

**A Computational Study on the Palladium-Catalyzed Allenylative
Dearomatization reaction**

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Contents:

Table S1 listing the single-point calculations by using B3LYP/SDD and PBE1PBE/LANL2DZ+p calculations were performed on reaction mechanism optimized at the B3LYP/LANL2DZ level, Table S2 giving total electronic energies and zero-point energies as well as thermal corrections to enthalpies and Gibbs free energies for all systems, and the optimized Cartesian coordinates for all species.

Table S1. Single-point energy of mechanism 1 and mechanism 2.

Structure	B3LYP/LANL2DZ	B3LYP/SDD	PBE1PBE/LANL2DZ+p
	Rel energy	Rel energy	Rel energy
Oxidative addition			
Pd(PH ₃) ₂	0.00	0.00	0.00
Monophosphine pathway			
Pd(PH ₃) ₂	0.00	0.00	0.00
PdPH ₃	25.16	28.15	28.15
TS(PdPH ₃ /1a)	20.71	21.93	25.54
1a	-8.07	-7.99	-6.57
Bisphosphine pathway			
Pd(PH ₃) ₂	0.00	0.00	0.00
TS(Pd(PH ₃) ₂ /1b)	11.90	12.52	9.21
1b	-20.09	-21.29	-24.12
TS(1b/1a)	-9.30	-9.31	-8.60
1a	-8.07	-7.99	-6.57
TS(1a/1c)	-4.67	-4.99	-3.49
1c	-18.33	-20.20	-21.64
Transmetalation			
Patht1			
2a	-13.99	-16.80	-22.17
2b	-15.44	-16.87	-22.69
TS(2/8)	-1.13	-1.84	-7.46
8	-6.59	-7.37	-8.92
Patht2			
2a	-13.99	-16.80	-22.17
2b	-15.44	-16.87	-22.69
TS(2a/3a)	-9.65	-9.94	-16.47
TS(2b/3b)	-6.03	-6.07	-11.14
3a	-12.83	-12.71	-17.72
3b	-12.27	-12.74	-17.13
TS(3/4)	2.21	2.21	-1.44
4	-4.08	-5.91	-7.44
TS(4/8)	0.14	0.33	-2.91
Reductive elimination			
Pathr1			
4	-4.08	-5.91	-7.44
TS(4/5)	12.94	16.12	16.99
5	4.41	3.82	1.86
TS(5/6)	12.14	13.65	12.64
6	-5.86	-6.05	-9.85
TS(6/7)	14.46	16.55	12.92
7	-6.76	-6.23	-16.55
Pathr2			
8	-6.59	-7.37	-8.92
TS(8/9)	1.47	1.05	-0.51

9	-14.02	-15.00	-18.15
TS(9/10)	0.47	0.89	-5.45
10	-13.68	-14.11	-23.49
Pathr3			
8	-6.59	-7.37	-8.92
TS(8/11)	-6.26	-5.99	-8.82
11	-11.72	-11.93	-16.33
TS(11/12)	5.60	5.91	-2.43
12	-21.02	-20.36	-29.94
Pathr4			
8	-6.59	-7.37	-8.92
TS(8/9)	1.47	1.05	-0.51
9	-14.02	-15.00	-18.15
TS(9/6)	4.65	5.705	2.39
6	-5.86	-6.05	-9.85
TS(6/13)	-5.81	-5.35	-10.99
13	-10.11	-10.35	-15.97
TS(13/14)	13.24	14.53	6.33
14	-8.88	-8.07	-19.65

Relative energies in kcal/mol.

Table S2. Total Electronic Energies (E_{tot}), Zero-point Energies (ZPEs), Thermal Corrections to Enthalpies (H_{corr}), Gibbs Free Energies (G_{corr}) (in a.u.) for all species involved in catalytic cycle. Gibbs energies of salvation ($G_{\text{solvation}}$) (in kcal/mol) for all species involved in catalytic cycle.

