2.84610900
H	-1.59157100	1.92311500	4.57419700
H	-0.13125900	4.06735900	1.15158400
C	-1.63044400	-0.55051700	3.55099400
H	-0.85686900	-1.31947100	3.46104400
H	-1.72165800	-0.33239700	4.62016800
C	-2.96646700	-1.10817100	3.04029900
H	-3.75926300	-0.35653400	3.12147900
H	-2.89604100	-1.40959300	1.98972200
H	-3.26599800	-1.98644000	3.62245600
H	-0.93850700	4.06421000	3.50260100
C	0.17886700	2.00381600	-0.50081000
C	1.51152200	2.41011800	-0.72685600
C	-0.65311300	1.76570400	-1.61902200
C	1.96676200	2.55218500	-2.04452600
C	-0.18321900	1.93750100	-2.92790600
C	1.13575000	2.32012500	-3.13915400
H	2.99679900	2.85390600	-2.20967500
H	-0.84925600	1.75541100	-3.76351800
H	1.51503300	2.43875500	-4.14898200
C	-2.05228100	1.31821500	-1.44231000
O	-2.43305100	0.48318500	-0.60969500
O	-2.90606500	1.87659000	-2.28335500

C	-4.27192600	1.38815200	-2.24376000
H	-4.78108400	1.90167000	-3.05752700
H	-4.28431500	0.30728100	-2.39421700
H	-4.72935000	1.63873200	-1.28477500
C	2.45659400	2.68095600	0.41776800
H	2.19808300	3.60272500	0.94784400
H	2.43586300	1.86758000	1.14721400
H	3.47894600	2.78557900	0.04805600
Br	-1.81411200	-2.60827300	-1.41853300
O	2.07256500	-1.90565700	-0.91862400
O	3.14721700	-0.68257600	0.67710100
C	4.43885700	-0.07383700	-1.34650700
C	4.96412800	-2.17338400	-0.02190500
C	5.34365100	0.09466000	0.99490700
C	4.48592200	-0.72290900	0.03396100
C	2.10799300	-1.35654500	0.16642100
C	1.00874200	-1.41739100	1.18503900
C	0.14234100	-2.49804600	1.18114900
H	3.79794900	-0.63293400	-2.02807000
H	5.45275500	-0.04739900	-1.75811800
H	4.07365500	0.95187200	-1.27706300
H	4.92120000	-2.62838200	0.97261100
H	6.00342000	-2.19413600	-0.36308600
H	4.36155000	-2.76722500	-0.71052300
H	4.97244700	1.12006000	1.07005800
H	6.37461000	0.12481500	0.63113300
H	5.34091600	-0.35319500	1.99308700
H	1.14872300	-0.82068000	2.07703200
H	0.21801400	-3.24272400	0.39858000
H	-0.43592000	-2.75570800	2.06092200

TS14'

Pd	-1.27223200	-0.73738700	-0.29488200
C	-0.73449900	-0.86946400	3.84913600
C	-0.43993700	0.46368400	4.11794000
C	0.00329300	1.28791600	3.08823200
C	0.15338900	0.79513100	1.78387300
C	-0.17493000	-0.55179800	1.51628900
C	-0.60458600	-1.40602400	2.56017500
H	-1.07524600	-1.52136200	4.64902100
H	0.23178200	2.33181600	3.28012900
C	-0.99066600	-2.85921500	2.37763600
H	-0.35229400	-3.34801200	1.63940400
H	-0.81274200	-3.37554800	3.32670900

C	-2.46307700	-3.04479500	1.98045700
H	-3.12734800	-2.59319800	2.72512900
H	-2.66610900	-2.56796900	1.01533000
H	-2.70981900	-4.10911900	1.90113900
H	-0.54962300	0.85759400	5.12371300
C	0.63138800	1.77196400	0.75772200
C	1.99335900	2.13660200	0.76803400
C	-0.25200600	2.43072300	-0.12664500
C	2.45391000	3.07209500	-0.16576200
C	0.23495900	3.37225400	-1.04598900
C	1.59135400	3.67065700	-1.08265500
H	3.50759300	3.33405700	-0.16785400
H	-0.45481500	3.86345400	-1.72186900
H	1.97229200	4.38566300	-1.80493900
C	-1.72171800	2.21915700	-0.05443300
O	-2.29980600	1.18255300	0.28368500
O	-2.40980100	3.30866600	-0.38649800
C	-3.84929800	3.16726000	-0.43770600
H	-4.21690300	4.12006700	-0.81594700
H	-4.12224600	2.34990400	-1.10773200
H	-4.24394900	2.97483900	0.56211500
C	2.94681800	1.55833500	1.78561400
H	2.70347800	1.90819900	2.79425800
H	2.90906900	0.46667500	1.80537800
H	3.97221700	1.86371000	1.56664500
Br	-2.82162600	-1.05078700	-2.25344300
O	1.69585400	-0.21026900	-1.65543200
O	3.11767500	-1.16375600	-0.15322800
C	4.60869500	0.48371700	-1.28476500
C	4.25425800	-1.85078700	-2.20270500
C	5.43556700	-1.51411400	-0.00286100
C	4.36364500	-0.98431500	-0.94935500
C	1.91351400	-0.87503900	-0.66178200
C	0.85765700	-1.64696200	0.09460000
C	-0.08486200	-2.30831700	-0.78153300
H	3.82019900	0.88595200	-1.91916400
H	5.56330100	0.56248200	-1.81488200
H	4.67746500	1.08303200	-0.37562600
H	4.02333300	-2.88611000	-1.93379500
H	5.21108600	-1.83847800	-2.73279500
H	3.48210100	-1.47814400	-2.87833200
H	5.46592400	-0.92100700	0.91594600
H	6.41488300	-1.45376000	-0.48585500
H	5.24073200	-2.55802800	0.25961300

