

DFT Calculations on Regioselectivity and Solvation effect in B-H Activation of O-carborane Guided by Directing group

Hui Li,^{*a,b} Wanyong Tang^a and Zifan Ma^a

^a Chemical Science and Engineering College, North Minzu University, Wenchang North Street 204th, Yinchuan 750021, P. R. China

* Corresponding author. Hui Li

E-mail: lihui@nun.edu.cn

Supporting Information

Table of Contents

Table S1. Energies calculated at ω B97X-D/BSI (6-311g**, SDD) level in gas phase of Path A, path C, and path B.	S2
Table S2. Correction energies calculated at ω B97X-D/BSII (6-311g**, SDD) of Path A, path B, and path C.	S4
Table S3. Energies calculated at ω B97X-D/BSI (6-311g**, SDD) level in gas phase of Path D, Path E, and path F.	S6
Table S4. Correction energies calculated at ω B97X-D/BSII (6-311g**, SDD) of Path D, Path E, and path F in DCE.	S7
Table S5. Correction energies calculated at ω B97X-D/BSII (6-311g**, SDD) of Path D, Path E, and path F in MeCN.	S8
Figure S1. Reaction mechanism of B(4)-H/B(7)-H/B(8)-H activation in Path A/B/C.	S9
Figure S2. Reaction mechanism of B(7)-H/B(8)-H activation in cation pathways (PathD/E/F) catalyzed by Pd ^{II} that 1, 10-o-phenanthroline as ligand.	S10
Figure S3. IRC profiles of all TSs in the pathways (a. IRC A1-A2, b. IRC A2-A3, c. IRC A3-A4, d. IRC B1-B2, e. IRC B2-B3, f. IRC B3-B4, g. IRC C1-C2, h. IRC C2-C3, i. IRC C3-C4).	S11
Cartesian coordinates of all stationary points optimized at ω B97X-D/BSI (6-311g**, SDD) level.	S12

Table S1. Energies calculated at ω B97X-D/BSI (6-311g, SDD) level in gas phase of Path A, path B, and path C. (unit: a.u.)**

	<i>E+ZPE</i>	<i>E</i>	<i>H</i>	<i>G</i>
L	-571.35899	-571.349882	-571.348937	-571.393671
CATA1	-1317.749617	-1317.735857	-1317.734913	-1317.794056
I-Pd-OTf	-1100.73328	-1100.722996	-1100.722052	-1100.773813
I-Pd-OTf-DCE	-2099.75554	-2099.73826	-2099.737316	-2099.807653
DCE	-998.976814	-998.971967	-998.971023	-999.005086
OTf_ion	-961.491852	-961.484825	-961.483881	-961.524164
HOAc	-229.017442	-229.013698	-229.012754	-229.043449
Ph-I	-242.94425	-242.938453	-242.937509	-242.975897
1	-618.47775	-618.462542	-618.461597	-618.517429
A1	-1936.256776	-1936.226469	-1936.225525	-1936.316876
TSA1-A2	-1936.232593	-1936.202188	-1936.201243	-1936.293406
A2	-1707.250039	-1707.224856	-1707.223912	-1707.305089
TSA2-A3	-1950.175269	-1950.1426	-1950.141656	-1950.241069
A3	-1950.213665	-1950.181146	-1950.180201	-1950.277155
TSA3-A4	-1950.201012	-1950.1695	-1950.168555	-1950.262885
A4	-849.431442	-849.411207	-849.410263	-849.47818
B1	-1936.249549	-1936.219737	-1936.218793	-1936.309126
TSB1-B2	-1936.224304	-1936.194005	-1936.193061	-1936.285443
B2	-1707.250983	-1707.2256	-1707.224655	-1707.306389
TSB2-B3	-1950.191926	-1950.159739	-1950.158795	-1950.255145
B3	-1950.21176	-1950.179492	-1950.178548	-1950.27439
TSB3-B4	-1950.19557	-1950.16387	-1950.162926	-1950.25836
B4	-849.431438	-849.411207	-849.410262	-849.47817
C1	-1936.258607	-1936.227775	-1936.226831	-1936.320321

TSC1-C2	-1936.252447	-1936.222152	-1936.221208	-1936.313208
C2	-1707.243248	-1707.217567	-1707.216623	-1707.299524
TSC2-C3	-1950.166766	-1950.13421	-1950.133266	-1950.230878
C3	-1950.21257	-1950.179671	-1950.178727	-1950.277471
TSC3-C4	-1950.206729	-1950.175015	-1950.174071	-1950.268312
C4	-849.43548	-849.415177	-849.414233	-849.482161

Table S2. Correction energies calculated at ω B97X-D/BSII (6-311g**, SDD) of Path A, path B, and path C. (unit: a.u.)

	$E+ZPE$ dichloroethane	E dichloroethane	H dichloroethane	G dichloroethane
L	-571.381674	-571.37247	-571.371526	-571.416712
CATA1	-1317.761092	-1317.748832	-1317.747888	-1317.802514
I-Pd-OTf	-1100.742527	-1100.732891	-1100.731947	-1100.781815
I-Pd-OTf-DCE	-2099.776322	-2099.760012	-2099.759068	-2099.825158
DCE	-998.987035	-998.982144	-998.9812	-999.015408
OTf_ion	-961.565394	-961.558352	-961.557408	-961.597691
HOAc	-229.025839	-229.022082	-229.021138	-229.051849
Ph-I	-242.953099	-242.947301	-242.946357	-242.984749
1	-618.491235	-618.475793	-618.474849	-618.531674
A1	-1936.28799	-1936.258434	-1936.25749	-1936.346886
TSA1-A2	-1936.2641	-1936.234174	-1936.23323	-1936.325188
A2	-1707.280388	-1707.255917	-1707.254972	-1707.33375
TSA2-A3	-1950.207184	-1950.175351	-1950.174407	-1950.270309
A3	-1950.244742	-1950.212864	-1950.211919	-1950.307307
TSA3-A4	-1950.235559	-1950.203878	-1950.202934	-1950.299276
A4	-849.45149	-849.431913	-849.430968	-849.497031
B1	-1936.289184	-1936.258864	-1936.25792	-1936.351802
TSB1-B2	-1936.262836	-1936.233989	-1936.233045	-1936.321424
B2	-1707.280954	-1707.25641	-1707.255466	-1707.334386
TSB2-B3	-1950.224146	-1950.192334	-1950.19139	-1950.28812
B3	-1950.244028	-1950.211663	-1950.210719	-1950.307606
TSB3-B4	-1950.235421	-1950.204292	-1950.203348	-1950.297479
B4	-849.451486	-849.431916	-849.430972	-849.497006
C1	-1936.297079	-1936.268643	-1936.267699	-1936.355258
TSC1-C2	-1936.289147	-1936.260388	-1936.259444	-1936.347315

C2	-1707.27801	-1707.25384	-1707.252896	-1707.332273
TSC2-C3	-1950.213861	-1950.1828	-1950.181856	-1950.275967
C3	-1950.249588	-1950.216333	-1950.215389	-1950.31741
TSC3-C4	-1950.238953	-1950.207819	-1950.206875	-1950.299686
C4	-849.455136	-849.434656	-849.433712	-849.502741

Table S3. Energies calculated at ω B97X-D/BSI (6-311g, SDD) level in gas phase of Path D, Path E, and path F. (unit: a.u.)**

	<i>E+ZPE</i>	<i>E</i>	<i>H</i>	<i>G</i>
D2	-1317.053342	-1317.026364	-1317.02542	-1317.108664
TSD2-D3	-1559.965366	-1559.931491	-1559.930547	-1560.029557
D3	-1559.978912	-1559.945402	-1559.944458	-1560.04111
TSD3-D4	-1559.956809	-1559.923366	-1559.922422	-1560.019468
A4	-849.431438	-849.411207	-849.410262	-849.47817
L_PdI	-710.54217	-710.529499	-710.528555	-710.584133
E2	-1317.053334	-1317.02636	-1317.025416	-1317.10864
TSE2-E3	-1559.963403	-1559.929498	-1559.928554	-1560.027255
E3	-1559.974211	-1559.940763	-1559.939819	-1560.036284
TSE3-E4	-1559.940824	-1559.907497	-1559.906553	-1560.003741
B4	-849.431438	-849.411207	-849.410262	-849.47817
L_PdI	-710.54217	-710.529499	-710.528555	-710.584133
F2	-1317.051256	-1317.023981	-1317.023036	-1317.107648
TSF2-F3	-1559.958092	-1559.923288	-1559.922344	-1560.024573
F3	-1560.002596	-1559.968343	-1559.967399	-1560.066365
TSF3-F4	-1559.984246	-1559.95017	-1559.949225	-1560.048265
C4	-849.43548	-849.415177	-849.414233	-849.482161
L_PFI	-710.54217	-710.529499	-710.528555	-710.584133

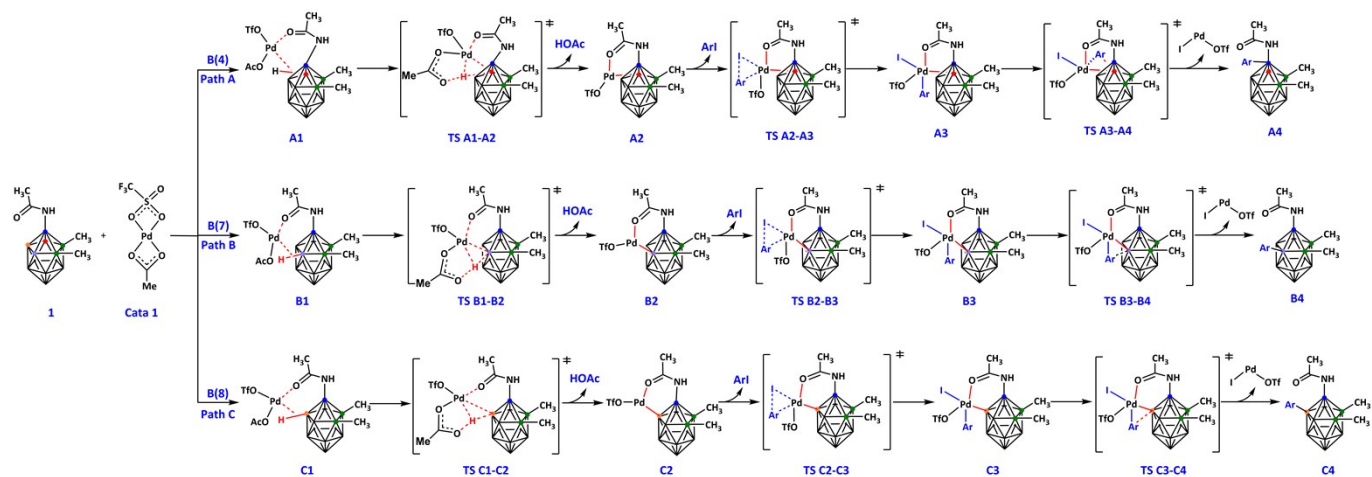
Table S4. Correction energies calculated at ω B97X-D/BSII (6-311g**, SDD) of Path D, Path E, and path F in DCE. (unit: a.u.)

	<i>E+ZPE</i> dichloroethane	<i>E</i> dichloroethane	<i>H</i> dichloroethane	<i>G</i> dichloroethane
D2	-1317.131293	-1317.105123	-1317.104178	-1317.184527
TSD2-D3	-1560.05162	-1560.018544	-1560.0176	-1560.114123
D3	-1560.077752	-1560.044259	-1560.043315	-1560.140333
TSD3-D4	-1560.055044	-1560.022509	-1560.021565	-1560.116065
A4	-849.45149	-849.431913	-849.430968	-849.497031
L_PdI	-710.640283	-710.62853	-710.627585	-710.68027
E2	-1317.131284	-1317.105121	-1317.104177	-1317.184468
TSE2-E3	-1560.05233	-1560.019346	-1560.018402	-1560.114022
E3	-1560.074202	-1560.040574	-1560.03963	-1560.137032
TSE3-E4	-1560.042497	-1560.010575	-1560.009631	-1560.103517
B4	-849.451486	-849.431916	-849.430972	-849.497006
L_PdI	-710.640283	-710.62853	-710.627585	-710.68027
F2	-1317.12797	-1317.10241	-1317.101466	-1317.182042
TSF2-F3	-1560.040503	-1560.008113	-1560.007168	-1560.102376
F3	-1560.089807	-1560.055265	-1560.054321	-1560.154567
TSF3-F4	-1560.072099	-1560.038745	-1560.037801	-1560.135186
C4	-849.455136	-849.434656	-849.433712	-849.502741
L_PFI	-710.640283	-710.62853	-710.627585	-710.68027

Table S5. Correction energies calculated at ω B97X-D/BSII (6-311g**, SDD) of Path D, Path E, and path F in MeCN. (unit: a.u.)

	$E+ZPE_{\text{acetonitrile}}$	$E_{\text{acetonitrile}}$	$H_{\text{acetonitrile}}$	$G_{\text{acetonitrile}}$
D2	-1317.136308	-1317.110022	-1317.109077	-1317.191005
TSD2-D3	-1560.057451	-1560.024346	-1560.023402	-1560.120161
D3	-1560.085549	-1560.052025	-1560.051081	-1560.147912
TSD3-D4	-1560.062678	-1560.029162	-1560.028218	-1560.126738
A4	-849.453379	-849.433749	-849.432805	-849.499196
L_PdI	-710.647524	-710.634837	-710.633892	-710.690615
E2	-1317.136283	-1317.110018	-1317.109074	-1317.190433
TSE2-E3	-1560.058568	-1560.025538	-1560.024594	-1560.12034
E3	-1560.081941	-1560.048271	-1560.047327	-1560.144994
TSE3-E4	-1560.051043	-1560.019083	-1560.018139	-1560.11184
B4	-849.453379	-849.433749	-849.432805	-849.499196
L_PdI	-710.647524	-710.634837	-710.633892	-710.690615
F2	-1317.132996	-1317.10737	-1317.10643	-1317.18631
TSF2-F3	-1560.045353	-1560.01284	-1560.01189	-1560.10778
F3	-1560.095417	-1560.06087	-1560.05992	-1560.16031
TSF3-F4	-1560.078126	-1560.04383	-1560.04289	-1560.14355
C4	-849.456728	-849.436159	-849.435215	-849.504725
L_PFI	-710.647524	-710.634837	-710.633892	-710.690615

Figure S1. Reaction mechanism of B(4)-H/B(7)-H/B(8)-H activation in Path A/B/C.



Description: The original picture is uploaded as an attachment.

Figure S2. Reaction mechanism of B(7)-H/B(8)-H activation in cation pathways (PathD/E/F) catalyzed by Pd^{II} that 1, 10-o-phenanthroline as ligand.