molecule	E_{tot}	ZPE	H_{corr}	G_{corr}	$\Delta G_{\text{solvation}}$
PH ₃	-8.2921807	0.023485	0.027338	0.003461	0.19
Pd(PH ₃) ₂	-143.374898	0.052316	0.061037	0.017895	0.87
PdPH ₃	-135.0425454	0.026013	0.030929	-0.000056	0.71
naphthalene allyl chloride	-517.0715253	0.199348	0.212048	0.159841	-2.16
(allenyl)SnMe ₃	-239.2559635	0.153041	0.165715	0.114841	4.25
ClSnMe ₃	-138.1630525	0.108998	0.120056	0.072324	1.73
TS(PdPH ₃ /1a)	-652.1217853	0.224406	0.242784	0.173746	-0.78
1a	-652.1672982	0.225855	0.244297	0.175790	-1.39
TS(1a/1c)	-652.1617387	0.225485	0.243166	0.177429	-3.36
1c	-652.1838315	0.225932	0.244041	0.178686	-2.05
TS(Pd(PH ₃) ₂ /1b)	-660.4183975	0.249661	0.272117	0.193134	2.40
1b	-660.478726	0.252329	0.274288	0.197721	-1.57
TS(1b/1a)	-660.4614675	0.250047	0.272707	0.189845	1.07
2a	-891.4351221	0.381153	0.413141	0.312977	6.19
2b	-891.4360829	0.380933	0.412999	0.312965	4.94
TS(2/8)	-891.4137829	0.379436	0.411086	0.311497	5.17
TS(2a/3a)	-891.4258303	0.379391	0.411261	0.313131	7.41
TS(2b/3b)	-891.4200334	0.379191	0.411118	0.379191	6.64
3a	-883.1386819	0.353940	0.382536	0.291966	4.98
3b	-883.1381881	0.353811	0.382443	0.291648	4.67
TS(3/4)	-883.1147915	0.352542	0.380660	0.290584	5.19
4	-744.9622572	0.243122	0.259954	0.198989	0.77
TS(4/8)	-753.2468606	0.266990	0.288114	0.214667	3.46
8	-753.258136	0.269229	0.290149	0.216751	1.29
TS(4/5)	-744.9343175	0.242091	0.259011	0.196099	2.63
5	-744.9480744	0.242020	0.259379	0.197615	1.7
TS(5/6)	-753.2314916	0.266400	0.287496	0.215967	3.50
6	-753.2564508	0.268616	0.289662	0.218262	4.13
TS(6/7)	-753.2241622	0.268130	0.288611	0.218515	3.08
7	-753.2578991	0.271143	0.291449	0.222627	2.55
TS(8/9)	-753.2449128	0.268531	0.288726	0.217679	2.36
9	-753.2696871	0.269303	0.290080	0.217440	2.57
TS(9/10)	-753.2465518	0.269521	0.289144	0.221629	0.51
10	-753.2691498	0.272078	0.291762	0.224348	-0.37
TS(8/11)	-761.5502923	0.293876	0.318788	0.234747	3.76
11	-761.5580162	0.295646	0.320395	0.237160	1.82
TS(11/12)	-761.5306732	0.293763	0.317965	0.238655	2.26
12	-761.5730946	0.297185	0.321500	0.239169	4.34
TS(9/6)	-753.2400218	0.267851	0.288475	0.216780	3.54
TS(6/13)	-761.548874	0.294004	0.318551	0.237711	3.82
13	-761.5554443	0.295438	0.320104	0.239179	4.39

TS(13/14)	-761.5187035	0.293699	0.318261	0.238566	3.39
14	-761.553875	0.297109	0.321541	0.242197	5.11
TS(4/15)	-744.9039489	0.242349	0.258890	0.197845	-2.19
15	-744.980854	0.246354	0.262437	0.202801	-1.41
TS(8/16)	-753.2141805	0.268637	0.289255	0.216326	1.56
16	-753.2983619	0.272618	0.292494	0.224022	0.56
TS(11/17)	-761.5086521	0.294382	0.319158	0.236470	3.95
17	-761.601839	0.298984	0.322988	0.241117	1.68
PPh ₃	-701.6004329	0.272733	0.289601	0.226807	0.63
Pd(PPh ₃) ₂	-1530.0035251	0.547542	0.583669	0.471694	8.59
PdPh ₃	-828.3582434	0.273826	0.292802	0.223813	1.73
TS(PdPPh ₃ /1a)	-1345.4378362	0.472006	0.504588	0.400905	4.00
TS(Pd(PPh ₃) ₂ /1b)	-2047.0453885	0.745399	0.796211	0.649782	19.94

Cartesian coordinates for the optimized geometries of all species involved in catalytic cycle (values in Angstrom).