H	1.25603700	-2.21158200	0.92732300
H	0.08316600	-2.22467000	-1.85085400
H	-0.51268900	-3.25268600	-0.45645100
22'			
Pd	-1.45106700	-0.54744500	-0.34490100
C	-1.42015400	-1.03695300	3.42923700
C	-1.44393300	0.34068800	3.61696300
C	-0.74303400	1.15307100	2.74022600
C	-0.00179100	0.61648100	1.67320300
C	0.02678200	-0.79843700	1.46171900
C	-0.71399000	-1.62257700	2.37652200
H	-1.95221700	-1.68442900	4.11993000
H	-0.74350600	2.22990000	2.87363100
C	-0.77750000	-3.13829900	2.31457300
H	-0.03207700	-3.55711900	1.64040800
H	-0.53316200	-3.51886000	3.31316100
C	-2.17239900	-3.65446600	1.92389800
H	-2.92681800	-3.33338600	2.64884800
H	-2.47088900	-3.27374900	0.94247600
H	-2.17984300	-4.74880200	1.88939500
H	-1.99782000	0.77505000	4.44350300
C	0.75332200	1.64330900	0.89070700
C	2.12126900	1.83308300	1.17178200
C	0.08671000	2.55152300	0.03556700
C	2.81840100	2.84403300	0.50162500
C	0.81717600	3.54820700	-0.63076600
C	2.18440700	3.67476900	-0.42006000
H	3.87394200	2.98273800	0.71469900
H	0.30354500	4.22484400	-1.30252500
H	2.74678000	4.44175600	-0.94295300
C	-1.39735100	2.56088400	-0.12540500
O	-2.17918000	1.61613500	-0.00799000
O	-1.85072300	3.78512100	-0.40781800
C	-3.27187000	3.90871900	-0.63415800
H	-3.43384000	4.95981600	-0.86972400
H	-3.58073700	3.27583400	-1.46876800
H	-3.82439600	3.62911000	0.26532800
C	2.82370900	1.00344100	2.21927000
H	2.27760900	1.02869200	3.16809300
H	2.91429100	-0.04572000	1.92678000
H	3.83169400	1.38680000	2.39467900
Br	-2.79351000	-1.09944400	-2.34728700
O	1.64129500	-0.05576700	-1.35095600

O	3.10350000	-1.35205600	-0.19036800
C	4.64316000	0.38640200	-1.04380900
C	3.98521800	-1.61146900	-2.46453200
C	5.36889300	-1.92851500	-0.38710300
C	4.28049900	-1.09500600	-1.05721200
C	1.88946100	-0.85786700	-0.47121700
C	0.83794300	-1.57880300	0.36861400
C	-0.22410700	-2.09631500	-0.61311700
H	3.85458200	0.99254500	-1.48791100
H	5.56475000	0.53024600	-1.61665000
H	4.82112300	0.72840300	-0.02123600
H	3.64889900	-2.65235100	-2.42539200
H	4.90163900	-1.57037500	-3.06092700
H	3.22150200	-1.01017800	-2.95923800
H	5.53285400	-1.59327700	0.64146900
H	6.30689700	-1.82332400	-0.93947800
H	5.09220300	-2.98687400	-0.36980000
H	1.35862600	-2.39334700	0.87629400
H	0.08857300	-2.11722800	-1.65519800
H	-0.68630300	-3.03657400	-0.32050000

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Pd	-0.50957100	-0.74790200	-0.64285800
C	3.54200700	3.42983300	0.48753600
C	4.05999600	2.68200100	1.53979500
C	3.41122600	1.51330600	1.93202600
C	2.25273300	1.08516300	1.27644900
C	1.72787300	1.84304900	0.20766400
C	2.38458000	3.02648700	-0.19304600
H	4.03912200	4.34401900	0.17471300
H	3.79976400	0.91834100	2.75294900
C	1.92417800	3.86244000	-1.37123700
H	0.83475000	3.97196500	-1.37574500
H	2.33125700	4.87202900	-1.25528700
C	2.39756600	3.28973000	-2.71745900
H	3.49041200	3.22367000	-2.74316900
H	2.00010700	2.28433900	-2.89196300
H	2.07458300	3.92806900	-3.54661600
H	4.96026600	3.00632300	2.05331700
C	1.60088700	-0.16183600	1.79065800
C	0.72936500	-0.05018200	2.89857000
C	1.89001300	-1.44253100	1.27253900
C	0.11133000	-1.19916100	3.40272800
C	1.27987200	-2.58094000	1.81931500