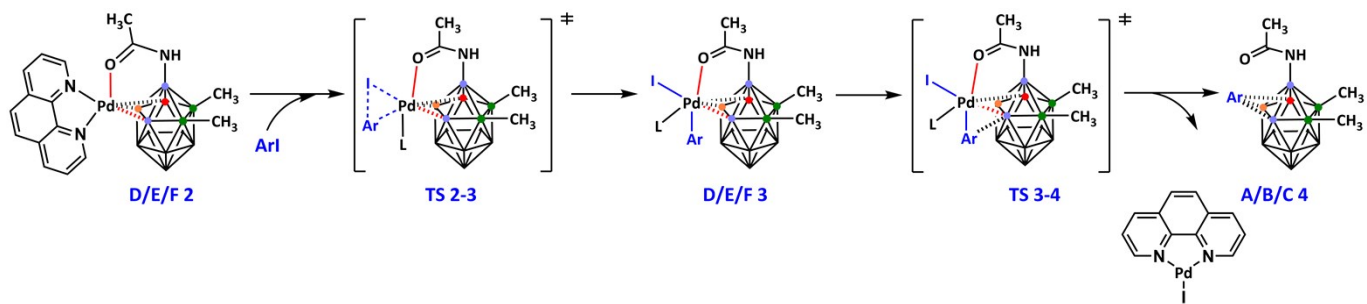
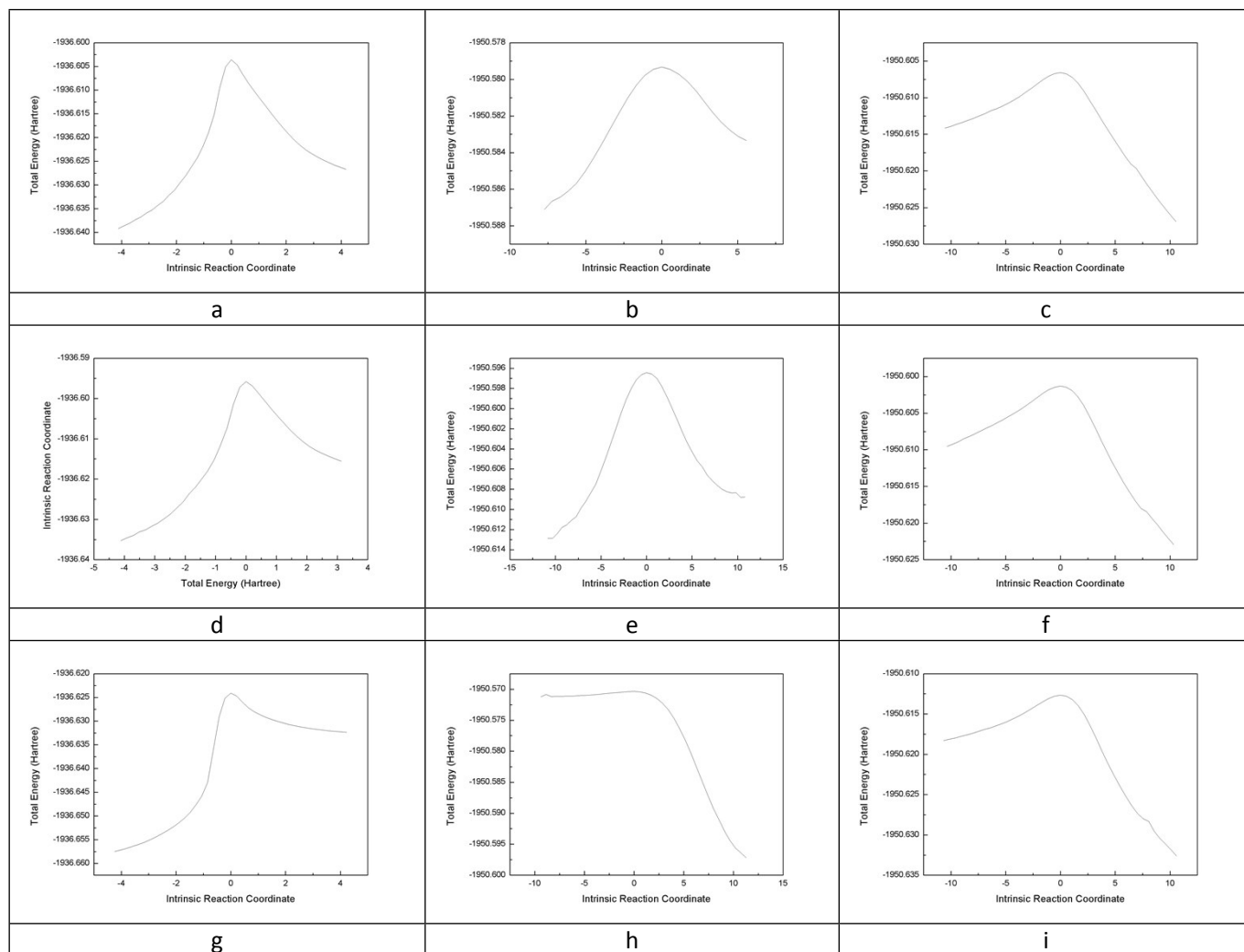


Figure S3. IRC profiles of all TSs in the pathways (a. IRC A1-A2, b. IRC A2-A3, c. IRC A3-A4, d. IRC B1-B2, e. IRC B2-B3, f. IRC B3-B4, g. IRC C1-C2, h. IRC C2-C3, i. IRC C3-C4).



Cartesian coordinates of all stationary points optimized at ω B97X-D/BSI (6-311g**, SDD) level

HOAc				H	-1.95823800	-0.15821600	-1.75809900
				B	-0.36488900	-0.34374400	-0.39417600
O	0.63420100	1.19566500	-0.00014300	B	0.29967300	-1.19027700	1.00554400
C	0.09233700	0.12526400	0.00018200	B	1.71454900	-0.30065400	1.58957800
O	0.78071900	-1.03381700	0.00003400	H	1.88486600	-0.17146600	2.75336400
C	-1.38995700	-0.11554400	-0.00003200	B	1.98531800	1.10711300	0.55693700
H	-1.66839400	-0.69850000	-0.88014000	H	2.25659200	2.18223900	0.96374100
H	-1.66882200	-0.69619800	0.88147300	B	0.88207000	-0.33089400	-1.65381600
H	-1.91166000	0.83843100	-0.00133400	H	0.50757400	-0.18481700	-2.77025300
H	1.71524400	-0.79684400	-0.00002200	B	0.65205400	-1.76619600	-0.63550800
C6H5I				H	0.14244800	-2.74513700	-1.06891000
				B	1.93226500	-1.75637500	0.59539400
C	-2.64335300	1.20136600	-0.00000300	H	2.35605000	-2.75524900	1.07191400
C	-1.25303500	1.20973300	-0.00000100	B	2.96282200	-0.33208900	0.32150300
C	-0.57358200	0.00000500	-0.00000100	H	4.11686600	-0.29869400	0.58735700
C	-1.25303300	-1.20973300	-0.00000200	B	2.31253600	0.54109700	-1.07902400
C	-2.64334400	-1.20137100	-0.00000300	H	2.89178300	1.26395500	-1.81585500
C	-3.33959400	-0.00000100	-0.00000400	B	2.29296000	-1.23221200	-1.06315700
H	-3.17953400	2.14336700	-0.00000300	H	2.97636200	-1.84714200	-1.81124300
H	-0.71237500	2.14729600	-0.00000100	H	-0.46460100	-1.64396600	1.78026600
H	-0.71236200	-2.14728900	-0.00000100	Cata1			
H	-3.17952900	-2.14336900	-0.00000300	O	2.66374200	0.16952900	-1.07651800
H	-4.42323000	-0.00000800	-0.00000600	C	3.32369100	0.30848800	0.00080800
I	1.55552200	0.00000000	0.00000200	O	2.66325800	0.16935900	1.07755500
I-Pd-OTf				C	4.78237500	0.58645500	0.00000200
Pd	0.53011300	-0.25843500	-0.00059400	H	5.07025800	1.07246400	0.93105900
O	-1.16605000	-0.66937500	-1.17661400	H	5.31350000	-0.36537800	-0.08158100
O	-3.06788700	-1.82723800	0.00106800	H	5.04236000	1.20151100	-0.86100200
C	-3.04731500	0.83874900	-0.00012700	Pd	0.97371500	-0.21935000	0.00014700
S	-2.10677900	-0.77459800	0.00034900	O	-0.72494600	-0.64137800	-1.18410100
O	-1.16619000	-0.66772700	1.17739000	O	-2.60001700	-1.83189800	-0.00058800
F	-3.79910400	0.89322400	1.08153500	C	-2.62234400	0.82471300	0.00001200
F	-3.80124700	0.89111900	-1.08035300	S	-1.64996900	-0.76650900	-0.00023300
F	-2.19088600	1.84648100	-0.00186200	O	-0.72518500	-0.64204800	1.18388300
I	2.99866600	0.22427200	0.00026200	F	-3.37958300	0.86849900	1.08044800
1				F	-3.37894500	0.86920300	-1.08084700
				F	-1.78976700	1.85554300	0.00059100
O	-2.80280700	-0.41224800	1.24409700	A1			
C	0.38970300	0.52712700	0.90877200	O	-0.83412500	2.62482300	1.02484200
C	0.74296500	1.01368300	-0.61752000	C	-0.98369400	3.05162300	-0.10255800
C	-0.47867400	1.42031300	1.76983700	O	-0.70501500	2.40356900	-1.20400400
H	-0.94209300	0.81545700	2.54558800	C	-1.54639200	4.42583600	-0.38551100
H	0.12144700	2.20889200	2.22352300	H	-2.60979200	4.31531900	-0.61175800
H	-1.28293800	1.86837700	1.18710000	H	-1.43344000	5.05280200	0.49730200
C	0.14430100	2.31087700	-1.11342100	H	-1.06238600	4.87885600	-1.25038500
H	0.57856700	2.54807200	-2.08394200	Pd	-0.30513400	0.47923000	-1.23417500
H	-0.93709500	2.21848400	-1.22329800	O	-2.30491000	0.08573300	-0.91747900
H	0.36250300	3.12860800	-0.42667500	O	-3.83423200	-1.83652400	-0.79492800
C	-2.87443400	-0.32479800	0.03967700	C	-3.70476000	-0.16854800	1.26721000
C	-4.19114600	-0.40820200	-0.70380800	S	-2.82823000	-1.07464100	-0.09873200
H	-4.26613500	-1.37840600	-1.20289700	O	-1.76462900	-1.80878100	0.58367100
H	-5.00514200	-0.31583700	0.01166800	F	-4.34377000	-1.04457300	2.03533300
H	-4.27518000	0.37208700	-1.46425800	F	-4.58168200	0.69062100	0.77011700
N	-1.76918000	-0.14601400	-0.76706700	F	-2.82485800	0.48967300	2.01142700
				O	-0.05984300	-1.51355200	-1.71801700

C	3.16247600	-0.81685300	1.34995000	H	2.47401600	-2.11587400	2.58859800
C	1.91738500	0.21156800	1.00620500	C	1.02966200	0.09045800	2.09762900
C	2.94774300	-1.84617400	2.44144900	H	0.39330600	0.97353500	2.03440400
H	3.68744500	-2.63926100	2.33102400	H	0.40536700	-0.77948000	1.88522700
H	3.07599200	-1.39162800	3.42281100	H	1.44081100	0.01769600	3.10472600
H	1.94758700	-2.27864700	2.39310800	C	0.42234700	-2.54432400	-0.73013900
C	0.65308500	0.04670200	1.81719600	C	-0.18685700	-3.90711200	-0.68735800
H	0.02700200	0.92844400	1.66362700	H	0.51806700	-4.68108500	-0.38233200
H	0.08934700	-0.83664000	1.51224300	H	-1.01134200	-3.84855500	0.03003800
H	0.89644500	-0.02658700	2.87739700	H	-0.61242800	-4.13706800	-1.66237000
C	0.46255400	-2.44775100	-1.09149700	N	1.50385300	-2.28725500	0.02507600
C	-0.10437900	-3.82045500	-1.25370900	H	1.88121700	-3.08014000	0.52079500
H	0.62425700	-4.60693100	-1.05432000	B	2.32650800	-1.06759300	-0.08726000
H	-0.93416300	-3.89067000	-0.54398400	B	4.06597700	-1.17759600	-0.36362700
H	-0.51108500	-3.92221700	-2.25798400	B	4.87104000	0.00377800	0.67417400
N	1.50184000	-2.27717100	-0.25505200	H	5.86927600	-0.29175900	1.23578600
H	1.85227900	-3.12734200	0.15971200	B	3.63967000	0.88324700	1.59478200
B	2.34258900	-1.07145700	-0.14230700	H	3.73917000	1.14203900	2.74155200
B	4.09924300	-1.19880700	-0.03421900	B	1.79021200	0.54586400	-0.58205200
B	4.67383600	-0.04749200	1.17613600	H	0.74227000	1.60030400	-0.87570400
H	5.52393600	-0.37206800	1.93141200	B	3.03932000	-0.31336000	-1.51910100
B	3.28593400	0.83914000	1.83086000	H	2.78967500	-0.77359200	-2.58047300
H	3.14235600	1.07013900	2.97804900	B	4.62774500	0.35005500	-1.04899500
B	1.95589200	0.56522800	-0.67814000	H	5.54024300	0.37288800	-1.80292700
H	1.20285500	0.96819500	-1.64993800	B	4.35695600	1.62458200	0.16530300
B	3.35479100	-0.29555400	-1.35947100	H	5.06147800	2.56735700	0.28832600
H	3.31528000	-0.71768700	-2.46498100	B	2.61400600	1.74609500	0.45464000
B	4.80932000	0.33792700	-0.54986100	H	2.02561900	2.69143200	0.84301300
H	5.86055600	0.36401500	-1.09338600	B	3.21687800	1.42154800	-1.19186800
B	4.29898700	1.59237200	0.60833200	H	3.08948100	2.23829800	-2.03974800
H	4.97486900	2.51864200	0.90011900	H	4.50648400	-2.26972400	-0.48730700
B	2.52914000	1.73881300	0.52105900				
H	1.85988100	2.67414200	0.77744100	A2			
B	3.47374400	1.43602100	-0.95877500				
H	3.53050000	2.26234200	-1.80410200	Pd	-0.59049100	0.72310800	-0.11730200
H	4.54858500	-2.29362800	-0.08134000	O	0.52868600	2.41898700	0.29409600

TS A1-A2

O	-0.63913000	2.63471700	1.17003700	C	3.68176800	-0.69079600	-0.29162800
C	-0.78289400	3.04793700	0.04899200	C	2.20323900	-0.53046600	-0.99500400
O	-0.37947900	2.40097400	-1.05403200	C	4.86395800	-0.00505300	-0.94384700
C	-1.43677200	4.35558700	-0.30507300	H	5.69921000	0.00459300	-0.24380900
H	-2.36555700	4.14808400	-0.84080100	H	5.17275700	-0.54018300	-1.84111600
H	-1.64992800	4.91200800	0.60502900	H	4.62610700	1.02364800	-1.22082100
H	-0.79153800	4.93223000	-0.96912800	C	2.10201700	0.29420500	-2.25982300
Pd	-0.31092500	0.33368500	-1.05600700	H	1.10670400	0.15968300	-2.68151800
O	-2.39489800	-0.08395100	-1.10412100	H	2.24589700	1.35562000	-2.05463800
O	-3.75388500	-2.09304500	-0.64241600	H	2.83910500	-0.03004900	-2.99478900
C	-4.02025800	0.02664200	0.92806800	C	1.71703900	2.68631600	0.49951000
S	-2.90835700	-1.06575300	-0.08229700	C	2.08636300	4.11531800	0.78131600
O	-1.86659800	-1.48772200	0.85582700	H	3.13762700	4.32499000	0.58046400
F	-4.53543800	-0.66469300	1.93865600	H	1.45396900	4.76915400	0.18331700
F	-5.01036900	0.50187100	0.18334300	H	1.88120000	4.31871100	1.83550100
F	-3.32764400	1.05038300	1.42060100	N	2.70568300	1.77001900	0.50340400
O	-0.10651600	-1.67856700	-1.44193400	H	3.61498300	2.12390800	0.75934300
C	3.44277800	-0.77789200	1.18563500	B	2.50984100	0.30378700	0.50183300
C	2.13779200	0.23391200	1.07839100	B	3.54602300	-0.78625800	1.41443300
C	3.47733500	-1.78080100	2.32123800	B	3.84620300	-2.22356200	0.42968900
H	4.07341500	-2.64341600	2.02133800	H	4.92636500	-2.70656400	0.41362200
H	3.93496100	-1.33868300	3.20497100	B	2.99146200	-2.05138100	-1.10932500
				H	3.46227500	-2.32524600	-2.15703600
				B	0.96457400	-0.48022200	0.20337700
				B	1.80865600	-0.69455100	1.76153100