PH₃

P	0.00000000	0.00000000	0.12807300
H	0.00000000	1.20886500	-0.64036700
H	-1.04690700	-0.60443200	-0.64036700
H	1.04690700	-0.60443200	-0.64036700

Pd(PH₃)₂

H	3.10048900	-0.92542800	0.80376200
P	2.37622500	-0.00000200	-0.00000400
H	3.10044400	1.15880900	0.39959400
H	3.10054800	-0.23333800	-1.20328400
Pd	0.00000000	0.00000000	0.00000000
P	-2.37622500	0.00000200	0.00000400
H	-3.10044400	-1.15880900	-0.39959700
H	-3.10048900	0.92542900	-0.80376200
H	-3.10054800	0.23333500	1.20328400

PdPH₃

H	0.00000000	1.22546400	-2.35785100
P	0.00000000	0.00000000	-1.63184000
H	-1.06128300	-0.61273200	-2.35785100
H	1.06128300	-0.61273200	-2.35785100
Pd	0.00000000	0.00000000	0.68589500

naphthalene allyl chloride

C	-3.96323900	-1.38142300	-0.08590600
C	-3.83078900	-0.01543700	-0.07123800
C	-2.55034600	0.59637900	-0.03733100
C	-1.37950700	-0.22951100	-0.02770600
C	-1.55784600	-1.63865500	-0.02585200
C	-2.81247500	-2.19950600	-0.05854500
H	-3.30318100	2.62203200	-0.01372400
H	-4.94727900	-1.83545700	-0.11172400
H	-4.70894600	0.62173400	-0.08195600
C	-2.40960100	2.00698400	-0.00438700
C	-0.08595100	0.39554800	0.00181600
H	-0.69176500	-2.28671500	0.01737900
H	-2.92097900	-3.27827100	-0.05741100
C	-0.00878300	1.77775200	0.02886200
C	-1.16451500	2.58342000	0.03274100
H	0.96534200	2.25215100	0.00902600
H	-1.06096200	3.66240100	0.04742600
C	1.14311400	-0.41319200	-0.03350000
H	1.11431000	-1.31792700	-0.63599900
C	2.28464700	-0.12151800	0.60350600
H	2.35288300	0.75657900	1.23866600

C	3.50114200	-0.95772900	0.50627100
H	3.94649800	-1.18177900	1.47211200
H	3.34830800	-1.86712000	-0.06800700
Cl	4.87709900	-0.03331100	-0.39930300
(allenyl)SnMe₃			
C	-3.65520400	-0.08254700	-0.00013800
H	-4.15395000	-0.35325700	0.92487300
H	-4.15427500	-0.33683600	-0.92962200
C	-2.50662400	0.54304800	0.00520300
C	-1.34032900	1.11808200	0.01001400
H	-1.28836000	2.20582600	0.01942400
Sn	0.49202500	-0.01319100	-0.00019100
C	2.11482400	1.39953000	-0.01152700
H	3.07496100	0.87922200	-0.01866500
H	2.07777100	2.03659800	0.87461600
H	2.06484200	2.03714200	-0.89663100
C	0.56935500	-1.24079800	1.76289400
H	1.48043700	-1.84303500	1.77332400
H	-0.29003900	-1.91327100	1.79398700
H	0.55323300	-0.62045300	2.66094500
C	0.54651600	-1.24444800	-1.76142200
H	1.45471100	-1.85083500	-1.77968300
H	0.52433200	-0.62565900	-2.66040800
H	-0.31615500	-1.91308800	-1.78277400
ClSnMe₃			
Sn	0.26449500	0.00000600	-0.00013600
C	0.84436100	-0.37820600	2.02013600
H	1.93402700	-0.40723000	2.09341500
H	0.44515200	-1.33572000	2.35651900
H	0.46985500	0.40810200	2.67649900
C	0.84027000	-1.56100800	-1.33881000
H	1.92994800	-1.61607700	-1.39497200
H	0.44633900	-1.36860800	-2.33738800
H	0.45817200	-2.52119100	-0.99032000
C	0.84082000	1.93938200	-0.68360100
H	1.93044100	2.01813000	-0.69590300
H	0.44111900	2.70928900	-0.02258800
H	0.46492000	2.11369200	-1.69242300
Cl	-2.17043700	-0.00009900	0.00162400
TS(PdPH₃/1a)			
C	5.04434900	2.38993600	-0.00970800
C	5.40571800	1.12454300	-0.39809000
C	4.48611600	0.04581100	-0.32433700
C	3.15696300	0.28319700	0.15619300
C	2.82752200	1.60177500	0.56303500
C	3.74152300	2.62630500	0.47828800
H	5.87485400	-1.42563300	-1.07898800