C	0.37401800	-2.45897200	2.86420900
H	-0.57721200	-1.10113600	4.23746700
H	1.51891200	-3.54866900	1.39524100
H	-0.11681600	-3.33900400	3.26822800
C	2.85822800	-1.70754200	0.16393900
O	3.48470200	-2.74658400	0.05883200
O	2.96440800	-0.69240200	-0.70647000
C	3.79008400	-0.92976900	-1.85853700
H	3.79004100	0.00867500	-2.41335100
H	4.80684600	-1.19426300	-1.55941900
H	3.35566000	-1.73055900	-2.46124600
C	0.47917200	1.28261000	3.56186400
H	-0.37956500	1.22291200	4.23534300
H	1.34935500	1.59204200	4.15250100
H	0.29622200	2.07989700	2.83650700
Br	0.29302600	-2.69947000	-2.09202600
O	-2.07533600	2.10540400	-1.62939800
O	-3.05145900	1.48861100	0.34094900
C	-4.76681200	0.77706600	-1.26800800
C	-4.66435000	3.17619000	-0.43112000
C	-5.24592100	1.30048200	1.14320100
C	-4.44708200	1.70210600	-0.09398600
C	-2.01689400	1.64376100	-0.49759000
C	-0.77030700	1.13658500	0.13777200
C	0.50373300	1.40217000	-0.56375600
H	-4.20660300	1.05688900	-2.16087800
H	-5.83607400	0.83848200	-1.49252500
H	-4.52919700	-0.25970900	-1.01133000
H	-4.36737000	3.80710700	0.41259900
H	-5.72681100	3.34896400	-0.62938500
H	-4.09159900	3.46945500	-1.31160000
H	-5.05713400	0.25407700	1.40055000
H	-6.31535200	1.42380600	0.95035000
H	-4.97331900	1.92497500	1.99932000
H	-0.79198500	1.11167000	1.21960700
H	0.31624200	2.01135000	-1.44394200
H	0.84259400	0.39224000	-1.10342800
N	-2.11535700	-1.63644400	0.23972000
C	-3.00016500	-2.07829700	0.83833000
C	-4.11278800	-2.62952200	1.58838600
H	-3.97771400	-3.70841500	1.70589800
H	-4.15529200	-2.15904000	2.57458200
H	-5.04601500	-2.43604200	1.05233900

TS12

Pd	-0.35064300	-0.70212000	-0.80536900
C	3.94533900	2.91088600	-0.14406200
C	4.30827900	2.40985900	1.10203800
C	3.43138700	1.57104200	1.78424700
C	2.19219000	1.23168900	1.23562600
C	1.80439500	1.76514000	-0.01733400
C	2.70950200	2.59975300	-0.72282700
H	4.62869800	3.55698000	-0.68759000
H	3.70766000	1.15541100	2.74824000
C	2.43163100	3.14043200	-2.11267400
H	1.41327400	3.53350400	-2.19389700
H	3.09715800	3.99210800	-2.28388000
C	2.67787000	2.09306000	-3.21142100
H	3.71389100	1.73995700	-3.17903600
H	2.02524600	1.22180300	-3.09729300
H	2.49519200	2.52315400	-4.20169000
H	5.27026200	2.66463100	1.53672300
C	1.34333900	0.29511000	2.03709300
C	0.48323000	0.84193200	3.01503300
C	1.43058100	-1.10745800	1.90046700
C	-0.32158300	-0.01333600	3.77539300
C	0.62822100	-1.93995500	2.69491900
C	-0.26104200	-1.39781600	3.61276300
H	-0.99794300	0.41644200	4.50885000
H	0.71633600	-3.01265600	2.56850000
H	-0.89415600	-2.04666700	4.20989300
C	2.36478900	-1.82007100	0.97043700
O	2.64189200	-3.00210600	1.08373400
O	2.87093300	-1.03653800	0.01099300
C	3.70695800	-1.67884600	-0.96610400
H	4.04179600	-0.87798100	-1.62564400
H	4.56279500	-2.15941400	-0.48594500
H	3.11930900	-2.41116100	-1.52343000
C	0.41861300	2.33337900	3.23751900
H	-0.36430600	2.58229100	3.95793600
H	1.37028800	2.71695100	3.62111000
H	0.21304700	2.87293000	2.30730700
Br	0.30625400	-2.72915000	-2.16386100
O	-2.05848400	1.99180400	-1.87059700
O	-3.04200900	1.42710700	0.11156000
C	-4.67199700	0.51265200	-1.47978500
C	-4.73320200	2.96324500	-0.79885400
C	-5.23976700	1.16045000	0.88223300

C	-4.43764000	1.52920200	-0.36285400
C	-2.00036200	1.60177600	-0.71310200
C	-0.74213900	1.23382300	-0.00639300
C	0.49160200	1.49512400	-0.65485900
H	-4.10146700	0.76503900	-2.37437100
H	-5.73585000	0.49843100	-1.73553000
H	-4.38511200	-0.48960000	-1.14743800
H	-4.48582900	3.66313500	0.00556700
H	-5.80064000	3.06117900	-1.02002100
H	-4.16434500	3.23199900	-1.68950500
H	-4.99444100	0.14692400	1.21281300
H	-6.30974800	1.20434200	0.66033100
H	-5.02615600	1.85557700	1.69982600
H	-0.81631400	1.12995300	1.06521600
H	0.35568900	1.96232300	-1.62328200
H	0.81864500	0.11152500	-1.46105800
N	-1.92755900	-1.62000700	0.28502900
C	-2.69193300	-1.97471600	1.07683100
C	-3.64044400	-2.41150900	2.08407700
H	-3.27742000	-3.32923700	2.55507100
H	-3.74554700	-1.63162500	2.84334900
H	-4.61196800	-2.60165300	1.61983800