H	1.41305600	-0.16232100	2.74387600	B	0.41613800	-2.62812800	0.53791400
B	2.62983900	-2.27076000	1.72595000	H	-0.60970900	-2.95956400	0.05898000
H	2.82233300	-2.89550100	2.71373200	B	0.71564700	-1.87991200	2.12835300
B	2.28842100	-3.04124900	0.15799900	H	-0.16935700	-1.71714800	2.89535100
H	2.22867000	-4.21389900	0.00751800	H	4.60296900	-1.22508200	1.59167300
B	1.26006800	-1.93295800	-0.77787600	C	-1.30234200	3.77588900	2.23034900
H	0.50678400	-2.20706600	-1.64506200	C	-1.39522000	2.94434900	1.12153100
B	1.02442400	-2.08401700	0.97572800	C	-0.23576600	2.30672700	0.68552800
H	0.04118800	-2.57584100	1.41213300	C	1.00459700	2.53399900	1.26515500
O	-1.86558100	-0.85605700	-0.65738900	C	1.06722700	3.36837800	2.37409300
O	-2.89192500	1.32781100	-0.69540000	C	-0.07927500	3.98556700	2.85661800
C	-4.09540600	-0.56383600	0.71954000	H	-2.19929300	4.25819400	2.59991300
S	-3.17176700	-0.11227900	-0.83079400	H	-2.34585200	2.77415400	0.63365000
O	-3.98700700	-0.56611900	-1.92328900	H	1.89931300	2.06446300	0.88478400
F	-5.26207800	0.06566100	0.74762500	H	2.02420800	3.52943800	2.85609100
F	-3.38938700	-0.20685900	1.79021300	H	-0.01952600	4.63837300	3.71921700
F	-4.30514100	-1.87130300	0.76181100	I	-0.12798000	1.85390000	-1.72586500
H	4.42749100	-0.29301600	2.03598500				

A3

TS A2-A3

Pd	-0.83263200	0.28027800	0.29361000	Pd	0.26807200	0.49838100	0.21556000
O	-2.18202500	-1.25632800	1.06562700	O	0.01495900	-0.33536500	2.19029400
O	-4.61839200	-0.93284700	1.46848100	C	-3.29510300	-2.23595300	-0.20156700
C	-3.82262700	-1.68871900	-0.94202100	C	-2.01181100	-1.49994000	-0.98060800
S	-3.49859200	-0.69899900	0.60072200	C	-3.26955100	-3.74264700	-0.04152200
O	-3.26549200	0.67188300	0.10388500	H	-3.79111700	-4.01522400	0.87678200
F	-4.92478800	-1.26214400	-1.53789100	H	-3.77587800	-4.22222000	-0.87797000
F	-3.95147100	-2.97319500	-0.64639400	H	-2.24870800	-4.12540700	0.00283400
F	-2.79746100	-1.55070200	-1.79141600	C	-0.90984900	-2.39170600	-1.50546000
O	5.26019700	0.33277500	-0.38243400	H	-0.23457100	-1.78629500	-2.10932200
C	3.08334200	-2.29005900	-0.07009400	H	-0.31745600	-2.81480500	-0.69647500
C	1.54813800	-1.92239800	-0.52031900	H	-1.32762400	-3.18134200	-2.12956000
C	4.12539300	-2.46993100	-1.15347900	C	-0.39094900	-1.47929200	2.43653900
H	3.99442900	-1.73621800	-1.94877500	C	0.21592600	-2.23508300	3.57488200
H	5.11083500	-2.31109900	-0.72064100	H	-0.32457300	-3.14969100	3.82008100
H	4.06494200	-3.47187700	-1.57756100	H	1.24629300	-2.46981500	3.28891800
C	1.24604500	-1.80157300	-1.99764600	H	0.25449300	-1.57971800	4.44514700
H	0.17528700	-1.65090100	-2.12985800	N	-1.34734900	-2.06826100	1.69411000
H	1.77378300	-0.95710900	-2.44101200	H	-1.63183700	-2.98499100	2.00155400
H	1.53585400	-2.71290600	-2.51978700	B	-2.20833300	-1.32625600	0.75502200
C	4.28162900	0.89628900	-0.81242600	B	-3.95087900	-1.22960100	1.02045400
C	4.35585900	2.17775700	-1.61651000	B	-4.75545700	-1.42253000	-0.53493500
H	3.84320700	2.06463400	-2.57563300	H	-5.72736300	-2.09178300	-0.61957300
H	3.86921700	2.99309000	-1.07369100	B	-3.52154500	-1.61147000	-1.78883200
H	5.40004500	2.42872900	-1.78746300	H	-3.58856700	-2.39912900	-2.66521200
N	2.99279800	0.43545600	-0.62059200	B	-1.71550700	0.04473100	-0.27188100
H	2.27785000	0.98592400	-1.07490100	B	-2.97409900	0.24996600	0.97924100
B	2.53672700	-0.65750300	0.23380100	B	-4.56336400	0.19092900	0.17531800
B	3.48437000	-1.55344400	1.42863100	H	-5.49262200	0.78994800	0.59916200
B	3.08704800	-3.27404700	1.31602800	B	-4.29961100	-0.05281800	-1.56581900
H	3.95408400	-4.07419600	1.39906700	H	-5.02734500	0.36580400	-2.39998800
B	1.86540600	-3.50902400	0.06917500	B	-2.54929800	-0.14051400	-1.84774700
H	1.88399300	-4.37262900	-0.73516200	H	-2.00637200	0.09415200	-2.86533000
B	0.82009500	-0.90312800	0.65396900	B	-3.18966100	0.97887700	-0.63087400
B	2.02486600	-0.68099800	1.93306500	H	-3.17087600	2.14391700	-0.80903300
H	2.09061700	0.31723000	2.56377200	C	-0.16471600	2.33112100	0.88628800
B	2.37458900	-2.28689100	2.60534600	C	-0.93017400	3.31590300	0.28820500
H	2.70610800	-2.42255100	3.73422700	C	0.49840500	2.54264000	2.08650100
B	1.37774400	-3.49032500	1.75399400	C	-1.07955200	4.53343300	0.94453800
H	0.98292600	-4.48680400	2.25595000	H	-1.39428100	3.16182600	-0.67264100
				C	0.34144300	3.77011300	2.72458100

H	1.13237900	1.78145100	2.52352200	C	-2.78112900	3.77969600	2.22579700
C	-0.45259600	4.76010500	2.16227400	H	-2.97405100	4.64092600	0.26469400
H	-1.68144500	5.30900700	0.48468400	H	-2.43650300	2.67333000	4.03772700
H	0.85102100	3.94271700	3.66568900	H	-3.31246200	4.58431400	2.72127500
H	-0.57043400	5.71315600	2.66480700	I	0.84773600	2.08474300	-1.59280300
I	0.76409900	1.42755900	-2.13535100	O	1.88565400	-0.62243600	-0.04516500
O	1.41176600	-1.54558500	-0.02330900	O	3.26417700	0.36230900	1.75106700
O	2.64081900	0.30215600	0.93568500	C	4.44738000	-0.56059600	-0.44501900
C	3.99411400	-1.42465500	-0.57310000	S	3.11137300	-0.74466700	0.83357800
S	2.66356100	-1.15031300	0.69453000	O	3.25649600	-2.09833600	1.34262500
O	3.01530100	-2.00783700	1.80749100	F	5.63436200	-0.72222200	0.12771400
F	5.16737500	-1.05726300	-0.07697600	F	4.39632300	0.64150500	-0.99844200
F	3.74689100	-0.72253100	-1.66821200	F	4.30121600	-1.47963900	-1.39540000
F	4.04325500	-2.71432900	-0.89206800	H	-3.61488400	-3.48093700	1.00464500
H	-4.35786300	-1.77690200	1.98835200	H	-3.16315300	-0.67287400	2.15196000
H	-2.74455800	0.86142500	1.96511800				

A4

TS A3-A4

Pd	0.16261400	0.53698700	0.39070400	O	1.50472200	1.96641700	1.01296500
O	0.07367900	-0.73015700	2.10689000	C	-2.32005100	0.56092100	0.35483800
C	-2.51260500	-2.64766800	-1.04361200	C	-1.00544600	-0.22760400	0.97280000
C	-1.62043900	-1.28602500	-1.33118900	C	-2.79887600	1.80952300	1.05887100
C	-1.91528900	-3.98591500	-1.43027300	H	-3.73060100	2.13477100	0.59721200
H	-2.43592700	-4.77499600	-0.88737400	H	-2.98311800	1.61839900	2.11580100
H	-2.04051000	-4.16478400	-2.49750800	H	-2.06270400	2.60898500	0.96186500
H	-0.85076300	-4.03712900	-1.19791800	C	-0.41528500	0.24438200	2.28638900
C	-0.29317300	-1.51019700	-2.02512700	H	-0.87801500	-0.29447100	3.11284300
H	0.03225400	-0.57781700	-2.48181100	H	0.65753500	0.06856500	2.27923300
H	0.48267600	-1.82656700	-1.32813900	H	-0.55407900	1.31462300	2.42491800
H	-0.40571600	-2.25303600	-2.81438600	C	1.02322900	2.46545900	0.02318100
C	-0.03882800	-1.96469600	2.03162100	C	1.63757900	3.67623000	-0.64797600
C	0.66905200	-2.82830500	3.02222900	H	2.18173100	3.34911700	-1.53872200
H	0.19357600	-3.80187900	3.14531000	H	0.88297000	4.40328600	-0.95767600
H	1.69442900	-2.95089800	2.65484300	H	2.33928900	4.14171000	0.04043300
H	0.71764900	-2.30464700	3.97541900	N	-0.10800200	1.98125700	-0.60012500
N	-0.76577400	-2.54463200	1.05819000	H	-0.37943600	2.49441200	-1.42544200
H	-0.81719500	-3.55073100	1.10970800	B	-0.76903600	0.67557700	-0.48220800
B	-1.82839900	-1.83524400	0.31497600	B	-2.31625100	0.47684400	-1.33811400
B	-3.46702000	-2.49767400	0.36090500	B	-3.41904900	-0.51920900	-0.37781100
B	-4.17775900	-2.35664700	-1.24952200	H	-4.56559800	-0.23386200	-0.31115300
H	-4.81723400	-3.24743400	-1.69282000	B	-2.58223600	-0.94567600	1.10952800
B	-2.99310000	-1.58098200	-2.31137700	H	-3.07123200	-0.93283100	2.18440800
H	-2.77675100	-1.92853700	-3.41773900	B	-0.03891100	-0.93977800	-0.29646200
B	-1.91783900	-0.07193400	-0.05650700	B	-0.91467000	-0.50898500	-1.78448300
B	-3.14334400	-0.87513000	0.98711500	H	-0.32618800	-0.30322400	-2.79394000
B	-4.60539300	-1.19901400	0.01649300	B	-2.53146000	-1.23918600	-1.73245200
H	-5.68034700	-1.18848200	0.51258100	H	-3.09809500	-1.56725300	-2.72042800
B	-4.30098300	-0.62965200	-1.63836400	B	-2.68549900	-2.12092900	-0.19188700
H	-5.14541700	-0.21287600	-2.35523100	H	-3.34542900	-3.09339200	-0.04308200
B	-2.64695700	0.03602700	-1.68524400	B	-1.15848200	-1.90211200	0.69125000
H	-2.23806200	0.83833700	-2.44916800	H	-0.72737900	-2.62327500	1.52463200
B	-3.67034800	0.28050800	-0.25329800	B	-1.13790300	-2.11630500	-1.06600700
H	-4.10497400	1.34134900	0.02355600	H	-0.68277800	-3.09424400	-1.55635300
C	-1.41193100	1.70579500	0.94723200	H	-2.72121100	1.42711400	-1.92140800
C	-1.91506900	2.78660500	0.21296300	C	3.52656700	-1.82055600	0.97599800
C	-1.60802600	1.68087900	2.33475500	C	2.14309600	-1.74430900	0.87808900
C	-2.58979700	3.81436800	0.85064600	C	1.52652700	-1.04672900	-0.16362800
H	-1.80918900	2.81339300	-0.86106300	C	2.35109700	-0.44274200	-1.11782500
C	-2.29172000	2.70956100	2.96433200	C	3.73393900	-0.51933500	-1.03020900
H	-1.23123800	0.85615100	2.92287000	C	4.32682900	-1.20540700	0.02239500
				H	3.98047300	-2.36415700	1.79722500

H	1.53472200	-2.24239100	1.62568400				
H	1.90143300	0.09571100	-1.94616300				
H	4.35128200	-0.04286700	-1.78400900				
H	5.40692300	-1.26504200	0.09696300				
B1				TS B1-B2			
O	-1.09628900	2.42524500	0.98313900	O	-0.79421300	2.51905000	1.21524500
C	-1.14754500	2.90706200	-0.12503700	C	-0.92162200	2.93904300	0.09769300
O	-0.78620700	2.28866400	-1.23055500	O	-0.52471200	2.26761200	-1.00154300
C	-1.66480300	4.30021100	-0.40379500	C	-1.54503100	4.25723400	-0.27223900
H	-2.73020800	4.22435400	-0.63509700	H	-2.48201100	4.06448200	-0.79918600
H	-1.54173800	4.91243800	0.48835800	H	-1.74142600	4.82834900	0.63257000
H	-1.16062500	4.75077600	-1.25820300	H	-0.89029900	4.81213600	-0.94533900
Pd	-0.34285300	0.38404600	-1.08308100	Pd	-0.33500300	0.22919300	-0.72740800
O	-2.35303000	-0.05206600	-0.93998800	O	-2.34158800	-0.28106200	-1.06863900
O	-3.45504300	-2.23154000	-0.57718000	O	-3.88940200	-2.16779000	-0.75315200
C	-4.18882300	-0.16438800	0.91086200	C	-4.34389500	0.09714100	0.54353100
S	-2.82487300	-1.09391400	0.05550400	S	-3.11505300	-1.14058300	-0.09786700
O	-1.82523300	-1.36878800	1.08143900	O	-2.32533100	-1.51585300	1.06951500
F	-4.72425600	-0.94800000	1.84195500	F	-5.09156300	-0.45544200	1.49195100
F	-5.12953500	0.16869400	0.03634500	F	-5.13566200	0.51743000	-0.43644000
F	-3.72096200	0.93010500	1.48396200	F	-3.71024000	1.14865400	1.05708800
O	0.03369400	-1.67128300	-1.23924000	O	-0.00900900	-1.82001000	-0.68832100
C	3.15618600	-0.29967100	-0.70561500	C	2.92836800	-0.28600800	-0.87414900
C	3.82110600	-0.83372600	0.68597700	C	3.97918700	-0.82834000	0.25781900
C	3.17890500	-1.20224900	-1.92118000	C	2.64897600	-1.17288800	-2.07080200
H	2.42086000	-0.87281400	-2.63060800	H	1.78238400	-0.78853500	-2.60604100
H	4.15450000	-1.16465800	-2.40396600	H	3.50603500	-1.17712400	-2.74354000
H	2.95619200	-2.23511400	-1.65231200	H	2.42931600	-2.19634900	-1.76984300
C	4.44066500	-2.21500000	0.70325200	C	4.58339000	-2.20299500	0.06844000
H	4.88330400	-2.38715900	1.68348300	H	5.32017600	-2.37261000	0.85274000
H	3.69599300	-2.98882300	0.51495700	H	3.82177300	-2.98107500	0.12894800
H	5.22487000	-2.29685100	-0.04894200	H	5.08297500	-2.27875500	-0.89697300
C	0.41386900	-2.40453800	-0.31048400	C	0.49703500	-2.46910900	0.23975600
C	-0.16262700	-3.77691100	-0.18704900	C	-0.11878700	-3.77260000	0.62275700
H	0.45926800	-4.44552500	0.40880100	H	0.52471600	-4.38864200	1.25106000
H	-1.14221000	-3.66260800	0.28513600	H	-1.04436800	-3.51880900	1.15037600
H	-0.32104700	-4.18623900	-1.18376800	H	-0.40094100	-4.30970600	-0.28231900
N	1.34458100	-2.01244800	0.57868200	N	1.58032100	-2.03024900	0.90726100
H	1.45730700	-2.61917600	1.37737000	H	1.86145500	-2.58488700	1.70195200
B	2.06516400	-0.72854200	0.60919100	B	2.27821500	-0.74819900	0.70083000
B	1.81055800	0.71718600	-0.37346000	B	1.70563900	0.68492100	-0.13636200
B	3.37148300	1.39057600	-0.86481500	B	3.05997400	1.39792400	-1.05214900
H	3.49956000	1.80430600	-1.96499500	H	2.85305100	1.84089900	-2.12892100
B	4.65558500	0.38816400	-0.18847700	B	4.50742000	0.41926600	-0.79771200
H	5.61662300	0.05254300	-0.78572400	H	5.25996800	0.11224400	-1.65301800
B	2.95912600	-0.23700000	2.04012000	B	3.55260400	-0.26759800	1.81791800
H	2.88449500	-0.95977200	2.97590200	H	3.76782700	-1.00811800	2.71818000
B	1.66802300	0.80371700	1.39885700	B	2.11910500	0.75663800	1.59921900
H	0.62573200	0.89284300	1.93929500	H	1.26824200	0.82379500	2.41526700
B	2.46364200	2.11774300	0.48609500	B	2.58790000	2.09035500	0.52274900
H	1.95772100	3.17760600	0.35276600	H	2.06173000	3.14844400	0.57476600
B	4.22912100	1.90114900	0.60242200	B	4.30644000	1.91030600	0.10709800
H	5.00101400	2.79765800	0.57858200	H	5.01809400	2.82637700	-0.12703100
B	4.52623800	0.44237300	1.56872100	B	4.90031200	0.44722200	0.91938600
H	5.48773200	0.17534300	2.20335200	H	6.01153600	0.19133300	1.23301400
B	3.18483000	1.52386100	1.99539400	B	3.73158300	1.49490300	1.74368600
H	3.21484600	2.15166400	2.99766800	H	4.04577100	2.11529800	2.70130600
H	1.19214000	0.86292300	-1.49226300	H	0.65226900	1.55052700	-0.73056100
				B2			
				Pd	-0.60160900	0.87653800	-0.55655000
				O	0.56827500	2.51514600	-0.06391400
				C	1.69934700	-0.76161000	0.88966300