H	5.75488100	3.20612200	-0.07075000
H	6.40652500	0.92682500	-0.76696100
C	4.86670600	-1.26237900	-0.71348100
C	2.23233300	-0.82445900	0.22485700
H	1.84404600	1.81432400	0.96066100
H	3.46000700	3.62441300	0.79416500
C	2.66918900	-2.08596000	-0.17348600
C	3.97458400	-2.30625900	-0.63679500
H	1.97228100	-2.91458200	-0.16746300
H	4.26868200	-3.30160600	-0.94859300
C	0.86437200	-0.62633200	0.66211400
H	0.46428600	0.38061100	0.60016100
C	0.01410000	-1.58493200	1.12973900
H	0.34150300	-2.61636700	1.20730900
C	-1.30282900	-1.29357300	1.54971500
H	-1.85115400	-2.00789800	2.14189100
H	-1.61840200	-0.25818500	1.63215400
Pd	-3.12202400	0.14434000	-0.22573200
Cl	-2.64416200	-2.25341100	-0.27925300
H	-2.85671500	3.37633800	0.46624300
P	-3.65109400	2.42295500	-0.23267300
H	-3.70607800	3.13110200	-1.46592700
H	-4.90833000	2.86252200	0.26890300
1a			
C	0.00000000	0.00000000	0.00000000
C	1.37223817	0.00000000	0.00000000
C	2.10616005	1.21518398	0.00000000
C	1.40083931	2.46319582	0.01239191
C	-0.01845063	2.42026150	-0.01050790
C	-0.69997563	1.22584721	-0.01186693
H	4.04446688	0.26096378	-0.03338747
H	-0.54804847	-0.93525340	-0.00038182
H	1.92167167	-0.93554247	-0.00467798
C	3.52334642	1.21226721	-0.02174404
C	2.15428586	3.69243906	0.02738686
H	-0.58278138	3.34290446	-0.04777094
H	-1.78407487	1.22463828	-0.03023426
C	3.54222408	3.62276809	0.00732400
C	4.22383389	2.39416808	-0.02521729
H	4.11903511	4.53848774	0.05152103
H	5.30772372	2.38810550	-0.03530237
C	1.48016778	4.98580661	0.10797494
H	0.47763586	4.98714234	0.52731261
C	1.98878939	6.18011883	-0.28057470
H	2.97057429	6.23448751	-0.73914811
C	1.29557840	7.44508789	-0.12478410
H	1.49670558	8.18475388	-0.89429585

H	0.23917716	7.37474608	0.13086568
Pd	2.26214720	8.37015020	1.46913200
Cl	3.97603715	9.18004458	0.03580214
H	0.91453854	6.51814202	3.89475286
P	0.65095960	7.68846802	3.13594789
H	0.33086701	8.56323139	4.20716095
H	-0.67113654	7.37396733	2.72497378
TS(1a/1c)			
C	-5.63838600	-1.38719500	-0.59830200
C	-5.43390100	-0.03667700	-0.45713000
C	-4.15522800	0.47868100	-0.12191200
C	-3.06116000	-0.42516700	0.06541500
C	-3.31527400	-1.81381700	-0.06925600
C	-4.56644500	-2.28272800	-0.39827400
H	-4.77936400	2.54694500	-0.11415200
H	-6.61992700	-1.76861100	-0.85542300
H	-6.25281200	0.66084300	-0.59848700
C	-3.94264400	1.87262400	0.03558700
C	-1.76699600	0.11178300	0.40535500
H	-2.51747100	-2.52470300	0.10570500
H	-4.73281200	-3.34955200	-0.49740800
C	-1.61622200	1.48851300	0.54595400
C	-2.70107000	2.36339700	0.36080800
H	-0.63020600	1.90259700	0.72195100
H	-2.54077500	3.43092400	0.45564100
C	-0.60507000	-0.74905700	0.52750300
H	-0.59346000	-1.65674200	-0.07047700
C	0.49005800	-0.49972200	1.30267500
H	0.48152900	0.35168600	1.97448400
C	1.69988800	-1.27792800	1.23286500
H	2.33734400	-1.27728100	2.11530800
H	1.61769000	-2.25649200	0.76126600
Pd	2.58891500	0.06829700	-0.08010700
Cl	1.87975300	2.36931500	-0.49563400
H	4.35959100	-2.76477200	-0.05471100
P	4.40245400	-1.40686300	-0.47181600
H	4.79867000	-1.60892300	-1.81862000
H	5.66402400	-1.05924700	0.07515700
1c			
C	-4.17414400	-2.07479100	0.58676000
C	-4.51087100	-0.94419900	-0.11386300
C	-3.58357000	0.11834100	-0.27406200
C	-2.28339100	0.01250700	0.31852200
C	-1.96040300	-1.18701900	1.00377900
C	-2.88160000	-2.19801700	1.14037000
H	-4.90720500	1.33943100	-1.46770600
H	-4.88937000	-2.88161500	0.70042000