TS13

Pd	1.30400500	-1.26491800	-0.52162300
C	-1.77653600	-0.19106600	3.45587300
C	-3.03965600	0.37370100	3.32628500
C	-3.46243900	0.82478000	2.07677500
C	-2.62547800	0.69725600	0.96814000
C	-1.33799400	0.12228500	1.10063200
C	-0.90548300	-0.32834200	2.36343400
H	-1.44045600	-0.53874400	4.42897200
H	-4.44027800	1.27988900	1.95316600
C	0.41834300	-1.00631200	2.63791900
H	1.13505000	-0.81616200	1.83712400
H	0.84760700	-0.55878700	3.54146500
C	0.26547600	-2.52001400	2.84143200
H	-0.42904900	-2.74072200	3.65901500
H	-0.10310400	-3.00079300	1.93123700
H	1.23258900	-2.97406700	3.08124600
H	-3.68963000	0.46781200	4.19117900
C	-3.09962000	1.26135100	-0.33650900
C	-2.78663900	2.60342600	-0.64219400
C	-3.91162400	0.52388100	-1.22324200

C	-3.27837200	3.16434200	-1.82722100
C	-4.41766300	1.11908300	-2.38639300
C	-4.09055700	2.43442800	-2.69479700
H	-3.02704500	4.19479700	-2.06286100
H	-5.05196900	0.53265700	-3.04209700
H	-4.46614100	2.89150600	-3.60502800
C	-4.28325800	-0.90547700	-1.00185700
O	-5.34605900	-1.39421300	-1.34241800
O	-3.29455600	-1.61329700	-0.43065500
C	-3.57504000	-2.99673800	-0.14839600
H	-2.67908700	-3.38012100	0.33901200
H	-4.43700800	-3.08368100	0.51726500
H	-3.77003500	-3.54512800	-1.07321300
C	-1.96987700	3.44681300	0.30542200
H	-1.64107300	4.36760600	-0.18310300
H	-2.56171500	3.72628900	1.18539700
H	-1.09017800	2.91763400	0.67788300
Br	1.72955300	-3.74529300	-0.59071000
O	1.16913400	1.77625000	1.51646700
O	2.20200200	2.37133600	-0.42563000
C	4.00645300	2.72129000	1.21390400
C	2.24896500	4.50773600	0.78267400
C	3.89546100	3.88270100	-1.01389000
C	3.09205400	3.38233000	0.18338100
C	1.32772100	1.66947600	0.31102000
C	0.56464600	0.75747800	-0.58245000
C	-0.58926900	0.04117700	-0.19215000
H	3.44080800	2.35432000	2.07050700
H	4.73939100	3.45424800	1.56486400
H	4.54900000	1.88563900	0.76300300
H	1.55314200	4.90023600	0.03444500
H	2.90695100	5.32318500	1.09848700
H	1.68106900	4.16263100	1.64721400
H	4.45421500	3.06225000	-1.47429800
H	4.60640500	4.64775100	-0.68942800
H	3.23488400	4.32010600	-1.76850300
H	0.67274700	0.96856900	-1.64274800
H	-1.23861400	-0.20614500	-1.02436600
H	-0.17028800	-1.63619000	-0.22289900
N	3.31996400	-0.70831500	-0.91383800
C	4.41212300	-0.36961500	-1.08580500
C	5.78348100	0.05719000	-1.29411300
H	5.80207200	1.12298900	-1.53713500
H	6.36119300	-0.11706300	-0.38198700

H	6.22470600	-0.51239600	-2.11681800
23			
Pd	-0.87760200	1.06563400	0.24214000
C	2.44043700	-2.14123200	3.34575800
C	3.65827200	-2.32287500	2.69902700
C	3.75409500	-2.05164700	1.33693000
C	2.63382800	-1.60949600	0.63281200
C	1.38380100	-1.45698400	1.27964800
C	1.29245600	-1.70191400	2.66706800
H	2.36389700	-2.33883500	4.41134000
H	4.69769000	-2.16975100	0.81327700
C	0.05164400	-1.47486600	3.50546500
H	-0.81976100	-1.95615700	3.05414200
H	0.19893400	-1.97525100	4.46776000
C	-0.22938600	0.01251100	3.76847000
H	0.60437700	0.46585100	4.31476700
H	-0.36024200	0.57772500	2.83917900
H	-1.13841800	0.13563700	4.36686200
H	4.52671400	-2.66625500	3.25338700
C	2.78780900	-1.32481800	-0.82979900
C	2.60378300	-2.38531900	-1.74241000
C	3.11725500	-0.03957100	-1.31384800
C	2.74977000	-2.14056400	-3.11220100
C	3.26164700	0.17465200	-2.69340900
C	3.07537800	-0.87133600	-3.58914400
H	2.60160300	-2.95924000	-3.81084900
H	3.51262800	1.16511400	-3.05173700
H	3.18134200	-0.69974700	-4.65586700
C	3.28926300	1.11026900	-0.37429400
O	2.96974200	1.11364900	0.80100900
O	3.85723600	2.17078300	-0.97765500
C	3.96503200	3.35855800	-0.17072600
H	4.45959400	4.09576200	-0.80384700
H	2.96788700	3.70164500	0.11433400
H	4.56489700	3.16473500	0.72198400
C	2.22140500	-3.76100400	-1.25650500
H	2.96565600	-4.16504400	-0.56278700
H	1.26676800	-3.73742300	-0.71862700
H	2.12163800	-4.45331600	-2.09601100
Br	0.12338500	3.32480900	-0.41068000
O	-1.67964800	-1.72179900	-1.58315800
O	-3.32650100	-1.49415700	-0.01935400
C	-4.30604200	-3.24664500	-1.43566600