C	3.33288900	-0.88136000	0.72914400	H	0.01218100	-2.31262000	4.04032900
C	1.14459600	-0.24098800	2.19826900	N	-1.56809100	-2.36482200	1.21876400
H	0.06591800	-0.39082000	2.19907200	H	-1.70143800	-3.36454600	1.22383700
H	1.57363700	-0.77985300	3.04336900	B	-2.14967300	-1.61198600	0.09645300
H	1.34087300	0.82485100	2.31975300	B	-1.55330100	-0.09949500	-0.62488900
C	4.19939300	-0.45784000	1.89650300	B	-2.96139200	0.90273800	-1.01935000
H	5.22275600	-0.31730400	1.54873800	H	-2.95089200	2.06929100	-0.84193600
H	3.84517600	0.47645500	2.33561500	B	-4.43879200	0.05153200	-0.55811900
H	4.20118300	-1.22365400	2.67121900	H	-5.35112800	0.56463300	-0.01194800
C	1.75711000	2.72817600	0.19690400	B	-3.14482400	-2.44311900	-1.09679200
C	2.18885400	4.14680100	0.43939700	H	-3.27571000	-3.61239900	-0.95258900
H	3.12155100	4.21367800	1.00062200	B	-1.66537200	-1.59305100	-1.59954800
H	2.32508200	4.63189000	-0.53057000	H	-0.69222300	-2.18705700	-1.91001900
H	1.39581100	4.67275900	0.96831400	B	-2.16706900	-0.03408200	-2.29992600
N	2.69743100	1.76569600	0.26425100	H	-1.54656700	0.49848800	-3.15248600
H	3.63831700	2.09606300	0.41627100	B	-3.94153800	0.06306600	-2.24198600
B	2.51831900	0.35930000	-0.15869300	H	-4.58501500	0.66982700	-3.02904800
B	0.97277400	-0.34178200	-0.61796800	B	-4.54021700	-1.43253500	-1.50179600
B	0.90082500	-1.99662600	0.02999100	H	-5.60364300	-1.93185300	-1.64092600
H	-0.11123100	-2.39455600	0.49086400	B	-3.14065100	-1.49010600	-2.59001700
B	2.40005200	-2.32796100	0.90428400	H	-3.21516600	-2.01884400	-3.64697300
H	2.46463600	-2.86946000	1.95162400	C	0.39059200	2.45516500	0.62861900
B	3.81639900	-0.57805500	-0.88750500	C	-0.78704200	3.17046800	0.80324500
H	4.86010300	-0.03270700	-1.02728900	C	1.44388000	2.54183900	1.53334200
B	2.31773400	-0.26884600	-1.78530800	C	-0.93926200	3.93406100	1.95378100
H	2.29921800	0.50376900	-2.68380100	H	-1.56546700	3.14101900	0.05645600
B	1.30887500	-1.73091000	-1.67900100	C	1.26557600	3.31007700	2.67861400
H	0.54560900	-2.02885400	-2.53159400	H	2.36635700	2.00145100	1.36809900
B	2.20021300	-2.94724800	-0.72548100	C	0.07956700	3.99928500	2.89648000
H	2.09490800	-4.11471200	-0.89076400	H	-1.86130700	4.48504300	2.10179900
B	3.74937100	-2.21991600	-0.23368700	H	2.07124200	3.36330100	3.40144400
H	4.75480000	-2.78028100	0.04072300	H	-0.04474800	4.59744200	3.79134500
B	3.07772000	-1.87489200	-1.84445900	I	0.96394500	2.04525400	-1.68640900
H	3.61329900	-2.27864400	-2.82073600	O	1.31132300	-2.10495400	-0.03668300
O	-1.92952700	-0.67690500	-1.02212900	O	2.53244000	-0.16074000	0.76879600
O	-3.03471800	1.38645700	-0.42360900	C	3.82518600	-1.83689200	-0.79280600
C	-3.53965200	-0.75764700	1.05018600	S	2.57347400	-1.63120300	0.56238200
S	-3.25346600	-0.04995000	-0.64831000	O	3.07454700	-2.40724500	1.67923400
O	-4.37252500	-0.47837200	-1.43925900	F	5.00054600	-1.34904900	-0.41419200
F	-4.66153200	-0.27635600	1.56440700	F	3.42596600	-1.18883600	-1.88450500
F	-2.52826500	-0.43106800	1.86553700	F	3.96928500	-3.12323900	-1.09075200
F	-3.61718600	-2.07915000	0.99261900				

TS B2-B3

Pd	0.28770400	0.29847700	0.15089100
O	-0.26184100	-0.71187300	2.02578900
C	-2.97999500	-0.10018100	0.35871200
C	-3.89225300	-1.44590500	0.06985700
C	-3.00706000	0.48613700	1.75520800
H	-2.15669600	1.15365900	1.88166300
H	-3.92943400	1.04505200	1.91079900
H	-2.93170700	-0.29270900	2.51320800
C	-4.66424500	-2.04613800	1.22429400
H	-5.25187100	-2.88454200	0.85199000
H	-3.99063100	-2.40939800	2.00089700
H	-5.34368000	-1.31389300	1.65992900
C	-0.63203900	-1.89068800	2.06795300
C	-0.04473700	-2.82369100	3.07936100
H	-0.60421800	-3.75417100	3.17986800
H	0.98054200	-3.04002700	2.76134200

B3

Pd	0.30755400	0.42113100	0.20440100
O	-0.19337900	-0.66075800	2.01826000
C	-2.92982700	-0.31347500	0.26531900
C	-3.68057500	-1.74932400	-0.05999900
C	-3.07985200	0.24206700	1.66733100
H	-2.33489600	1.01599100	1.83595100
H	-4.07124900	0.67594300	1.79111100
H	-2.93790000	-0.53373400	2.41898800
C	-4.41489400	-2.44091400	1.06858600
H	-4.89461600	-3.33599400	0.67432500
H	-3.73259200	-2.73298600	1.86716100
H	-5.18369500	-1.79080600	1.48519300
C	-0.50568100	-1.86058200	2.06702600
C	0.02991000	-2.71713800	3.16846900
H	-0.51504800	-3.65475000	3.28119800
H	1.07946300	-2.91961400	2.92859100
H	0.00543800	-2.15139600	4.09939400

N	-1.31472400	-2.41693400	1.14971300	H	-0.99113400	-3.61509000	-0.15427000
H	-1.40254200	-3.42106600	1.18851900	B	-1.78168200	-1.66215700	-0.54173000
B	-1.93154200	-1.72316500	0.00593800	B	-1.74773900	0.13336300	-0.36850900
B	-1.48292900	-0.15309500	-0.69062600	B	-3.45737900	0.67990500	-0.46044700
B	-2.98422600	0.70060800	-1.10410600	H	-3.85646000	1.53293500	0.24772900
H	-3.11618000	1.85472700	-0.90878200	B	-4.51802900	-0.70812900	-0.66976900
B	-4.37101200	-0.31483100	-0.69043400	H	-5.53291000	-0.85160700	-0.08451900
H	-5.34483300	0.09176700	-0.16228200	B	-2.45692200	-2.06474300	-2.11880800
B	-2.80032200	-2.64766100	-1.21441200	H	-2.16486900	-3.12811200	-2.55168800
H	-2.80216800	-3.82525700	-1.07916700	B	-1.38110400	-0.66892700	-1.94595500
B	-1.41178400	-1.63638100	-1.67860300	H	-0.28315500	-0.70927900	-2.37831100
H	-0.37569500	-2.12030900	-1.97035200	B	-2.40930300	0.78842300	-1.88996700
B	-2.06560800	-0.13168200	-2.37818700	H	-2.03154400	1.83276000	-2.29397600
H	-1.49968100	0.47199100	-3.21732700	B	-4.10603700	0.27609800	-2.06053800
B	-3.83856700	-0.23301900	-2.35720300	H	-4.93733800	0.95191600	-2.56321600
H	-4.52429400	0.30886800	-3.15535400	B	-4.12664300	-1.49151400	-2.20130300
B	-4.28788000	-1.79289300	-1.64630600	H	-4.95683700	-2.17074500	-2.69967100
H	-5.28937700	-2.39987200	-1.81219200	B	-2.82853600	-0.55937500	-2.97149400
B	-2.86772400	-1.68472600	-2.69991900	H	-2.73877000	-0.48871000	-4.14930800
H	-2.85577500	-2.20715900	-3.76207400	C	-1.13922300	1.55521400	1.13965300
C	-0.29813700	2.13411700	1.02224200	C	-1.55058100	2.80670600	0.66335600
C	-1.11064500	3.12428500	0.49217000	C	-1.27303900	1.28113900	2.50783300
C	0.24733800	2.25087600	2.29556400	C	-2.10064800	3.74148200	1.52373800
C	-1.43751200	4.22161900	1.28238500	H	-1.46394500	3.04230900	-0.38716400
H	-1.47423200	3.06216900	-0.52200100	C	-1.82382500	2.22472700	3.36603700
C	-0.08033400	3.36088100	3.06917900	H	-0.92678200	0.33907900	2.91053600
H	0.92100300	1.49678300	2.68604800	C	-2.24374900	3.45384200	2.87617200
C	-0.93090100	4.33872300	2.57046400	H	-2.41728900	4.70088400	1.13165600
H	-2.07770100	4.99555700	0.87406500	H	-1.90960400	1.99900300	4.42281100
H	0.34301600	3.45659600	4.06258000	H	-2.67053600	4.19006400	3.54776700
H	-1.18284400	5.20089900	3.17717200	I	1.19749900	2.21762700	-1.24945200
I	1.07404000	1.75383000	-1.86179700	O	1.91625000	-0.86134800	-0.30533800
O	1.45675400	-1.53739100	-0.22445800	O	3.14152000	-0.30625600	1.76057400
O	2.59082500	0.08828100	1.16135100	C	4.52731000	-0.74226700	-0.46254500
C	4.09569300	-1.37412400	-0.47870400	S	3.07536200	-1.18463400	0.61026700
S	2.63423600	-1.29974900	0.66644600	O	3.19103100	-2.61780700	0.82377500
O	2.86924200	-2.34428400	1.64387000	F	5.65116800	-1.06540400	0.16885400
F	5.20861700	-1.16040500	0.21153100	F	4.53684900	0.55782500	-0.71520100
F	3.99239400	-0.45746900	-1.42741700	F	4.47406500	-1.40653900	-1.61074500
F	4.15932800	-2.57473400	-1.04213600				

TS B3-B4

Pd	0.29320000	0.35264600	0.32338500
O	-0.04586900	-1.28334900	1.69748800
C	-3.07554100	-0.80429400	0.27807300
C	-3.46216600	-2.05695800	-0.74119800
C	-3.31353000	-1.02959700	1.75592000
H	-3.44758600	-0.06138500	2.23399000
H	-4.21717900	-1.61805200	1.91052400
H	-2.47230900	-1.52888200	2.23138800
C	-3.94744700	-3.35600600	-0.13125500
H	-3.85233500	-4.14884800	-0.87315900
H	-3.36419700	-3.62966400	0.74839800
H	-4.99612700	-3.27757300	0.15343400
C	-0.22578000	-2.43830300	1.27483300
C	0.41489100	-3.59328900	1.96854500
H	-0.09062000	-4.53846400	1.76799800
H	1.45309100	-3.63680100	1.61740300
H	0.44134600	-3.39229000	3.03870600
N	-0.99552900	-2.66960100	0.19762800

B4

O	-1.50475900	1.96641700	1.01234700
C	1.00558500	-0.22750200	0.97272200
C	2.32031500	0.56032900	0.35472300
C	0.41572800	0.24480200	2.28636600
H	-0.65716100	0.06940000	2.27941000
H	0.87834400	-0.29418100	3.11279200
H	0.55506700	1.31498500	2.42480800
C	2.79962100	1.80890500	1.05850800
H	3.73144600	2.13372600	0.59674800
H	2.06371200	2.60859100	0.96140000
H	2.98384700	1.61790600	2.11546700
C	-1.02262000	2.46588700	0.02308400
C	-1.63601500	3.67746300	-0.64746400
H	-0.88090100	4.40489800	-0.95507000
H	-2.17887100	3.35158800	-1.53945000
H	-2.33867900	4.14208400	0.04055300
N	0.10865100	1.98154400	-0.60006800
H	0.38065100	2.49501000	-1.42500900
B	0.76909900	0.67558100	-0.48231600

B	0.03852600	-0.93952600	-0.29631100	H	0.37432800	-3.42962600	-3.08340300
B	1.15793400	-1.90213800	0.69143800	H	0.96372000	-3.72526100	-1.44038200
H	0.72640400	-2.62278000	1.52504900	N	-1.32330600	-2.07704400	-0.62335800
B	2.58213900	-0.94629500	1.10952100	H	-1.52648500	-2.95860900	-0.17827000
H	3.07106600	-0.93345500	2.18443200	B	-1.94564900	-0.84232500	-0.11715500
B	2.31624700	0.47617400	-1.33815300	B	-1.28908500	0.16741000	1.20839200
H	2.72172100	1.42608400	-1.92168100	B	-2.64953800	0.65474200	2.22448800
B	0.91436600	-0.50923100	-1.78438300	H	-2.53218700	0.64203800	3.40058100
H	0.32590800	-0.30329300	-2.79382400	B	-4.13719600	-0.02660200	1.54103500
B	1.13709600	-2.11650900	-1.06578200	H	-4.98525600	-0.53617700	2.18584600
H	0.68157700	-3.09439900	-1.55587000	B	-3.04507700	0.17633500	-1.08950900
B	2.68478500	-2.12168200	-0.19182800	H	-3.20869500	-0.14657000	-2.21479100
H	3.34442700	-3.09435700	-0.04314000	B	-1.55296600	0.85316000	-0.40813800
B	3.41887400	-0.52021300	-0.37795400	H	-0.84926900	1.40667700	-1.35378700
H	4.56553500	-0.23523100	-0.31167100	B	-1.97663000	1.79195800	1.04558500
B	2.53087400	-1.23997000	-1.73246000	H	-1.35052000	2.73377800	1.38635500
H	3.09730900	-1.56820600	-2.72049400	B	-3.73892200	1.67161100	1.26548200
C	-1.52690400	-1.04642000	-0.16337300	H	-4.38929900	2.52045900	1.77166000
C	-2.35136400	-0.44234100	-1.11762100	B	-4.38927300	0.69181600	-0.05766300
C	-2.14360000	-1.74405800	0.87821600	H	-5.48762300	0.70783300	-0.49433300
C	-3.73421700	-0.51896700	-1.03021700	B	-3.05035700	1.80775700	-0.37726300
H	-1.90158700	0.09624100	-1.94581800	H	-3.19124600	2.75935900	-1.06267600
C	-3.52708600	-1.82033200	0.97592100	H	-0.27232300	-0.19455200	1.68220900
H	-1.53534200	-2.24217000	1.62588400				
C	-4.32723800	-1.20515200	0.02224300				
H	-4.35145700	-0.04242800	-1.78405700				
H	-3.98109200	-2.36398500	1.79706100				
H	-5.40734100	-1.26482600	0.09665900				