H	-5.49309300	-0.84676100	-0.56435200
C	-3.92127500	1.27504300	-1.01967400
C	-1.36245600	1.10976100	0.17689000
H	-0.95806400	-1.33756900	1.37862900
H	-2.60372600	-3.10950600	1.65703600
C	-1.74893100	2.21334800	-0.56874100
C	-3.01634100	2.29603400	-1.17266100
H	-1.07892400	3.05820500	-0.67151400
H	-3.27763500	3.18009200	-1.74293800
C	-0.07616000	1.09440100	0.88708600
H	-0.05424500	0.51618600	1.80628600
C	0.96234200	2.03068600	0.71361500
H	0.90147500	2.76859600	-0.07875400
C	2.19500500	1.84130800	1.37041800
H	3.02347200	2.50037600	1.13952100
H	2.22963000	1.37005200	2.34830300
Pd	1.82951000	0.12561000	0.08940000
Cl	0.97875400	-1.85176300	-1.06969400
H	4.31057700	-2.05918500	0.01198500
P	4.04135500	-0.74941100	-0.45312200
H	4.27589900	-0.94505600	-1.83509400
H	5.27536500	-0.13459400	-0.10322400
TS(Pd(PH₃)₂/1b)			
C	0.00000000	0.00000000	0.00000000
C	1.37215266	0.00000000	0.00000000
C	2.10432889	1.21613392	0.00000000
C	1.39861894	2.46349383	0.00716385
C	-0.02005041	2.42110097	-0.01004349
C	-0.70003075	1.22558769	-0.00828816
H	4.04223565	0.26254531	-0.01651366
H	-0.54808786	-0.93513075	0.00039408
H	1.92219668	-0.93508555	-0.00289858
C	3.52144755	1.21411875	-0.01331664
C	2.15470775	3.69259697	0.00988151
H	-0.58665103	3.34243689	-0.03813282
H	-1.78409041	1.22424778	-0.01915813
C	3.54427526	3.62313812	0.00005433
C	4.22492927	2.39512511	-0.01542574
H	4.12027859	4.53917425	0.04495012
H	5.30870188	2.38662771	-0.01314761
C	1.48282526	4.98195406	0.05950266
H	0.47439093	5.00275203	0.45977988
C	1.99997482	6.17573248	-0.33570566
H	2.99990711	6.23213936	-0.75201793
C	1.26687751	7.39105802	-0.24367548
H	1.55066445	8.22811292	-0.85968894
H	0.20969451	7.33150921	0.01462500

Pd	0.22530495	7.88596547	2.16198851
Cl	2.65426187	8.60605492	1.35128158
H	1.09045984	6.60808220	5.11843667
P	0.68460189	6.13936194	3.83540084
H	-0.26260462	5.19159694	4.32747287
H	1.74962612	5.20220279	3.68258506
H	-1.59300986	10.62156063	2.53479354
P	-1.63301245	9.40925535	1.78705547
H	-2.99281491	9.10085765	2.08996315
H	-1.91735201	10.02740142	0.53042328
1b			
C	-5.64648000	1.80309600	0.55337300
C	-5.74593900	0.45762800	0.80342100
C	-4.68535500	-0.43112300	0.48444200
C	-3.49116900	0.08585700	-0.11890400
C	-3.42307700	1.48685400	-0.34668600
C	-4.46746900	2.32126900	-0.02509200
H	-5.69637300	-2.19600800	1.21595700
H	-6.46504000	2.46911500	0.80196100
H	-6.64353400	0.04827900	1.25538300
C	-4.78782800	-1.81726900	0.76011000
C	-2.41836900	-0.82030400	-0.44720000
H	-2.52692100	1.91541600	-0.77550500
H	-4.38541300	3.38596300	-0.21430300
C	-2.58466600	-2.16839800	-0.15800000
C	-3.75264300	-2.66409400	0.44767700
H	-1.80343500	-2.86709700	-0.43127700
H	-3.83480100	-3.72596300	0.65101500
C	-1.19451800	-0.33688100	-1.09164500
H	-1.27452100	0.59029800	-1.65247000
C	0.01279600	-0.94639500	-1.07350800
H	0.14621400	-1.86520900	-0.50987100
C	1.20953000	-0.44947500	-1.74447400
H	1.83109900	-1.22646900	-2.18113400
H	1.03141000	0.37180300	-2.43919100
Pd	2.49028000	0.15870200	-0.19176000
Cl	3.23303000	-2.15945100	-0.06204400
H	0.93355800	2.94295600	0.66444400
P	1.71851500	2.42282500	-0.39782900
H	2.64891600	3.49019700	-0.50618700
H	0.86818400	2.77227000	-1.47880000
H	3.87896900	-0.43783200	2.83978700
P	4.12916100	0.44315000	1.75818600
H	4.46535300	1.60229400	2.52124200
H	5.44792700	0.02614100	1.44822000
TS(1b/1a)			
C	-5.80262100	1.93066300	0.48916100