C	-4.50767500	-0.79010000	-2.06000500
C	-5.66393500	-1.67796200	-0.01230200
C	-4.44901900	-1.81334500	-0.92625000
C	-2.06036800	-1.43766600	-0.45561300
C	-1.16978900	-0.94591400	0.63343900
C	0.27210000	-0.99118200	0.36613000
H	-3.43780200	-3.35068000	-2.08715100
H	-5.20336300	-3.52154400	-1.99870400
H	-4.20447600	-3.93988200	-0.59470700
H	-4.53429700	0.22624800	-1.65626000
H	-5.42096000	-0.95196400	-2.64069200
H	-3.64948700	-0.88153500	-2.72638200
H	-5.59466300	-2.37517000	0.82806400
H	-6.57626400	-1.89999700	-0.57297800
H	-5.73840100	-0.66080200	0.38315700
H	-1.57863900	-1.05277700	1.62706100
H	0.42036300	-1.38229000	-0.63997500
H	0.62626400	0.16361000	0.15855100
N	-2.81432300	1.69178400	0.46225600
C	-3.93172400	1.96646800	0.57528000
C	-5.33522600	2.30878100	0.70790500
H	-5.43786000	3.38593500	0.86684200
H	-5.86549200	2.02380100	-0.20503000
H	-5.76411500	1.77303700	1.55916000

TS15

Pd	-0.77657300	0.99075600	0.21144900
C	2.40401800	-1.90831900	3.45166600
C	3.63337900	-2.07803500	2.82150300
C	3.72805700	-1.89590600	1.44544800
C	2.59662300	-1.55130400	0.70650900
C	1.33207400	-1.41340000	1.33631600
C	1.24314700	-1.57280900	2.74166000
H	2.32954100	-2.04116500	4.52720800
H	4.68026900	-2.00583100	0.93633500
C	-0.01690100	-1.37113400	3.55533900
H	-0.86167300	-1.89754300	3.10440000
H	0.13544200	-1.83840900	4.53320200
C	-0.35614000	0.11229500	3.77129600
H	0.44238900	0.60517000	4.33553500
H	-0.46949200	0.64853400	2.82294200
H	-1.28976800	0.21868500	4.33376300
H	4.51185300	-2.34573400	3.40116200
C	2.75286900	-1.35488700	-0.76944100

C	2.56831800	-2.46553100	-1.62074300
C	3.08650200	-0.09890300	-1.32360700
C	2.70141500	-2.29462800	-3.00292300
C	3.21497600	0.04006100	-2.71430200
C	3.01683200	-1.05180300	-3.55058400
H	2.55293900	-3.15092300	-3.65469200
H	3.46746900	1.00793200	-3.12845200
H	3.11169000	-0.93770000	-4.62598700
C	3.30358400	1.09184700	-0.44503700
O	3.08267400	1.13587900	0.75143600
O	3.80542200	2.13510500	-1.13192200
C	3.97082400	3.35071000	-0.37976400
H	4.40235200	4.06811500	-1.07839500
H	2.99902200	3.69865700	-0.02313900
H	4.64654900	3.19289300	0.46461300
C	2.20755100	-3.81794200	-1.05835700
H	2.94445300	-4.15648300	-0.32308700
H	1.23881700	-3.78942200	-0.54630700
H	2.14715300	-4.56341000	-1.85491300
Br	0.14997400	3.22443800	-0.51349600
O	-1.71584000	-1.73626200	-1.59926500
O	-3.36989100	-1.45309800	-0.05222600
C	-4.42029400	-3.10640000	-1.53896300
C	-4.48705600	-0.62181700	-2.07753700
C	-5.71397400	-1.52063800	-0.07579200
C	-4.49629400	-1.68621800	-0.98090100
C	-2.09794500	-1.45660600	-0.47185700
C	-1.19712500	-1.05642300	0.64807500
C	0.19989800	-1.14069900	0.41264200
H	-3.55383700	-3.23071600	-2.18906200
H	-5.32650400	-3.31652200	-2.11549700
H	-4.35920900	-3.83246300	-0.72212100
H	-4.46926000	0.37932700	-1.63674800
H	-5.39780000	-0.71632200	-2.67679400
H	-3.62383700	-0.73294800	-2.73459700
H	-5.69303100	-2.25127100	0.73837000
H	-6.62909700	-1.67266700	-0.65500400
H	-5.73980000	-0.51637400	0.35668100
H	-1.63938200	-1.07932400	1.63175000
H	0.40515100	-1.45573000	-0.60669300
H	0.62990100	0.34917000	-0.02635000
N	-2.74921900	1.69128700	0.56283300
C	-3.85321100	1.99598200	0.72281900
C	-5.24098900	2.37651500	0.91255200