C1

O	-0.09157100	3.55365400	-1.41653200
C	0.74406800	3.39934900	-0.54739400
O	1.21444900	2.24251800	-0.14640400
C	1.36923900	4.54541700	0.21570500
H	1.20526600	4.40607600	1.28569700
H	2.44720700	4.55034500	0.04452200
H	0.93160600	5.48490900	-0.11583700
Pd	0.59728300	0.63080200	-1.08517200
O	2.52817600	-0.12391900	-0.94267300
O	1.61077200	-1.99769400	0.38007900
C	3.32317800	-0.37830200	1.55122200
S	2.81898100	-1.26817800	-0.00264800
O	3.97004500	-2.03126400	-0.41509600
F	3.72626400	-1.26383800	2.45778000
F	2.28959400	0.29549100	2.05336400
F	4.30961800	0.46887400	1.30690300
O	0.11086100	-1.12735700	-2.10727200
C	-2.63284400	-0.86318200	1.44278400
C	-3.66421100	-0.84085300	0.11204400
C	-2.47071200	-2.13928600	2.24289900
H	-1.40923600	-2.36992800	2.34348600
H	-2.89587300	-2.01010800	3.23696400
H	-2.97238600	-2.98546500	1.76975700
C	-4.42848200	-2.09259100	-0.25948800
H	-5.25355000	-1.80418600	-0.90978100
H	-3.80072500	-2.79670100	-0.80655100
H	-4.84869300	-2.58074600	0.61968000
C	-0.38322500	-2.13761500	-1.58717400
C	0.07877900	-3.48647700	-2.03751500
H	-0.67674900	-4.26057900	-1.89717800

TS C1-C2

O	-0.50783800	3.31619500	-1.29310100
C	0.44357900	3.42738700	-0.49702000
O	1.10553400	2.42611000	-0.05855900
C	0.84038400	4.77561600	0.03136700
H	0.10472500	5.06870000	0.78457900
H	1.82719700	4.73883900	0.48705300
H	0.80893500	5.50871200	-0.77377100
Pd	0.56213600	0.70755800	-0.96380100
O	2.58575100	0.01981000	-0.94019400
O	1.79723600	-1.99752300	0.23400300
C	3.36655900	-0.34914700	1.53516800
S	2.95298400	-1.15800600	-0.08700200
O	4.16064500	-1.81634400	-0.52089400
F	3.75856200	-1.26716000	2.41372900
F	2.28999700	0.26868100	2.02829900
F	4.33410400	0.54353700	1.38580200
O	0.13996800	-1.00442700	-2.07719300
C	-2.65448800	-1.04613000	1.41276600
C	-3.58749700	-0.96761800	0.01559600
C	-2.53360800	-2.36003600	2.15688900
H	-1.47914900	-2.59548300	2.30814500
H	-3.01380000	-2.27958200	3.13087800
H	-3.00517100	-3.18162400	1.61475100
C	-4.30099500	-2.20939700	-0.47037900
H	-5.04554800	-1.90634000	-1.20547400
H	-3.61143500	-2.90151100	-0.95471700
H	-4.81808100	-2.71642400	0.34411400
C	-0.26634000	-2.07747700	-1.60800700
C	0.26343100	-3.36430400	-2.15316500
H	-0.44932000	-4.18439800	-2.05683700
H	0.53950900	-3.22122500	-3.19609600
H	1.16768800	-3.59248900	-1.58190500
N	-1.18146400	-2.12650500	-0.62110100
H	-1.31580300	-3.03209100	-0.19945700
B	-1.85977700	-0.93460100	-0.08958700

B -1.31105300 0.00843400 1.31889100
 B -2.74215000 0.43085200 2.26447300
 H -2.70772400 0.36243100 3.44430200
 B -4.16977000 -0.23069200 1.44535600
 H -5.05637700 -0.77681800 2.00308700
 B -2.89457300 0.11640600 -1.09198500
 H -2.98681400 -0.15920800 -2.23804200
 B -1.45071200 0.77667000 -0.28424600
 H -0.69085800 1.82502200 -1.21615100
 B -2.00468900 1.62893200 1.18628600
 H -1.41809200 2.55971500 1.62187900
 B -3.77561700 1.48220600 1.28049200
 H -4.47179600 2.30027400 1.77722900
 B -4.31755700 0.55968000 -0.13047600
 H -5.38385100 0.58941900 -0.64053700
 B -2.97867800 1.70341900 -0.30320300
 H -3.10752100 2.68896700 -0.94034500
 H -0.32009600 -0.36491000 1.83966200

C2

Pd 0.71650000 0.79388500 -0.31917400
 O 2.03321300 -0.75521100 -0.84274500
 O 4.35122300 -0.47229200 -1.69432100
 C 3.98897100 -0.66692500 0.91469100
 S 3.36936400 -0.05743900 -0.73042100
 O 3.12481800 1.37888600 -0.52840800
 F 5.15312100 -0.09766400 1.19979700
 F 4.14530200 -1.98328100 0.88884900
 F 3.11828100 -0.35996600 1.87635400
 O -0.46462600 2.45010900 0.15560700
 C -3.57215600 -0.65096400 -0.67791600
 C -3.31364000 -0.81281000 0.97966200
 C -4.83946600 0.01787400 -1.16748200
 H -4.58691800 0.76011000 -1.92526900
 H -5.50630100 -0.71970300 -1.61158900
 H -5.37817100 0.51550500 -0.35882100
 C -4.35268600 -0.29147500 1.94740600
 H -4.19624400 -0.78029900 2.90829300
 H -4.25084100 0.78422400 2.10096200
 H -5.36577300 -0.51930800 1.61595400
 C -1.66444300 2.71011600 0.27157500
 C -2.06319000 4.14721400 0.46112500
 H -3.13511200 4.28359300 0.60748800
 H -1.52557600 4.54300400 1.32359000
 H -1.74057700 4.71271100 -0.41470900
 N -2.64375800 1.78170800 0.23687800
 H -3.58312900 2.14163400 0.29402600
 B -2.39702900 0.33400100 0.07241400
 B -2.09363500 -0.41572700 -1.50157600
 B -2.90423500 -1.98421200 -1.51155300
 H -3.48859200 -2.34410500 -2.47539900
 B -3.70769000 -2.19865100 0.05603900
 H -4.80019700 -2.63111200 0.18281400
 B -1.65966900 -0.67269600 1.33569400
 H -1.38973400 -0.13249700 2.35383500
 B -0.85164600 -0.43237900 -0.23145300
 B -1.15314300 -1.88633500 -1.22289900
 H -0.38015600 -2.26398800 -2.03402700
 B -2.16394800 -3.00230300 -0.26382000
 H -2.13116400 -4.17976800 -0.38130900

B -2.45907800 -2.25099600 1.31096200
 H -2.72408200 -2.79251000 2.32873500
 B -0.87904000 -2.04611400 0.52937000
 H 0.09298500 -2.53901200 0.98898000
 H -2.13508400 0.30502500 -2.43924500

TS C2-C3

Pd -0.68832800 -0.33420200 -0.22639400
 O -1.09915400 1.46066200 0.82202200
 O -0.76143300 2.16306800 -1.47985300
 C -0.45220300 3.98820100 0.44413800
 S -1.40679600 2.52882900 -0.22049400
 O -2.77415900 2.97407800 -0.22192900
 F -0.83723100 5.08464600 -0.19523500
 F 0.85815900 3.83907300 0.26039600
 F -0.68430200 4.13933300 1.74137200
 O 0.06801200 -1.73682500 -1.70718600
 C 3.81218700 0.42700800 -0.47944300
 C 3.79287500 -1.17702200 0.00536200
 C 4.70002600 0.84099400 -1.63517100
 H 4.16397200 1.55750300 -2.25837100
 H 5.60690800 1.31634300 -1.26447300
 H 4.99219800 -0.01158700 -2.25182100
 C 4.64646200 -2.17490200 -0.74389800
 H 4.69860300 -3.09102700 -0.15677900
 H 4.20888400 -2.41890500 -1.71317400
 H 5.66116200 -1.80286000 -0.88569700
 C 0.97089700 -1.54311700 -2.52924500
 C 0.77570800 -2.00602300 -3.94235400
 H 0.30915800 -2.99025600 -3.92491100
 H 0.07332100 -1.31977100 -4.42228800
 H 1.70273300 -2.03885600 -4.51572900
 N 2.12732200 -0.92131100 -2.21108000
 H 2.75176300 -0.71955000 -2.97588000
 B 2.43038200 -0.49646700 -0.83273700
 B 2.28422500 1.16723100 -0.24939800
 B 3.61325800 1.45381200 0.87368200
 H 4.19608400 2.48233900 0.84537200
 B 4.57863600 -0.03014300 0.99770400
 H 5.75969800 -0.04368500 0.99484200
 B 2.24536300 -1.60234400 0.54584300
 H 1.88649400 -2.70143900 0.30440900
 B 1.27353000 -0.11485300 0.42017200
 B 1.98722900 1.10113400 1.49953000
 H 1.35176300 1.93419400 2.03994500
 B 3.41753800 0.36762200 2.26543200
 H 3.80749100 0.67513700 3.33973300
 B 3.55922100 -1.29877800 1.68728400
 H 4.08852100 -2.20855300 2.22656400
 B 1.94689400 -0.61274300 1.98674800
 H 1.27126500 -1.02515400 2.86576000
 H 1.96823500 1.96662400 -1.05599100
 C -1.59038600 -1.73971900 3.58832400
 C -1.71331100 -0.99501700 2.41922300
 C -1.32072300 -1.59816500 1.24022700
 C -0.90433900 -2.91270200 1.14834000
 C -0.78486400 -3.63145000 2.33444200
 C -1.12021100 -3.04706700 3.54964000
 H -1.86968900 -1.28506000 4.53183500
 H -2.07439900 0.02472200 2.42926300

H	-0.67180700	-3.35975400	0.19141900	F	3.53605800	-3.14113800	-1.11400400
H	-0.44112100	-4.65910000	2.29606400	F	4.94721300	-1.98725900	0.04775100
H	-1.03205200	-3.61690500	4.46713800	F	3.78911100	-1.03289500	-1.50446400
I	-3.24865000	-1.09466000	-0.86074800				

C3

Pd	0.41247600	0.54674300	0.22477400
O	-0.13988100	-0.30578700	2.15872100
C	-3.83433500	-0.97380400	0.31753700
C	-3.11626900	-2.08444200	-0.71520800
C	-4.62847900	-1.47438200	1.50296100
H	-3.97277300	-1.87987800	2.27430500
H	-5.16966500	-0.63055200	1.92931000
H	-5.35565900	-2.22954600	1.20497300
C	-3.29550800	-3.56617000	-0.45364000
H	-3.94927500	-4.00156500	-1.20771200
H	-2.32677200	-4.06471000	-0.50886100
H	-3.73733200	-3.75564100	0.52638900
C	-0.62899900	-1.42525200	2.34020900
C	-0.18541300	-2.25255600	3.50508600
H	-0.90965800	-3.02062100	3.77939800
H	0.76379300	-2.71828200	3.21782600
H	0.00646400	-1.59409400	4.35084900
N	-1.54523900	-1.94614700	1.49645700
H	-1.76345600	-2.91956900	1.63985500
B	-2.10949100	-1.22119900	0.34839300
B	-2.85460300	0.40256000	0.46809800
B	-4.31855400	0.41254700	-0.53427800
H	-5.28944000	0.96279700	-0.14392800
B	-4.49645600	-1.19704400	-1.24050300
H	-5.51478100	-1.79097300	-1.31083200
B	-1.63304400	-1.48568700	-1.34662000
H	-0.78210100	-2.28001700	-1.52659100
B	-1.45916300	0.12395600	-0.60006000
B	-2.81939800	1.12095200	-1.15835300
H	-2.75494200	2.28787700	-1.31920800
B	-3.84843500	0.11907500	-2.21432000
H	-4.48111200	0.56290400	-3.11042100
B	-3.11248400	-1.48899000	-2.30995500
H	-3.24630900	-2.28541100	-3.17366000
B	-2.07606200	-0.04804000	-2.27502100
H	-1.46245700	0.26064300	-3.23355200
H	-2.82423800	0.93363200	1.52261400
I	1.19061100	1.64974500	-1.96112900
C	0.04701100	2.35465400	0.97229100
C	0.74935100	2.49783600	2.16229500
C	-0.74415500	3.37327800	0.47103000
C	0.61588800	3.68159600	2.88227700
H	1.39415800	1.70802900	2.53239300
C	-0.87532700	4.54602100	1.20818900
H	-1.23854100	3.27739200	-0.48296900
C	-0.20250400	4.70073300	2.41291800
H	1.15845600	3.79903300	3.81352500
H	-1.49776700	5.34585500	0.82266400
H	-0.30352600	5.62077000	2.97715200
O	2.72672400	-0.22127300	1.16629500
O	2.49714800	-2.65788300	1.65347700
C	3.76567000	-1.95656500	-0.55631000
S	2.43812200	-1.57818300	0.68629100
O	1.18760700	-1.57324300	-0.13816500

TS C3-C4

Pd	-0.08969800	0.89180600	0.71602900
O	-0.43255800	-0.40006500	2.41830600
C	-2.20064500	-2.99430800	-0.35140600
C	-0.87313200	-2.78070900	-1.34928700
C	-2.31982200	-4.26910000	0.45336000
H	-2.21197200	-5.14722300	-0.18288600
H	-1.57829800	-4.30313400	1.25160700
H	-3.31047600	-4.29563500	0.90583900
C	0.19192200	-3.85585900	-1.42745500
H	0.01730900	-4.64697200	-0.69598200
H	0.19157600	-4.30412100	-2.41973000
H	1.16881000	-3.40773000	-1.23559500
C	0.07842900	-1.53137300	2.32607600
C	0.93016100	-2.05458700	3.43598800
H	0.47284200	-1.78328600	4.38728100
H	1.08181800	-3.13182200	3.37867200
H	1.90042600	-1.55085400	3.37346200
N	-0.09756600	-2.28885200	1.23035900
H	0.62504600	-2.98060200	1.07727400
B	-0.95071000	-1.88103800	0.10105900
B	-2.67824000	-1.50626000	0.31971300
B	-3.57772800	-2.25947200	-1.01147700
H	-4.61684600	-2.77838200	-0.79048100
B	-2.41615200	-3.10007100	-2.04504400
H	-2.58336100	-4.17752500	-2.49791700
B	-0.41657100	-1.13414000	-1.42921000
H	0.73399200	-0.92602500	-1.55441400
B	-1.57688200	-0.27919700	-0.37107800
B	-3.21256900	-0.52874000	-1.05868000
H	-4.08477400	0.25775000	-0.93288600
B	-3.04281800	-1.52373300	-2.52761400
H	-3.77058000	-1.43352300	-3.45644500
B	-1.32159600	-1.89238400	-2.73699200
H	-0.76753000	-2.16205900	-3.74528500
B	-1.81312700	-0.29643700	-2.13507000
H	-1.65290300	0.67366100	-2.79200600
H	-3.09544300	-1.53156900	1.42460000
I	0.75340500	2.59841900	-1.04996000
C	-2.00334000	1.57387300	0.67817800
C	-2.67319700	1.39893700	1.89759200
C	-2.54859400	2.44881700	-0.27024100
C	-3.85789900	2.07413300	2.15101100
H	-2.27688900	0.72417900	2.64288200
C	-3.72813900	3.12631000	-0.00419000
H	-2.07615400	2.57848500	-1.23183400
C	-4.38791400	2.94096700	1.20332700
H	-4.36452100	1.92248200	3.09723700
H	-4.13452400	3.79546000	-0.75367000
H	-5.31497000	3.46602700	1.40376200
O	3.93315200	-0.93160500	1.84743600
O	2.48060600	-2.00153900	0.15366400
C	3.98900300	0.00401500	-0.63380900
S	3.01184300	-0.77107100	0.74304200
O	1.96192200	0.24786300	1.03925600
F	3.25842300	0.05489400	-1.74346000