C	-5.85997800	0.65762700	0.99666400
C	-4.80510900	-0.26821300	0.78133200
C	-3.65922400	0.13082200	0.01586300
C	-3.63661600	1.46084100	-0.48367800
C	-4.67488600	2.33349900	-0.25793800
H	-5.74310000	-1.86561100	1.89259700
H	-6.61521000	2.62725100	0.66081300
H	-6.71833600	0.33533600	1.57672200
C	-4.87006300	-1.57795700	1.31677400
C	-2.59299000	-0.81928400	-0.19622300
H	-2.78554400	1.80950400	-1.05299600
H	-4.62697200	3.34093300	-0.65607300
C	-2.72285300	-2.09064700	0.35110300
C	-3.84550900	-2.46854100	1.10470700
H	-1.94562100	-2.82463700	0.17903700
H	-3.90043100	-3.47277300	1.50902400
C	-1.41260500	-0.45865100	-0.97760100
H	-1.48329500	0.44394900	-1.57646200
C	-0.24295100	-1.13869000	-1.04890000
H	-0.08905800	-2.03962300	-0.46431300
C	0.87954800	-0.72836900	-1.87318700
H	1.45381700	-1.54027000	-2.31027000
H	0.67297400	0.07332900	-2.58147800
Pd	2.30267600	-0.02746100	-0.53137700
Cl	3.18213800	-2.22066100	-0.24899000
H	0.62319600	2.76402500	0.20048900
P	1.62871500	2.28912000	-0.68194200
H	2.59427200	3.30734100	-0.47275500
H	1.07670400	2.76989000	-1.89877900
H	5.27704200	-0.11008600	3.11441500
P	5.61036700	1.00803500	2.28911500
H	6.82129900	0.42813900	1.79651300
H	6.25774900	1.73180400	3.34360500
2a			
C	-6.88668400	-0.24677900	-1.38965600
C	-6.60151400	1.01583200	-0.93462800
C	-5.44028400	1.27398400	-0.15942300
C	-4.55077800	0.19402500	0.15665600
C	-4.87792500	-1.09572100	-0.34205000
C	-6.01152800	-1.31297700	-1.08899700
H	-5.82935700	3.38898800	0.05700200
H	-7.77767400	-0.42850900	-1.97983100
H	-7.26445300	1.84407200	-1.16240000
C	-5.14743200	2.58167300	0.30141600
C	-3.37176000	0.46100100	0.94170700
H	-4.22342900	-1.93202400	-0.13506500
H	-6.23492300	-2.30984800	-1.45240600

C	-3.15119400	1.76044500	1.37677100
C	-4.02359000	2.81577100	1.05451600
H	-2.29624000	1.96724700	2.00927800
H	-3.80833200	3.81363500	1.41996800
C	-2.43705800	-0.61673300	1.28986800
H	-2.84420000	-1.62307700	1.32707800
C	-1.12929100	-0.46874700	1.59180400
H	-0.69594200	0.52838800	1.55734100
C	-0.20898400	-1.54674900	1.97037600
H	0.39488400	-1.26718600	2.83356300
H	-0.70655300	-2.50222500	2.14986400
Pd	1.21650000	-1.86003400	0.44089800
Cl	2.81076000	-2.15276000	-1.47367600
H	-1.79864000	-2.84297800	-0.80835900
P	-0.44553600	-2.60928000	-1.16968700
H	-0.64884800	-1.75266200	-2.27700800
H	-0.15168600	-3.81550400	-1.84724400
C	2.89892200	-0.65240000	1.57832600
C	2.82019800	-1.93856900	1.97764000
H	3.52412700	-2.65314900	1.56229100
H	2.29832400	-2.21993200	2.88432400
C	3.20791300	0.57432300	1.29804500
H	4.00775600	0.98539300	1.92012300
Sn	2.71111300	1.85401900	-0.38312200
C	4.47330700	1.81082600	-1.60256200
H	4.35735300	2.46711300	-2.46772800
H	4.63244700	0.78934700	-1.95059500
H	5.34850900	2.13410600	-1.03586700
C	2.43411600	3.80539400	0.48618100
H	2.27518000	4.54976800	-0.29731700
H	3.31330700	4.10059000	1.06300200
H	1.56732500	3.81722400	1.15009700
C	0.98219300	1.26298200	-1.49644100
H	0.75746700	2.03629800	-2.23515700
H	0.10762500	1.12706100	-0.85979200
H	1.20967800	0.32913100	-2.00987700
2b			
C	7.45679400	-2.03183500	-0.47311100
C	7.73453400	-0.73668000	-0.11506300
C	6.72303200	0.25985300	-0.11506600
C	5.38814400	-0.09295500	-0.50263600
C	5.14033600	-1.44712400	-0.85429300
C	6.14220600	-2.38860400	-0.84424800
H	8.02621900	1.84782300	0.55751200
H	8.23962900	-2.78176400	-0.46828600
H	8.73960200	-0.45185600	0.17844400
C	7.01239400	1.59336900	0.26763200