H	-5.30267600	3.44557600	1.13442200
H	-5.80387000	2.16269000	-0.00028600
H	-5.66769700	1.80802000	1.74333000

TS16

Pd	2.28322200	-0.23483000	0.45573100
C	-0.84235800	-3.47119400	-2.29230100
C	-2.19503400	-3.62529400	-2.00614400
C	-2.74223900	-2.94224200	-0.92691600
C	-1.94286200	-2.10952400	-0.14079400
C	-0.55931300	-1.96696000	-0.42034400
C	0.00087500	-2.66170700	-1.51535500
H	-0.40915500	-4.00186900	-3.13565300
H	-3.79690700	-3.03627600	-0.68774200
C	1.45021600	-2.58221800	-1.94948200
H	2.12626700	-2.61333100	-1.09278900
H	1.67009400	-3.47362200	-2.54664700
C	1.76018200	-1.33146100	-2.78279100
H	1.16233000	-1.32158200	-3.70151900
H	1.52411300	-0.42262300	-2.22476900
H	2.81951000	-1.30906200	-3.05845000
H	-2.81483100	-4.27348900	-2.61865000
C	-2.57447400	-1.40197800	1.02043000
C	-2.36323500	-1.89269400	2.32685500
C	-3.40255800	-0.26489900	0.84043300
C	-2.90506600	-1.20127500	3.41852500
C	-3.93166700	0.40253300	1.95436700
C	-3.66536700	-0.05015400	3.24200600
H	-2.72586700	-1.58334000	4.42016800
H	-4.55371100	1.27522000	1.80207500
H	-4.06817900	0.47882100	4.10010800
C	-3.77490300	0.22481200	-0.52413300
O	-3.24529200	-0.08174900	-1.57406700
O	-4.83629100	1.06386300	-0.47029600
C	-5.31557700	1.54295700	-1.73837900
H	-6.16461000	2.18559400	-1.50516000
H	-4.54370400	2.11137800	-2.26054200
H	-5.63479600	0.70715400	-2.36634200
C	-1.57871800	-3.15378600	2.60439200
H	-1.30661500	-3.68463700	1.69169400
H	-0.65924100	-2.93279800	3.15942500
H	-2.16841300	-3.83348000	3.22844300
Br	4.64280800	-1.07700000	0.23953300
O	-0.34304800	0.91011400	-1.51304000

O	-0.44092200	2.39644700	0.21389000
C	-2.24652000	3.30063200	-1.16894900
C	0.17395200	3.84216100	-1.69601700
C	-0.87777100	4.69054300	0.42336000
C	-0.85331600	3.55890500	-0.60028400
C	-0.22939300	1.18883100	-0.33379600
C	0.19838500	0.24532200	0.73791500
C	0.16541900	-1.15334300	0.61993500
H	-2.23211600	2.46681800	-1.87077000
H	-2.59756700	4.19680500	-1.68995600
H	-2.95122600	3.07415000	-0.36391400
H	1.17436900	3.94954100	-1.26901300
H	-0.08641800	4.78360900	-2.18969100
H	0.19116400	3.04806800	-2.44203200
H	-1.57552900	4.46283400	1.23480000
H	-1.19681200	5.61900400	-0.05871800
H	0.11703000	4.84634400	0.85199900
H	0.21867800	0.66095400	1.74119700
H	0.21664800	-1.65953800	1.57847200
H	1.91438800	-1.71885900	0.52611500
N	2.82073300	1.84261400	0.47985900
C	3.08722500	2.96229500	0.59141000
C	3.41597600	4.36903700	0.73109600
H	4.49846400	4.48597200	0.83316500
H	3.07263200	4.91332900	-0.15291100
H	2.92166800	4.77260500	1.61919100

P

O	2.71505400	1.99640600	-0.86131800
O	3.06219200	0.17400900	0.47016600
O	-2.16573900	-2.89074300	2.33008600
O	-1.50555200	-0.75165500	2.04266500
C	5.01095400	1.55133900	1.06464200
C	5.03394100	0.05815400	-0.99242900
C	4.94054000	-0.95069400	1.30791100
C	4.53643900	0.23929300	0.44124700
C	2.29805100	1.05807700	-0.19722500
C	0.87109000	0.71916300	-0.01653500
C	-0.08029800	1.45306700	-0.61770100
C	-1.52788600	1.21290400	-0.57311300
C	-2.40448300	2.32367600	-0.50100600
C	-1.88370700	3.74195500	-0.41728000
C	-1.32157000	4.08794300	0.97004100
C	-3.78353800	2.10329100	-0.42903000