F 5.06908000 -0.73200600 -0.87412500
 F 4.36611000 1.22885600 -0.30422600

C4

O -0.07806800 2.96401200 -1.05556600
 C -2.10432400 0.31654300 -0.58906700
 C -2.09191000 -0.21720700 0.96574100
 C -2.81326900 1.61674900 -0.90379800
 H -2.39415000 2.02905300 -1.81889600
 H -3.88264900 1.44806400 -1.02850600
 H -2.64948300 2.35249200 -0.11670600
 C -2.75366800 0.63978300 2.02115900
 H -2.74620300 0.09963800 2.96730100
 H -2.21277200 1.57862800 2.14839600
 H -3.78797500 0.85791400 1.75534700
 C 0.35938200 2.73468100 0.04973100
 C 1.40834900 3.60242900 0.70767100
 H 2.37348500 3.09122100 0.63747600
 H 1.46922800 4.55277700 0.18207600
 H 1.19174200 3.77452700 1.76467700
 N -0.03854200 1.64560300 0.79994400
 H 0.46987100 1.53003500 1.66479700
 B -0.60270200 0.40289500 0.26665200
 B -0.66879800 -0.14210200 -1.41063900
 B -2.18885800 -1.00324800 -1.66645300
 H -2.79048600 -0.83659900 -2.67144800
 B -3.09681200 -1.03581300 -0.15141700
 H -4.25839700 -0.83876400 -0.07139700
 B -0.63679200 -1.03284800 1.29638200
 H -0.18117200 -0.90936200 2.38491900
 B 0.30323100 -1.04109600 -0.21987400
 B -0.68169400 -1.91461900 -1.42425300
 H -0.18322800 -2.50864500 -2.32018100
 B -2.18716100 -2.45831500 -0.64437600
 H -2.76890800 -3.43951500 -0.96397700
 B -2.14625500 -1.91659500 1.04435700
 H -2.70856600 -2.39008500 1.97181500
 B -0.65313200 -2.46916900 0.26093400
 H -0.13188000 -3.47477000 0.61251200
 H -0.27231600 0.59328200 -2.24243200
 C 1.87941200 -0.92631600 -0.16269800
 C 2.64261400 -1.80971800 0.60607700
 C 2.55436600 0.10361200 -0.82862000
 C 4.02164400 -1.67216800 0.71026100
 H 2.14882200 -2.62051300 1.13241200
 C 3.93283800 0.24771600 -0.72843000
 H 1.99384300 0.80436200 -1.44042200
 C 4.67145300 -0.63982600 0.04510400
 H 4.59065500 -2.37155900 1.31322500
 H 4.43139300 1.05229700 -1.25857900
 H 5.74703700 -0.52891500 0.12716400

1, 10-o-phenanthroline

C -2.68809500 -1.54344500 -0.00016600
 H -3.17454100 -2.51580100 -0.00018200
 C -3.46472400 -0.37276800 -0.00023700
 H -4.54610200 -0.43680900 -0.00032300
 C -2.81701300 0.83590200 -0.00019900

H -3.36999100 1.76978200 -0.00025100
 C -1.41028800 0.86382200 -0.00009400
 C -0.72895700 -0.37311100 -0.00007500
 C 0.72895500 -0.37310700 0.00015300
 C 1.41028600 0.86381900 0.00013800
 C 0.67505200 2.09596300 0.00008700
 H 1.22832200 3.02935000 0.00013200
 C -0.67505200 2.09596400 -0.00001000
 H -1.22832000 3.02935200 -0.00005600
 C 2.81701600 0.83590100 0.00023100
 H 3.36998800 1.76978400 0.00032900
 C 3.46472600 -0.37276500 0.00022900
 H 4.54610300 -0.43681300 0.00036900
 C 2.68809100 -1.54344600 -0.00001200
 H 3.17454500 -2.51579800 0.00012100
 N -1.37340400 -1.55495800 -0.00008300
 N 1.37340600 -1.55496000 0.00002600

L-Pd-I

Pd -0.73955700 -0.68543400 -0.00053900
 C 1.60075600 -2.69072500 -0.00015900
 H 0.83238600 -3.45548300 -0.00034400
 C 2.96070300 -3.02803400 0.00008800
 H 3.24435900 -4.07197500 0.00005600
 C 3.90494400 -2.02998900 0.00033200
 H 4.96214600 -2.26988500 0.00052100
 C 3.49437200 -0.68123400 0.00034600
 C 2.11787700 -0.43732900 0.00008000
 C 1.61917200 0.89762800 -0.00000500
 C 2.50848200 1.97676000 0.00016700
 C 3.91883500 1.70759500 0.00049000
 H 4.60295000 2.54782700 0.00064900
 C 4.39154900 0.43861900 0.00057300
 H 5.45831600 0.24928200 0.00081200
 C 1.95509300 3.27222200 -0.00004400
 H 2.60893300 4.13692400 0.00006000
 C 0.59101600 3.42440400 -0.00040400
 H 0.13073100 4.40330600 -0.00061200
 C -0.23717300 2.29613300 -0.00054900
 H -1.31280700 2.39088400 -0.00081200
 N 1.19585600 -1.43212000 -0.00014900
 N 0.26584000 1.06709300 -0.00033200
 I -3.20175500 -0.01362300 0.00042100

D2

Pd 0.34775900 0.36521000 -0.04885100
 O -0.52292300 2.25994500 -0.08698200
 C -4.18095400 -0.15387400 0.37449200
 C -2.66705400 -0.33203200 1.00938400
 C -5.15203400 0.77219400 1.07722500
 H -5.97743800 0.99832900 0.40248000
 H -5.55937100 0.29770500 1.96906500
 H -4.67434100 1.70790200 1.37157700
 C -2.33695900 0.42872300 2.27627000
 H -1.33268300 0.15359000 2.59616700
 H -2.35831300 1.50642100 2.11159200
 H -3.03829700 0.18013000 3.07237700
 C -1.63683500 2.75818000 -0.31975000

C	-1.72859900	4.25014500	-0.45600400	C	1.96904800	0.34145900	2.58402000
H	-2.75453200	4.61308600	-0.51202000	C	2.37463600	0.93600100	3.90272500
H	-1.22542500	4.71346100	0.39318100	H	2.92027200	1.86264500	3.70729500
H	-1.19631200	4.54643300	-1.36246800	H	1.47730400	1.19831000	4.46232100
C	2.65283900	2.58290400	0.02891200	H	3.00363400	0.27439600	4.49834900
H	1.81989400	3.27720500	0.03030800	C	-1.75336900	-1.08347400	2.65777900
C	3.98261100	3.02587900	0.02545300	H	-0.98840800	-0.64272000	3.28870500
H	4.19443800	4.08702100	0.02609600	C	-2.80057000	-1.83247600	3.20996300
C	4.99198400	2.09572200	0.02062100	H	-2.85580100	-1.98109200	4.28048100
H	6.03148400	2.40436200	0.01706200	C	-3.74183600	-2.36556500	2.36503700
C	4.67607400	0.72289700	0.02101500	H	-4.56496200	-2.95638800	2.75119800
C	3.31636000	0.37571700	0.02431700	C	-3.64153600	-2.14131600	0.97925600
C	2.92229100	-1.00829600	0.03021700	C	-2.56016400	-1.36515200	0.52587800
C	3.91912700	-1.99613900	0.04350300	C	-2.41710300	-1.09801300	-0.88805000
C	5.30204300	-1.61238300	0.03257300	C	-3.34376000	-1.66566000	-1.78161300
H	6.05089500	-2.39565700	0.03561900	C	-4.43632000	-2.44957900	-1.28150600
C	5.66761600	-0.31126900	0.02046600	H	-5.14103400	-2.85921700	-1.99566900
H	6.71437000	-0.03072400	0.01272100	C	-4.58424800	-2.67410700	0.04107300
C	3.51423300	-3.34377800	0.07075000	H	-5.41187300	-3.26648100	0.41362500
H	4.26163200	-4.12897700	0.07851800	C	-3.15636800	-1.45720500	-3.15842400
C	2.17729900	-3.63803100	0.09179000	H	-3.85715700	-1.88758900	-3.86486600
H	1.81881600	-4.65839800	0.11884700	C	-2.08047100	-0.72549200	-3.58872000
C	1.24607200	-2.59397600	0.07135400	H	-1.88631500	-0.55971400	-4.63984100
H	0.19110800	-2.81270800	0.07901200	C	-1.21525200	-0.18432300	-2.63795600
N	-2.75475100	2.03626200	-0.45138100	H	-0.34512800	0.37612400	-2.94718200
H	-3.58068100	2.55554200	-0.70961000	N	2.64255600	-0.73346800	2.14069000
N	2.33535100	1.30339300	0.02880900	H	3.31683100	-1.11999400	2.78405500
N	1.58960800	-1.31625500	0.03185700	N	-1.63719800	-0.86772900	1.36592600
B	-2.84169200	0.55747500	-0.46208300	N	-1.38221100	-0.33821800	-1.33682000
B	-4.13841600	-0.25131300	-1.33554500	B	2.35532900	-1.49172700	0.90693000
B	-4.71996800	-1.59844900	-0.34552500	B	2.73813200	-3.20788400	0.78652200
H	-5.87884800	-1.82180400	-0.28108800	B	3.42272000	-3.52443500	-0.81387100
B	-3.78816500	-1.63775800	1.15569800	H	4.33931800	-4.26206000	-0.92376700
H	-4.25331200	-1.81576400	2.22533300	B	3.46665100	-2.00573800	-1.71727400
B	-1.47862600	-0.55210100	-0.24034000	H	4.37483000	-1.64844700	-2.37971000
B	-2.43925900	-0.55084500	-1.75676700	B	1.12510000	-1.08904100	-0.29019600
H	-1.97788600	-0.11676800	-2.75822200	B	1.06901400	-2.64523700	0.58762800
B	-3.60205400	-1.89934600	-1.69264400	H	0.26545800	-2.85041800	1.43071100
H	-3.96353200	-2.45556900	-2.67233900	B	1.72261100	-3.91082800	-0.47975600
B	-3.37886800	-2.74866600	-0.14083700	H	1.35099400	-5.03153300	-0.40414800
H	-3.56914800	-3.90716900	0.00651000	B	2.17462200	-3.15343200	-2.02519800
B	-2.09215700	-1.90263100	0.75154700	H	2.12884000	-3.71276600	-3.06641500
H	-1.40163800	-2.36366800	1.59683700	B	1.81228400	-1.41669600	-1.89685700
B	-1.97495600	-2.08748500	-1.01169200	H	1.60791500	-0.66690900	-2.78858600
H	-1.16970700	-2.79743200	-1.51403200	B	0.72628800	-2.60551900	-1.15188600
H	-4.90202000	0.44051600	-1.92008900	H	-0.35606200	-2.80411800	-1.58694900
TS D2-D3				C	1.35576700	3.38756600	-2.68820200
Pd	-0.13044100	0.53098400	0.16467800	C	0.38474200	2.64202800	-2.02533600
O	1.05791400	0.88787000	1.95057200	C	0.50455700	2.43395100	-0.65737200
C	3.71583700	-2.05286900	-0.01052200	C	1.49022900	3.09144900	0.07485400
C	2.79934900	-0.83556800	-0.64561500	C	2.44043900	3.84789400	-0.59879700
C	5.09736700	-1.71413700	0.51057800	C	2.39482800	3.97921600	-1.98233100
H	5.42808300	-2.50707000	1.18124400	H	1.26659100	3.53598800	-3.75827800
H	5.81119000	-1.64143000	-0.30900200	H	-0.48095500	2.29197300	-2.56740800
H	5.09933000	-0.76941900	1.05622300	H	1.51037800	3.01972800	1.15259400
C	3.41583400	0.54155800	-0.71544400	H	3.21159800	4.35429000	-0.02897800
H	2.86016300	1.14132800	-1.43406600	H	3.13375100	4.57850100	-2.49993600
H	3.37544800	1.04875100	0.24690100	I	-1.78126800	2.69211300	0.56963100
H	4.45211800	0.48172400	-1.04646200	H	3.20227100	-3.71510400	1.75093000

D3				C	-0.81488300	2.15167200	2.22051200
				C	-0.50692100	2.16040400	0.86959100
Pd	0.28452800	0.57792900	-0.13129000	C	-0.75133400	3.30029300	0.10961800
O	-0.81844900	1.15017800	-1.80568600	C	-1.32658100	4.41448500	0.70967300
C	-3.95683600	-1.44887700	-0.12962700	C	-1.64820100	4.40767700	2.06200100
C	-2.98558000	-0.27550900	0.53794500	H	-1.62300200	3.25091200	3.87439300
C	-5.20933400	-1.02300400	-0.86794400	H	-0.66002600	1.27352200	2.82884000
H	-5.59284100	-1.87651900	-1.42642800	H	-0.47857000	3.33916900	-0.93572300
H	-5.97954300	-0.70097300	-0.16819500	H	-1.50233300	5.30257300	0.11341300
H	-5.01221700	-0.20767300	-1.56534000	H	-2.08887800	5.28306800	2.52362900
C	-3.47412600	1.15332300	0.40448300	I	2.48475300	2.09558000	-0.99230400
H	-3.17786200	1.71823800	1.28541800	H	-3.42216100	-3.30616200	-1.67101500
H	-3.04982900	1.65020900	-0.46508300				
H	-4.56064100	1.17942100	0.33611000	TS D3-D4			
C	-1.68703500	0.63270100	-2.52991700	Pd	0.28085300	0.57281100	-0.28475700
C	-1.92512100	1.26880300	-3.86710000	O	-0.82086100	0.69106700	-2.06604800
H	-2.55289200	0.66379500	-4.52116700	C	-3.87841100	-1.65086200	-0.10410700
H	-2.40809100	2.23515500	-3.70311200	C	-3.28651800	-0.11531400	0.14941000
H	-0.96362800	1.46363000	-4.34213400	C	-4.86578900	-1.86944000	-1.23236900
C	1.23584600	-1.40769300	-2.45439100	H	-5.86006000	-1.53011700	-0.94442800
H	0.69141900	-0.74717900	-3.11828700	H	-4.57031000	-1.34127000	-2.13975300
C	1.86382800	-2.56236400	-2.93394700	H	-4.92145000	-2.93610800	-1.44951600
H	1.80068800	-2.80691600	-3.98597500	C	-3.85983800	0.97634900	-0.72968500
C	2.55368600	-3.36180400	-2.05485500	H	-3.78811900	1.92355500	-0.19961800
H	3.04551000	-4.26555100	-2.39623100	H	-3.32479700	1.07466600	-1.67156200
C	2.64860100	-2.98561500	-0.70201400	H	-4.91104500	0.78255200	-0.93845300
C	1.98426200	-1.81329000	-0.31759300	C	-1.35860300	-0.27029200	-2.64362300
C	2.10941200	-1.31997300	1.02055400	C	-1.36828100	-0.27184100	-4.14103600
C	2.93462900	-1.99691000	1.92844000	H	-1.81452400	-1.16950700	-4.56892800
C	3.55026200	-3.23049200	1.52970700	H	-1.92366200	0.60457200	-4.48192500
H	4.15313800	-3.76065500	2.25746500	H	-0.34169900	-0.15212600	-4.49248200
C	3.41041500	-3.70902400	0.27312400	C	1.35051400	-2.27171400	-1.89253700
H	3.89671700	-4.63041500	-0.02454000	H	0.74678500	-1.95438600	-2.73554000
C	3.15317500	-1.40603000	3.18497300	C	2.03371600	-3.49455100	-1.93502400
H	3.78114500	-1.90681100	3.91290500	H	1.95365700	-4.12847300	-2.80848700
C	2.60455300	-0.17783800	3.45190000	C	2.79774900	-3.85788500	-0.85573600
H	2.79383100	0.33848300	4.38320000	H	3.33786400	-4.79788500	-0.84649300
C	1.78121500	0.42922100	2.50158100	C	2.90304900	-2.98553200	0.24399200
H	1.36355100	1.40849000	2.67444800	C	2.17636900	-1.78410500	0.18988700
N	-2.42922400	-0.42584400	-2.18090600	C	2.31046500	-0.82943800	1.26010300
H	-3.04926400	-0.77249400	-2.89787500	C	3.21280000	-1.09391000	2.30496400
N	1.27380100	-1.06554200	-1.18410900	C	3.88777500	-2.35807000	2.35887300
N	1.48945800	-0.15098800	1.34816400	H	4.54551300	-2.55248600	3.19778800
B	-2.42371300	-1.12209600	-0.87404500	C	3.73624600	-3.26906000	1.37412300
B	-3.03734400	-2.76957000	-0.68778400	H	4.26448600	-4.21465500	1.40752000
B	-3.95726200	-2.85911800	0.82079800	C	3.46824000	-0.07702500	3.24069600
H	-4.96719900	-3.47095700	0.86011000	H	4.16161800	-0.26092200	4.05348400
B	-3.92882700	-1.26576200	1.58264800	C	2.88146600	1.15095000	3.07827300
H	-4.86254500	-0.74770700	2.08349700	H	3.10128500	1.98080900	3.73602800
B	-1.31513200	-0.75266100	0.44627800	C	1.97557300	1.33588700	2.03498500
B	-1.36073700	-2.39218700	-0.29117700	H	1.50481400	2.29289600	1.86962900
H	-0.51353000	-2.80778900	-0.99753900	N	-1.93925800	-1.28018900	-1.98102300
B	-2.29289400	-3.46531200	0.76283600	H	-2.28188300	-2.04004900	-2.55006500
H	-2.05587100	-4.62281100	0.82383800	N	1.39774600	-1.45802100	-0.86190400
B	-2.84154100	-2.52143500	2.16271000	N	1.64605100	0.36017900	1.19995400
H	-3.00631400	-2.98051200	3.23998400	B	-2.22651600	-1.32241300	-0.52528100
B	-2.25225800	-0.85952200	1.95850400	B	-2.70612800	-2.82879200	0.26277600
H	-2.10151300	-0.09986100	2.84353900	B	-4.04954000	-2.49902300	1.36356400
B	-1.22931900	-2.21786700	1.46555000	H	-4.95102500	-3.25983500	1.43121500
H	-0.23628700	-2.48000600	2.05717000	B	-4.42532200	-0.77897000	1.27021300
C	-1.38336800	3.27595900	2.81728100				