C	4.36386900	0.92107500	-0.50224000
H	4.14026100	-1.75281900	-1.13207400
H	5.92172400	-3.41388600	-1.12000000
C	4.71488100	2.21096900	-0.12965500
C	6.02397100	2.54629900	0.26139400
H	3.96687600	2.99385600	-0.16949500
H	6.24916200	3.56913200	0.54213900
C	2.98953800	0.60483500	-0.91013500
H	2.86654700	-0.21955800	-1.60711600
C	1.87357200	1.25715200	-0.51962300
H	1.97537700	2.07349100	0.19254200
C	0.50822600	0.94196900	-0.95346900
H	-0.07332500	1.82582900	-1.21957200
H	0.47478000	0.22027800	-1.77149200
Pd	-0.57595800	0.12235000	0.65883500
Cl	-1.88393900	-0.99450600	2.48310900
H	1.39628000	-2.34782600	-0.61387600
P	0.49309900	-2.04464500	0.44045600
H	1.31706600	-2.36430600	1.54519800
H	-0.32266100	-3.19927100	0.40596200
C	-2.25727500	1.86108300	0.62945300
C	-1.12800400	2.18054600	1.29172900
H	-0.37801900	2.81317800	0.83184300
H	-1.11702200	2.09288600	2.37396700
C	-3.42669300	1.71523200	0.09639500
H	-4.07540200	2.59095400	0.17760800
Sn	-4.43508700	-0.05073700	-0.66112500
C	-5.61793700	-0.78191200	0.96639600
H	-6.18355000	-1.66543000	0.66277900
H	-6.31996600	-0.01888300	1.30770300
H	-4.94855900	-1.04596900	1.78607400
C	-3.08292900	-1.53748600	-1.40224800
H	-3.63607500	-2.26667600	-1.99899900
H	-2.62647300	-2.04208400	-0.55163100
H	-2.30333800	-1.09435400	-2.02306900
C	-5.68066600	0.69697900	-2.25036800
H	-6.29308500	-0.10726800	-2.66429300
H	-5.07503000	1.11623000	-3.05633200
H	-6.35007600	1.47673200	-1.88040500
TS(2/8)			
C	6.88887500	1.85063500	1.76696800
C	6.95103000	2.09959600	0.41892300
C	6.09553400	1.42772100	-0.49370000
C	5.15599200	0.46469200	0.00266900
C	5.11321500	0.24777900	1.40615200
C	5.95470400	0.91584100	2.26390500
H	6.86629800	2.43016700	-2.24711700

H	7.54867700	2.37171400	2.45144900
H	7.65883100	2.82232200	0.02626200
C	6.15121700	1.70005600	-1.88349600
C	4.29219700	-0.22068200	-0.92517300
H	4.39715900	-0.45251100	1.81561700
H	5.89919800	0.72742600	3.33037000
C	4.40337900	0.08353200	-2.27459400
C	5.31609900	1.04196400	-2.75217400
H	3.79202900	-0.45566100	-2.98839700
H	5.36693500	1.24271300	-3.81658200
C	3.33923800	-1.23552800	-0.45973600
H	3.60605700	-1.77334100	0.44604900
C	2.17979700	-1.57247100	-1.06387800
H	1.88399300	-1.02889300	-1.95846700
C	1.24805300	-2.60730100	-0.60041200
H	0.87310100	-3.23557600	-1.40675600
H	1.65777500	-3.23316500	0.19428500
Pd	-0.42415200	-1.62102700	0.17615500
Cl	-2.37463900	-0.26780800	1.28378200
H	1.87296600	-1.94063600	2.66137800
P	0.63965400	-1.29985000	2.36767500
H	1.00091300	0.02295400	2.72962400
H	-0.07039600	-1.65449100	3.54288400
C	-2.50563200	-1.28138100	-1.85464100
C	-1.33722300	-2.02554400	-1.74837200
H	-1.50404700	-3.10032300	-1.66647900
H	-0.58049600	-1.76616800	-2.48741400
C	-3.52943000	-0.57424800	-1.85110300
H	-4.35706200	-0.44068700	-2.52432500
Sn	-4.11887300	1.16374700	-0.06097100
C	-6.09991500	0.34389000	-0.28486600
H	-6.80283500	0.90604800	0.33280400
H	-6.10302700	-0.69907000	0.03514100
H	-6.41992900	0.38601200	-1.32769900
C	-3.34914200	2.56042300	-1.50802900
H	-3.61984500	3.57704600	-1.21446500
H	-3.73799300	2.34717800	-2.50416900
H	-2.26140700	2.48097600	-1.54069200
C	-4.25092100	2.32841500	1.75947100
H	-4.98134600	3.12993600	1.61042100
H	-3.28601900	2.77256800	2.00707200
H	-4.57321600	1.70952800	2.59775700
TS(2a/3a)			
C	-5.50752700	-0.85149700	1.96332100
C	-5.33005400	-1.94134400	1.14832800
C	-4.38125800	-1.91875700	0.09303700
C	-3.60877100	-0.73314700	-0.13124200