C	-4.30868600	0.81355800	-0.44302200
C	-3.44995100	-0.27905200	-0.53814600
C	-2.06484800	-0.09599100	-0.60541000
C	-1.22181200	-1.32056100	-0.77039300
C	-0.63631100	-1.60859100	-2.02185500
C	-0.75918800	-0.65354000	-3.18074100
C	0.06793400	-2.80749300	-2.18152000
C	0.17935000	-3.73371700	-1.14473400
C	-0.41907400	-3.46575000	0.08042500
C	-1.10133300	-2.25847000	0.27470000
C	-1.66332800	-2.02384800	1.63749800
C	-2.08324000	-0.41441000	3.31754300
H	4.73003000	2.40698600	0.45015800
H	6.10079100	1.53091000	1.16236500
H	4.58110400	1.67508000	2.06359700
H	4.61849100	-0.85730600	-1.42532200
H	6.12461600	-0.03096500	-0.98744400
H	4.75450400	0.90485100	-1.61992900
H	4.54511600	-0.84236000	2.32224700
H	6.03076200	-1.01518600	1.36531900
H	4.55940500	-1.88426400	0.88337300
H	0.64134900	-0.12964300	0.61308900
H	0.25777100	2.32101300	-1.17959200
H	-2.70379000	4.42713900	-0.65428100
H	-1.10858700	3.91075800	-1.17338600
H	-0.47904900	3.43974100	1.23000600
H	-2.08968100	3.96484000	1.74087700
H	-0.97235100	5.12531800	0.99855300
H	-4.44903700	2.95915400	-0.35978500
H	-5.38213200	0.65898700	-0.39035100
H	-3.84882000	-1.28815500	-0.56904100
H	-1.78779900	-0.30263000	-3.30584200
H	-0.44024000	-1.13228200	-4.10984900
H	-0.13365600	0.23381800	-3.02959300
H	0.52186600	-3.02181200	-3.14497200
H	0.72381200	-4.66027900	-1.29688800
H	-0.35366500	-4.17179400	0.90112700
H	-1.62638800	-1.00315600	4.11626400
H	-3.16156700	-0.59027600	3.30391800
H	-1.87475800	0.64555000	3.45938700
P'			
C	0.68902800	2.69299300	1.92292000
C	1.66441600	1.95702600	2.59323400

C	2.04478500	0.70910800	2.10383400
C	1.44671000	0.19896600	0.94858600
C	0.44010900	0.93036300	0.28893100
C	0.06616800	2.20236800	0.76892400
H	0.40351300	3.67367800	2.29368500
H	2.80907000	0.12621700	2.60874700
C	-0.91141200	3.08382600	0.02472000
H	-1.78837700	2.50826300	-0.27674900
H	-1.26727400	3.86478600	0.70497900
C	-0.27698000	3.74086400	-1.21010400
H	0.58655300	4.35217400	-0.92689500
H	0.06472100	2.98646300	-1.92627200
H	-0.99825900	4.38728500	-1.72146700
H	2.13122800	2.35752400	3.48817700
C	1.86403400	-1.14665500	0.44372000
C	1.13531400	-2.28438600	0.85276400
C	3.00489700	-1.31596000	-0.36803300
C	1.55157000	-3.55032700	0.42601000
C	3.41808900	-2.59777000	-0.75606500
C	2.68400900	-3.71275900	-0.37179700
H	0.98224100	-4.42164500	0.73717400
H	4.30835500	-2.69876500	-1.36675300
H	2.99238200	-4.70484200	-0.68642400
C	3.84897800	-0.18317600	-0.85301200
O	5.05321200	-0.25861800	-1.02432900
O	3.13501600	0.92096100	-1.12760500
C	3.88248100	2.07592600	-1.55167900
H	3.14366500	2.86609300	-1.68139400
H	4.61254000	2.35929600	-0.79007500
H	4.39716500	1.87632500	-2.49447900
C	-0.05645200	-2.14912700	1.76603300
H	-0.54987700	-3.11480000	1.90201000
H	0.24880700	-1.78290400	2.75317700
H	-0.78860700	-1.43504400	1.38088000
O	-2.45083800	0.25317700	0.81112300
O	-3.56904400	-0.47820800	-1.03433000
C	-5.34660700	0.74472900	0.14665100
C	-4.78272600	-1.66137000	0.74707100
C	-5.78075600	-1.11016900	-1.49387500
C	-4.87951000	-0.61749400	-0.36477800
C	-2.47806900	-0.05464600	-0.37189100
C	-1.32075900	-0.03787800	-1.29384100
C	-0.08036500	0.36911500	-0.98101800
H	-4.71499600	1.10289100	0.95975300

H	-6.37470100	0.65897500	0.51163300
H	-5.33259800	1.47956700	-0.66435900
H	-4.37914800	-2.59946700	0.35347900
H	-5.78362100	-1.85968500	1.14252600
H	-4.14646400	-1.31659400	1.56236900
H	-5.81168300	-0.38221600	-2.31004800
H	-6.79798300	-1.25464100	-1.11939300
H	-5.41821200	-2.06319200	-1.89049500
H	-1.51339800	-0.41967200	-2.29108000
H	0.67648100	0.25404600	-1.75540900