H	-5.51311000	-0.32640600	1.22000000	C	-2.17733100	-3.63801500	0.09214300
B	-1.61916800	-0.16808300	0.70006600	H	-1.81886300	-4.65838200	0.11938200
B	-1.29072800	-1.94162800	0.83238000	C	-1.24610400	-2.59396900	0.07152600
H	-0.22585900	-2.40962400	0.66910700	H	-0.19113700	-2.81268900	0.07919900
B	-2.40525600	-2.65856700	2.00270700	N	2.75470300	2.03622000	-0.45128900
H	-2.08239000	-3.59146100	2.65471400	H	3.58060700	2.55547700	-0.70964400
B	-3.46940000	-1.37742500	2.61291100	N	-2.33538200	1.30339600	0.02860900
H	-3.92768300	-1.36629300	3.70273000	N	-1.58965600	-1.31625100	0.03182000
B	-3.01955800	0.13530200	1.80415200	B	2.84165800	0.55741100	-0.46193800
H	-3.24219600	1.21346000	2.22012400	B	1.47860600	-0.55212100	-0.24016700
B	-1.75584100	-1.01931700	2.26815900	B	2.09229400	-1.90270800	0.75151900
H	-0.97725200	-0.77770200	3.12957900	H	1.40196400	-2.36395200	1.59685200
C	-1.23895500	3.43365700	2.58548400	B	3.78835200	-1.63774800	1.15541600
C	-0.86580400	2.18858700	2.10451800	H	4.25361500	-1.81586900	2.22498300
C	-0.95909100	1.89333700	0.74253200	B	4.13823600	-0.25125400	-1.33571900
C	-1.42539100	2.88000700	-0.12992000	H	4.90160000	0.44074100	-1.92038500
C	-1.79940300	4.12709200	0.35861300	B	2.43902100	-0.55075300	-1.75671700
C	-1.71072000	4.40885900	1.71430800	H	1.97755100	-0.11647300	-2.75804100
H	-1.17465900	3.63365300	3.64883000	B	1.97480600	-2.08746600	-1.01170800
H	-0.54511400	1.43172100	2.80893300	H	1.16953500	-2.79742600	-1.51398700
H	-1.46399300	2.69936100	-1.19537700	B	3.37889800	-2.74866900	-0.14110300
H	-2.14051800	4.88559400	-0.33626200	H	3.56921900	-3.90716800	0.00620500
H	-2.00173200	5.38217800	2.09069700	B	4.71992600	-1.59842400	-0.34592300
I	2.36064400	1.78477700	-1.66710500	H	5.87880300	-1.82182200	-0.28155200
H	-2.69685800	-3.80004500	-0.41550800	B	3.60182400	-1.89923600	-1.69290200
				H	3.96319200	-2.45537100	-2.67268700

E2

Pd	-0.34773900	0.36521700	-0.04878200
O	0.52294700	2.25995600	-0.08644800
C	2.66715200	-0.33213800	1.00942200
C	4.18106500	-0.15389900	0.37431200
C	2.33716900	0.42860400	2.27634200
H	1.33248000	0.15433600	2.59569000
H	3.03790700	0.17916400	3.07271100
H	2.35958600	1.50632000	2.11190900
C	5.15228400	0.77217100	1.07683400
H	5.97725500	0.99873100	0.40170300
H	4.67453500	1.70767200	1.37175400
H	5.56021300	0.29749300	1.96830400
C	1.63684500	2.75815500	-0.31943700
C	1.72860200	4.25013500	-0.45556000
H	2.75448900	4.61298900	-0.51294300
H	1.19504700	4.54667400	-1.36118900
H	1.22667600	4.71332800	0.39444100
C	-2.65285500	2.58291300	0.02866500
H	-1.81990800	3.27721100	0.03007200
C	-3.98262600	3.02589500	0.02516700
H	-4.19445100	4.08703700	0.02576900
C	-4.99200500	2.09573800	0.02035900
H	-6.03150500	2.40437900	0.01677800
C	-4.67609900	0.72291300	0.02082300
C	-3.31639000	0.37573300	0.02414500
C	-2.92232100	-1.00829500	0.03016000
C	-3.91916400	-1.99613000	0.04359200
C	-5.30208900	-1.61236600	0.03261800
H	-6.05093500	-2.39564500	0.03575800
C	-5.66765300	-0.31125600	0.02036700
H	-6.71440300	-0.03069600	0.01258600
C	-3.51427100	-3.34375900	0.07105200
H	-4.26166700	-4.12896000	0.07895600

TS E2-E3

Pd	0.16019700	0.53609000	-0.15171200
O	-0.94565100	0.71565100	-2.04480000
C	-1.73366700	-2.20850000	-0.39353800
C	-3.36222400	-2.46496100	-0.33221300
C	-1.01386100	-2.62905400	-1.65668600
H	0.01348800	-2.88211800	-1.40532700
H	-1.48336400	-3.51030300	-2.09232400
H	-0.99759300	-1.83166900	-2.39663900
C	-4.04824500	-3.04379600	-1.55201000
H	-5.12324800	-2.89569900	-1.45261900
H	-3.71120300	-2.55870500	-2.46908400
H	-3.85841500	-4.11350000	-1.63293400
C	-2.12454100	0.59237000	-2.40298900
C	-2.57736700	1.28023900	-3.65771900
H	-3.47981900	0.84065000	-4.08316000
H	-2.77628200	2.32873000	-3.41732400
H	-1.77105700	1.25982000	-4.38910700
C	1.82611600	-1.01823900	-2.61617400
H	1.08522300	-0.53189300	-3.24256600
C	2.87686200	-1.76137300	-3.16881300
H	2.96391400	-1.86184900	-4.24282000
C	3.78185900	-2.35113100	-2.32065100
H	4.60428000	-2.94180800	-2.70869900
C	3.65300500	-2.17410500	-0.93026100
C	2.57426100	-1.39424500	-0.47515800
C	2.42749300	-1.12882900	0.93754400
C	3.35063300	-1.70058800	1.83129600
C	4.42014900	-2.51783800	1.33417700
H	5.11418700	-2.94234000	2.05021200
C	4.57194100	-2.74088500	0.01139300
H	5.39070100	-3.34700900	-0.35858400
C	3.19744000	-1.44149300	3.20483800

H	3.89541400	-1.87430200	3.91260200	C	1.99718200	2.45621200	3.00669600
C	2.16856200	-0.64240600	3.62648000	H	2.05471000	2.60513500	4.07678200
H	2.00847400	-0.42105300	4.67311600	C	2.58407000	3.33814000	2.12999900
C	1.30179900	-0.10398800	2.67305100	H	3.10529300	4.21670500	2.49319200
H	0.47283800	0.51565900	2.97916500	C	2.54922400	3.07073000	0.74922300
N	-3.03188600	-0.11280900	-1.70784600	C	1.86276500	1.91906700	0.33922300
H	-3.97774900	-0.07770000	-2.05834000	C	1.93477300	1.48477800	-1.02431000
N	1.67280000	-0.86167800	-1.31797200	C	2.68004400	2.23424800	-1.94423300
N	1.41890200	-0.32701200	1.37736100	C	3.27374400	3.47225300	-1.52360400
B	-2.79667100	-0.82130800	-0.43416900	H	3.80836800	4.05995500	-2.26047200
B	-1.30761100	-0.79583600	0.51327000	C	3.21726200	3.87269800	-0.23390500
B	-1.02807700	-2.43896200	1.13567300	H	3.70609600	4.78623600	0.08338000
H	0.07054200	-2.87892600	1.15352700	C	2.86678300	1.69951800	-3.23098000
B	-2.32391800	-3.50250600	0.57568100	H	3.43084900	2.25818500	-3.96904100
H	-2.15520500	-4.58976900	0.14961300	C	2.37631700	0.45095600	-3.51331800
B	-4.13783100	-1.27242600	0.61500800	H	2.54694900	-0.02413300	-4.46978600
H	-5.21956400	-0.94344400	0.26213300	C	1.64046400	-0.23436300	-2.54457100
B	-2.84733800	-0.21173100	1.21313800	H	1.27106600	-1.23011300	-2.73239400
H	-3.04071400	0.93863300	1.39534300	N	-3.06947400	-0.78088200	1.44716900
B	-1.75661800	-1.21155400	2.18774000	H	-3.98642800	-1.11067500	1.71231900
H	-1.17891800	-0.77138900	3.11858600	N	1.21118000	1.11836300	1.20411200
B	-2.37338200	-2.87725600	2.21439900	N	1.37214900	0.28879000	-1.35912100
H	-2.21236200	-3.61583000	3.12408500	B	-2.97598900	0.17377800	0.32093800
B	-3.85410000	-2.90944900	1.23120800	B	-1.46437900	0.52674800	-0.50480100
H	-4.75392600	-3.67159400	1.30788400	B	-1.45439000	2.26909600	-0.85652300
B	-3.50393000	-1.50033200	2.25133300	H	-0.46228600	2.89870600	-0.72366400
H	-4.16290200	-1.24816200	3.20077700	B	-2.95166100	3.00722100	-0.26742700
C	-1.47820300	3.30882100	2.65560400	H	-2.99561900	4.03294500	0.31412700
C	-0.45100700	2.64101300	1.99665100	B	-4.33113300	0.54460300	-0.75509000
C	-0.57467900	2.38416200	0.63859200	H	-5.35319200	-0.01702200	-0.55042400
C	-1.62106900	2.93503100	-0.09572800	B	-2.85611000	-0.17934800	-1.38705300
C	-2.63260000	3.61046800	0.57447100	H	-2.89677500	-1.30701300	-1.71738600
C	-2.58063400	3.77571600	1.95322200	B	-1.88073200	1.10893400	-2.12950000
H	-1.39015000	3.49121800	3.72037200	H	-1.14137000	0.91151400	-3.03604100
H	0.45335800	2.38814000	2.52979700	B	-2.78525700	2.63524800	-1.97824000
H	-1.63172800	2.86431800	-1.17306200	H	-2.70480900	3.51931200	-2.75963300
H	-3.45684700	4.02720200	0.00672300	B	-4.30703700	2.27640500	-1.12931600
H	-3.37073400	4.30701900	2.46924000	H	-5.32279400	2.87767900	-1.17945600
I	1.72437800	2.74983500	-0.61477200	B	-3.65307600	1.11404300	-2.29665300
E3				H	-4.20503600	0.89654500	-3.31982700
Pd	0.26503400	-0.56130700	0.14555800	C	-1.07385700	-3.47273400	-2.77708700
O	-0.84378700	-1.18918600	1.80210800	C	-0.70073200	-2.27058300	-2.18127100
C	-2.20062800	1.70355200	0.56268000	C	-0.36610500	-2.23814200	-0.83735300
C	-3.84412100	1.68879300	0.39875400	C	-0.42344300	-3.40088700	-0.07658900
C	-1.67822900	2.06431600	1.93646700	C	-0.81162700	-4.59474600	-0.67702500
H	-0.83310200	2.73985900	1.82946100	C	-1.13059700	-4.63754700	-2.02758900
H	-2.44113300	2.58239900	2.51477900	H	-1.33774200	-3.48223900	-3.82845500
H	-1.36163300	1.18290300	2.48778200	H	-0.73598900	-1.36966300	-2.77879100
C	-4.70724600	1.94973700	1.61540400	H	-0.11791000	-3.40486700	0.96068600
H	-5.74382100	1.73704500	1.35618000	H	-0.83029100	-5.50131300	-0.08272100
H	-4.42292800	1.31367000	2.45518400	H	-1.41790500	-5.57293500	-2.49238700
H	-4.64265900	2.99227800	1.92556700	I	2.62202700	-1.88596700	0.95337500
C	-2.04790700	-1.40200700	2.05140100	TS E3-E4			
C	-2.35945100	-2.42893000	3.09569800	Pd	0.30495400	0.45500000	-0.23113700
H	-3.34509200	-2.29841500	3.54253100	O	-0.75883600	0.67064200	-2.03331700
H	-2.31463700	-3.40811100	2.60890900	C	-2.09725300	-1.72449500	-0.15712200
H	-1.58852900	-2.40604000	3.86383700	C	-3.70873500	-1.96146700	-0.36065800
C	1.31612100	1.34531200	2.49885600	C	-1.23607800	-2.35901300	-1.22775200
H	0.84265100	0.62155400	3.15211200	H	-0.33283100	-2.74477800	-0.76587500