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O	-2.87131100	0.77155300	1.09775500
O	-3.05764500	-0.13313400	-0.98772800
C	-5.32386600	0.76941900	-0.68051200
C	-4.66851100	-1.49931000	0.26594500
C	-4.77830300	-1.14238700	-2.21952100
C	-4.48428200	-0.49328400	-0.86952200
C	-2.38520200	0.43099800	0.02744100
C	-0.96436200	0.60271500	-0.34049400
C	-0.09644700	1.13110300	0.53435500
C	1.29966700	1.45020800	0.18593700
C	1.58313300	2.83997900	0.19631400
C	0.64125600	3.85115900	0.82457600
C	-0.44732900	4.35154000	-0.13735300
C	2.70535900	3.33014800	-0.47501200
C	3.50270900	2.46253700	-1.21011700
C	3.27284900	1.09560800	-1.13591100
C	2.25538300	0.52428300	-0.33933800
H	-5.11878500	1.24157300	0.28057500
H	-6.38564700	0.50767500	-0.72481500
H	-5.11570200	1.48717400	-1.48024100
H	-3.98331300	-2.34195100	0.13693900
H	-5.69417500	-1.88046500	0.24705100
H	-4.48155700	-1.04089000	1.23709900
H	-4.59265900	-0.43827400	-3.03610400
H	-5.82580400	-1.45363600	-2.26153400
H	-4.14779200	-2.02384000	-2.36931000
H	-0.65770800	0.27210100	-1.32685700
H	-0.49004800	1.47154400	1.48694000
H	1.24223600	4.70657800	1.15142700
H	0.17237600	3.44211800	1.72466100
H	-1.09714800	3.53490200	-0.46382000
H	0.00147600	4.80214800	-1.02878000

H	-1.07154500	5.10850100	0.34907000
H	2.90204700	4.39861100	-0.47176700
H	4.31174300	2.83873600	-1.82850000
H	3.89866200	0.44908600	-1.73042800
C	2.31868400	-0.97657600	-0.19532700
C	1.22631400	-1.85811800	0.09361600
C	3.56480500	-1.63358300	-0.44901300
C	1.27811700	-3.21122000	-0.26070800
C	3.58903900	-3.00187900	-0.76185300
C	2.44193600	-3.77956900	-0.76561400
H	0.40287200	-3.82060200	-0.06666300
H	4.54988300	-3.45563200	-0.98902100
H	2.47248200	-4.82531300	-1.05332400
C	0.08971500	-1.61121800	1.03169300
C	4.94070800	-1.00878900	-0.27611800
O	-1.01706000	-2.11086600	0.93660500
O	0.50341900	-0.93766200	2.12330100
C	-0.48526500	-0.77411600	3.16347200
H	-1.39184700	-0.31702400	2.76490700
H	-0.72478400	-1.74363600	3.60742200
H	-0.01959100	-0.12584600	3.90539100
H	4.91508700	-0.08388000	0.29994900
H	5.56701100	-1.72687200	0.26350400
H	5.44635700	-0.79989400	-1.22483900

P''

O	-2.28885900	2.00331600	0.90088800
O	-3.07520800	0.40327800	-0.52668100
C	-4.95566100	1.98850300	-0.52657800
C	-4.71408000	0.23049000	1.29425400
C	-5.18553500	-0.45434900	-1.07829700
C	-4.49969800	0.57176900	-0.17998700
C	-2.10857200	1.12927700	0.06485900
C	-0.78787900	0.69984500	-0.43842000
C	0.33418200	1.25544300	0.04903500
C	1.72212500	0.91290100	-0.28712800
C	2.69156700	1.94891600	-0.28958900
C	2.31611500	3.39213400	-0.02975800
C	1.57266700	4.04131000	-1.20663800
C	4.02018100	1.64234700	-0.59625200
C	4.41091600	0.33621800	-0.88256400
C	3.46674300	-0.68609900	-0.85787000
C	2.12809100	-0.41803200	-0.55899600
H	-4.46873000	2.72748600	0.11005600

H	-6.03878700	2.06341300	-0.38891700
H	-4.72798900	2.21565800	-1.57275000
H	-4.30853500	-0.76163300	1.51595600
H	-5.78683800	0.21811700	1.50991500
H	-4.23408900	0.96160600	1.94529500
H	-4.99196700	-0.23556400	-2.13271700
H	-6.26613500	-0.43088100	-0.91173000
H	-4.82189900	-1.46276800	-0.85945200
H	-0.78163700	-0.08526300	-1.18302700
H	0.19560400	2.05909500	0.76836100
H	3.23235100	3.95600100	0.17204100
H	1.70059400	3.47022700	0.87379100
H	0.63210800	3.52330100	-1.41800300
H	2.18360700	4.01079700	-2.11494000
H	1.34035000	5.08840200	-0.98645400
H	4.75435500	2.44294900	-0.60810700
H	5.44893800	0.11344800	-1.11028800
H	3.76781800	-1.71132800	-1.04716600
C	1.18149800	-1.57362900	-0.49239900
C	0.81955700	-2.23982300	-1.68294000
C	0.59454600	-1.97801500	0.72496600
C	-0.10605800	-3.28868000	-1.62235800
C	-0.35029200	-3.00945200	0.75352400
C	-0.69100300	-3.67562400	-0.41774300
H	-0.38389800	-3.79447200	-2.54274000
H	-0.80471100	-3.27901600	1.70052600
H	-1.41465600	-4.48436000	-0.39656300
C	1.36800700	-1.80791400	-3.02107900
H	1.28108500	-0.72506400	-3.15554700
H	2.42903600	-2.05644000	-3.12697100
H	0.82623800	-2.29968700	-3.83276500
C	0.86219600	-1.29339200	2.02508600
O	0.00938600	-1.09769000	2.87335000
O	2.14871100	-0.94059300	2.17672200
C	2.45318400	-0.15565800	3.34432100
H	3.51894700	0.06114000	3.27926800
H	1.87696800	0.77272700	3.33775200
H	2.23285100	-0.71528100	4.25625200