H	-1.75622700	-3.20260200	-1.67760800	H	-1.51763700	2.64141600	-0.99982300
H	-0.96425300	-1.65988000	-2.01102700	H	-2.16488800	4.75354300	-0.01283100
C	-4.19319900	-2.61718000	-1.63704800	H	-2.01368200	5.10126800	2.44089000
H	-5.27222200	-2.48416500	-1.70655200	I	2.33357300	2.12544000	-1.28208100
H	-3.73221700	-2.17274000	-2.52003300				
H	-3.98370900	-3.68655400	-1.62900400	F2			
C	-1.91894900	0.72549300	-2.47960200	Pd	0.44447600	0.36034200	0.01688400
C	-2.10544600	1.34764500	-3.83125400	O	-0.46913100	2.24789600	0.04177900
H	-3.08737700	1.15465500	-4.26280700	C	-4.02519800	-0.26975100	-0.84071300
H	-1.96217900	2.42634800	-3.72499800	C	-4.02453000	-0.25340500	0.84533100
H	-1.32422600	0.98669600	-4.49938100	C	-5.02680000	0.58397100	-1.59039100
C	1.70317900	-1.75775600	-2.27513300	H	-4.50328800	1.25203900	-2.27530400
H	1.15320500	-1.25203600	-3.06164500	H	-5.69111100	-0.05269300	-2.17258500
C	2.49962400	-2.87840400	-2.54336600	H	-5.64145800	1.18212700	-0.91585100
H	2.57611200	-3.25396200	-3.55536500	C	-5.03646400	0.59622200	1.58299000
C	3.16789600	-3.48413800	-1.50620500	H	-5.08357800	0.24741100	2.61395000
H	3.77904600	-4.36312100	-1.67755100	H	-4.75021800	1.64873800	1.60243000
C	3.09730500	-2.92609600	-0.21580700	H	-6.03224800	0.49730100	1.15171400
C	2.28494300	-1.79308400	-0.05372800	C	-1.60379500	2.74022900	-0.02960800
C	2.31283300	-1.06300200	1.18109900	C	-1.72678100	4.23617800	-0.07936100
C	3.17311100	-1.48288000	2.20644700	H	-2.75857400	4.58263500	-0.13699700
C	3.88741700	-2.71994900	2.06034400	H	-1.25834900	4.65312100	0.81361200
H	4.49687600	-3.05990900	2.88938400	H	-1.17575300	4.60269800	-0.94697200
C	3.85408900	-3.41286500	0.90047700	N	-2.72715700	2.00895700	-0.06298600
H	4.43275800	-4.32138700	0.78204200	H	-3.58277200	2.53313500	-0.16243900
C	3.36720400	-0.62126900	3.30024200	B	-2.75791200	0.53004600	-0.02029100
H	4.02092200	-0.92131600	4.11125900	B	-2.43604700	-0.46844100	-1.44103800
C	2.78466400	0.62026500	3.28486200	B	-3.58806900	-1.81219600	-1.41829900
H	2.97366200	1.34802200	4.06227400	H	-4.10071500	-2.16817100	-2.42183200
C	1.92986100	0.96356200	2.23648300	B	-4.61471400	-1.63539200	0.01738100
H	1.48092700	1.94284300	2.18071700	H	-5.78338500	-1.80094700	0.01703900
N	-3.00513400	0.28358900	-1.82892800	B	-2.43926500	-0.42410600	1.43598300
H	-3.88350500	0.46092100	-2.29436200	H	-2.18419700	0.16713900	2.42899400
N	1.56476600	-1.26537600	-1.06223800	B	-1.38234300	-0.57795800	0.00017200
N	1.63065900	0.11615700	1.26174800	B	-1.92117800	-2.05127500	-0.86995300
B	-3.06318800	-0.32990300	-0.48171400	H	-1.18096500	-2.70709800	-1.52464300
B	-1.77776300	-0.14599000	0.73230500	B	-3.27401900	-2.78681500	0.02793600
B	-1.66674600	-1.79003700	1.48310700	H	-3.49024800	-3.94980700	0.04283600
H	-0.60264900	-2.24337800	1.74173600	B	-3.58358200	-1.78098900	1.45137700
B	-2.87192800	-2.91812100	0.79999900	H	-4.08675600	-2.11314600	2.46754700
H	-2.63129900	-4.03542200	0.50711800	B	-1.91895100	-2.02666200	0.90638700
B	-4.61163800	-0.69625300	0.31461100	H	-1.17467000	-2.66422200	1.57451900
H	-5.60243300	-0.38892300	-0.25708400	H	-2.18921300	0.10143800	-2.44830900
B	-3.46232200	0.40412700	1.07008900	C	2.73507200	2.61008400	0.04307800
H	-3.70468500	1.55798600	1.13033500	H	1.89587900	3.29668400	0.06135300
B	-2.57653700	-0.51514000	2.30621800	C	4.06036800	3.06656500	0.03681000
H	-2.18616000	-0.03350000	3.30881600	H	4.26205000	4.12962800	0.05094600
B	-3.19868500	-2.16545600	2.33861700	C	5.07843900	2.14630600	0.01355500
H	-3.21261700	-2.82307800	3.32144400	H	6.11499700	2.46475800	0.00809800
B	-4.48504700	-2.28075700	1.11282700	C	4.77532700	0.77087500	-0.00265500
H	-5.39261800	-3.03644400	1.07907200	C	3.41875800	0.41027000	0.00487500
B	-4.30864900	-0.80187800	2.05683100	C	3.03946000	-0.97885800	-0.00845500
H	-5.12358700	-0.46618300	2.84523200	C	4.04724400	-1.95575500	-0.02575600
C	-1.23486900	3.13212800	2.80594700	C	5.42602700	-1.55737300	-0.03509700
C	-0.85832700	1.92247500	2.24351800	H	6.18288700	-2.33281400	-0.05006200
C	-0.98545500	1.68715500	0.87161500	C	5.77771600	-0.25260300	-0.02475900
C	-1.45887800	2.74091000	0.07276300	H	6.82137200	0.03945800	-0.03169000
C	-1.81872100	3.95465100	0.63197800	C	3.65770100	-3.30798600	-0.03177300
C	-1.72160000	4.15434700	2.00330100	H	4.41399200	-4.08456600	-0.04489200
H	-1.15215000	3.26937500	3.87776500	C	2.32426000	-3.61774700	-0.01914900
H	-0.51413800	1.13710500	2.90008400				

H	1.97772800	-4.64261700	-0.02121100	C	-1.85120300	3.72506700	-1.96229900
C	1.38114400	-2.58419200	-0.00386300	H	-1.46511200	4.47913100	-2.63575000
H	0.32817500	-2.81373100	0.00593700	C	-1.17247300	2.50780700	-1.82076900
N	2.42913800	1.32813000	0.02728200	H	-0.26166800	2.32736200	-2.37670500
N	1.71091600	-1.30232000	-0.00082600	N	-2.64082900	-0.62217300	0.28564800
TS F2-F3				N	-1.57178500	1.53949900	-1.02103600
Pd	-0.32050000	-0.35953500	-0.22583500	C	0.57115900	-3.19429900	2.56431800
O	-0.30479300	0.79716300	1.79293800	C	-0.10887200	-2.58969900	1.50933700
C	4.03357400	1.05648000	0.56010600	C	0.48815700	-2.53203600	0.25076400
C	3.27137000	2.46020500	0.07845900	C	1.72923800	-3.13667400	0.04328000
C	4.92537400	1.07794600	1.78530000	C	2.37436500	-3.76654900	1.09444600
H	4.65926300	0.25138700	2.44538900	C	1.80550500	-3.79093300	2.36281300
H	5.96768700	0.96075900	1.49318300	H	0.10671600	-3.20986600	3.54379500
H	4.83407200	2.01455300	2.33787100	H	-1.07191500	-2.14787500	1.70773400
C	3.47629600	3.72746500	0.87838100	H	2.18813000	-3.13051400	-0.93459500
H	3.09880800	4.56546600	0.29375800	H	3.32921200	-4.24586200	0.91251700
H	2.92574500	3.69827400	1.81967900	H	2.31287400	-4.28732300	3.18128900
H	4.53270700	3.90544100	1.07817500	I	-0.57178600	-2.46078400	-1.87335400
C	0.57717400	1.12944700	2.57917200	F3			
C	0.26261500	1.29168200	4.04165700	Pd	-0.31744100	-0.30313500	-0.12732100
H	1.00584800	1.88112500	4.57985900	O	-0.08722000	0.16664600	1.99597200
H	-0.71701500	1.75679500	4.14195200	C	4.22194900	0.45875300	0.61361900
H	0.20791900	0.29676800	4.49121000	C	3.55404800	1.98145100	0.73732200
N	1.86101700	1.34289900	2.19568500	C	5.17919800	-0.02414500	1.68472400
H	2.51325200	1.53311900	2.94053200	H	4.84453600	-0.98797100	2.07100700
B	2.34527300	1.17563600	0.81615600	H	6.17320800	-0.15471500	1.26009600
B	3.07841300	-0.31345000	0.21798500	H	5.25691900	0.68376000	2.51162200
B	4.45808600	0.11039800	-0.79738600	C	3.90519300	2.85173900	1.92357900
H	5.46073600	-0.51048900	-0.71956800	H	3.52217800	3.85417300	1.73652100
B	4.58845300	1.87840200	-0.84821300	H	3.44606200	2.48397700	2.84205700
H	5.60932500	2.46213400	-0.75005500	H	4.98392100	2.92315300	2.05962700
B	1.76064000	2.10272200	-0.57452500	C	0.86357400	0.14638100	2.78801400
H	0.91464600	2.89427400	-0.35023700	C	0.58471400	-0.06747400	4.24705000
B	1.59201600	0.31948500	-0.54452100	H	1.39415600	0.27510300	4.89214100
B	2.91447900	-0.34497500	-1.54220000	H	-0.34018400	0.44403100	4.50895100
H	2.80363300	-1.35988900	-2.13872700	H	0.43312000	-1.13867800	4.40832300
B	3.85957900	1.01254600	-2.20295600	N	2.14625500	0.27709400	2.40513700
H	4.41428100	0.96570200	-3.24614300	H	2.83390300	0.15382300	3.13261400
B	3.13129900	2.51733200	-1.61737700	B	2.56895200	0.56953500	1.02251100
H	3.18399400	3.58585700	-2.12001600	B	3.14194600	-0.64232200	-0.12625800
B	2.08796600	1.14715200	-2.03786100	B	4.48664500	0.05773400	-1.02558900
H	1.38114200	1.19340800	-2.98777700	H	5.43548300	-0.60478700	-1.26344800
H	3.16101400	-1.17606500	1.01562000	B	4.76356000	1.70884600	-0.44349600
C	-3.24993600	-1.70153400	0.73947300	H	5.83146800	2.16122900	-0.22635000
H	-2.72596500	-2.64340000	0.61429300	B	1.98200300	1.97677700	0.12228700
C	-4.50920800	-1.68191700	1.35026100	H	1.20792400	2.67038600	0.68539800
H	-4.94711900	-2.60392300	1.70956100	B	1.66809200	0.31973300	-0.47519000
C	-5.15440100	-0.47922500	1.47998800	B	2.86879000	-0.00936900	-1.75516700
H	-6.12431600	-0.41358500	1.96057200	H	2.64728400	-0.73733500	-2.65907400
C	-4.56780400	0.67968300	0.94054800	B	3.88552500	1.44317500	-1.95336800
C	-3.30423300	0.55565700	0.33186700	H	4.37642800	1.75137300	-2.98361700
C	-2.74318100	1.69440800	-0.36262000	B	3.32347700	2.66740800	-0.80295500
C	-3.48133700	2.89150700	-0.41585500	H	3.43462600	3.84122900	-0.88417800
C	-4.71875600	3.00707700	0.29981900	B	2.14595200	1.61238700	-1.60564900
H	-5.24272900	3.95578700	0.27613800	H	1.39420500	2.05554800	-2.40490000
C	-5.23972500	1.94650500	0.95207900	H	3.21765800	-1.74576300	0.28098700
H	-6.19195000	2.02307800	1.46429500	C	-2.91423600	-2.11021100	0.69762400
C	-2.99056600	3.92993700	-1.22915400	H	-2.22084400	-2.92372100	0.51434600
H	-3.53587700	4.86536100	-1.29099000	C	-4.21277900	-2.35910000	1.16042100

H	-4.53218700	-3.37783600	1.33663800	B	-4.81991700	0.20044600	-0.61389800
C	-5.05253900	-1.29625800	1.37627100	H	-5.85041500	0.77151000	-0.52514400
H	-6.06347200	-1.44931600	1.73765200	B	-4.85079800	-1.56767000	-0.68410500
C	-4.60420900	0.00994500	1.10281700	H	-5.83445500	-2.21110000	-0.58344900
C	-3.28651200	0.16085100	0.63782100	B	-2.00797600	-1.62243100	-0.43124700
C	-2.80766200	1.47208000	0.26752200	H	-1.13055000	-2.38732300	-0.22915100
C	-3.68206100	2.56894400	0.36250200	B	-1.93068600	0.18809900	-0.36331500
C	-5.00256900	2.38738500	0.89264500	B	-3.31073500	0.75466100	-1.36813900
H	-5.64670700	3.25483900	0.97931100	H	-3.29166800	1.78291100	-1.94696200
C	-5.44472400	1.16222600	1.24985500	B	-4.17627300	-0.64885800	-2.03101900
H	-6.44943500	1.02557700	1.63286300	H	-4.74000500	-0.61990600	-3.06960100
C	-3.22719300	3.81412500	-0.10837300	B	-3.36115400	-2.10857600	-1.46055200
H	-3.87954700	4.67848100	-0.05088000	H	-3.34020400	-3.17560400	-1.96801700
C	-1.97851200	3.90758100	-0.66582200	B	-2.39666300	-0.67809700	-1.88057000
H	-1.60573500	4.83742300	-1.07447500	H	-1.69453400	-0.70616200	-2.82918600
C	-1.17200700	2.76487000	-0.70790200	H	-3.60321800	1.59711500	1.16889700
H	-0.19087800	2.80705500	-1.16003400	C	2.74582000	1.96344200	1.53826600
N	-2.46198200	-0.89396000	0.46440000	H	1.97561500	2.72830000	1.59022200
N	-1.55186100	1.59512000	-0.22868700	C	3.99726700	2.15221800	2.14486800
C	0.71267100	-4.01274600	1.60068100	H	4.20885300	3.07314100	2.67286000
C	0.24925600	-2.72799200	1.32600000	C	4.93468600	1.15473100	2.04382600
C	0.44811200	-2.16325200	0.06661500	H	5.91411700	1.26400800	2.49646500
C	1.08738400	-2.90675600	-0.92043600	C	4.62565100	-0.02105500	1.33284200
C	1.54004800	-4.19057200	-0.64051200	C	3.34392900	-0.11043800	0.76309400
C	1.36361400	-4.74661500	0.61961600	C	2.98748600	-1.28235400	-0.00824000
H	0.54983600	-4.43935600	2.58450200	C	3.94007900	-2.30335300	-0.17937400
H	-0.28636600	-2.19079000	2.09868300	C	5.23109000	-2.18639100	0.43749700
H	1.25761600	-2.49424900	-1.90373300	H	5.94285400	-2.99173600	0.29700900
H	2.03794100	-4.75463200	-1.42096500	C	5.56031800	-1.09524000	1.16238800
H	1.72153800	-5.74721300	0.83127000	H	6.54062000	-1.00812700	1.61680600
I	-0.80254200	-0.61128900	-2.66651800	C	3.58888900	-3.40536700	-0.97825600

TS F3-F4

Pd	0.29532000	0.19884900	-0.18034100	C	2.35325000	-3.44529500	-1.57385900
O	0.10488900	-0.84425300	1.77275500	H	2.05718400	-4.26443800	-2.21555000
C	-4.33256300	-0.72206600	0.73362000	C	1.46570700	-2.38968600	-1.35194500
C	-3.49901700	-2.07224600	0.23143000	H	0.49246700	-2.37471400	-1.82668600
C	-5.21561100	-0.81049900	1.96259100	N	2.43355800	0.86966000	0.87951300
H	-5.13813200	0.11786600	2.52924400	N	1.76214900	-1.35670500	-0.58046100
H	-6.25595600	-0.94875700	1.67257800	C	-1.09160600	3.39326400	2.13932100
H	-4.93512300	-1.64422700	2.60941500	C	-0.81877200	2.12409900	1.65487400
C	-3.62534400	-3.35086000	1.02858700	C	-0.88214100	1.83674600	0.27979700
H	-3.22721100	-4.16891800	0.42956700	C	-1.19009900	2.89226500	-0.58755900
H	-3.05609400	-3.30134400	1.95771500	C	-1.47122800	4.16093200	-0.10069100
H	-4.66796100	-3.57383200	1.25422200	C	-1.43093700	4.41729800	1.26218200
C	-0.78097700	-1.05530400	2.60530200	H	-1.03220800	3.58352400	3.20504900
C	-0.38883900	-1.42037500	4.00866300	H	-0.53449500	1.36016900	2.36318700
H	-1.22621600	-1.76325500	4.61668800	H	-1.23804500	2.72180100	-1.65209900
H	0.37523300	-2.19644900	3.96508400	H	-1.72084600	4.95116300	-0.79874900
H	0.06242400	-0.54344900	4.47910400	H	-1.65083700	5.40903500	1.63971100
N	-2.09740700	-0.94204700	2.32648300	I	0.95133200	1.10078100	-2.54950100
H	-2.72175000	-1.04019500	3.11225100				
B	-2.63917200	-0.73653500	0.97083700				
B	-3.46670100	0.71611300	0.39440800				