C	-3.80180300	0.36246900	0.74873000
C	-4.72811000	0.30818300	1.76349800
H	-4.76840800	-3.94418200	-0.55228300
H	-6.23297900	-0.88212300	2.76818000
H	-5.91078000	-2.84456100	1.30329000
C	-4.17778300	-3.05241200	-0.73306600
C	-2.65779400	-0.71268900	-1.21273000
H	-3.18770100	1.24604200	0.64266300
H	-4.85025400	1.15721800	2.42631400
C	-2.50349600	-1.85566900	-1.98663400
C	-3.25137400	-3.02159900	-1.74682900
H	-1.81968500	-1.83992300	-2.82666500
H	-3.10453800	-3.88835600	-2.38092700
C	-1.91904600	0.50473700	-1.54067600
H	-2.40120500	1.44841500	-1.30867600
C	-0.72124000	0.56282600	-2.20843800
H	-0.20830100	-0.36291500	-2.44828700
C	-0.03058000	1.79304800	-2.48196300
H	0.83255500	1.73390100	-3.13795800
H	-0.62355500	2.69491200	-2.61179300
Pd	0.45772300	1.73753800	-0.44546100
Cl	0.63445500	1.25002900	1.99313300
H	-2.05999700	4.93829600	0.19203500
P	-1.23203700	3.84178000	0.60354600
H	-2.00461000	3.48220800	1.74281500
H	-0.28376300	4.63366800	1.30732600
C	2.69995200	1.45300700	-0.67809100
C	2.35015800	2.76213100	-0.82991800
H	2.50638500	3.44131800	0.00254000
H	2.25766400	3.20578700	-1.81499100
C	3.38751800	0.36457200	-0.49814800
H	4.46367200	0.48784800	-0.65362600
Sn	2.86850500	-1.55798500	0.35983600
C	3.44044600	-1.45384000	2.42205800
H	3.29856100	-2.42285300	2.90575100
H	2.81583400	-0.70833900	2.91465300
H	4.48923300	-1.16637600	2.51878700
C	4.15329800	-2.94047000	-0.68712000
H	4.03420600	-3.94962900	-0.28575800
H	5.20221400	-2.65500700	-0.57820600
H	3.91421900	-2.96698200	-1.75259100
C	0.82734700	-2.13231600	0.09695900
H	0.67513600	-3.11440600	0.55108300
H	0.56285200	-2.20110600	-0.95888900
H	0.17827400	-1.41093200	0.59172000
TS(2b/3b)			
C	5.56531000	2.70158700	-0.57310500

C	6.34999700	1.60434800	-0.31503500
C	5.76956200	0.36624300	0.06342200
C	4.34714700	0.27753400	0.20776900
C	3.56516400	1.41838600	-0.10570400
C	4.16027200	2.59954300	-0.48467500
H	7.64276700	-0.70805400	0.16345600
H	6.02014500	3.64003300	-0.86976900
H	7.42909900	1.66378800	-0.41174900
C	6.56650500	-0.78817600	0.27454700
C	3.76617300	-0.97368000	0.61022100
H	2.48528500	1.34759300	-0.11633100
H	3.53961500	3.44963800	-0.74329500
C	4.59124700	-2.07605700	0.77793700
C	5.98686300	-1.98750000	0.60589200
H	4.16037000	-3.01505200	1.10609000
H	6.59951400	-2.86790300	0.76313600
C	2.33910800	-1.09347300	0.93836100
H	1.90241200	-0.31696700	1.55938100
C	1.56959700	-2.18495900	0.61649000
H	2.01079400	-2.94406600	-0.02402800
C	0.16799900	-2.29075700	0.91050300
H	-0.32462600	-3.22973700	0.67890900
H	-0.20989500	-1.80624000	1.80900200
Pd	-0.03980400	-0.75436300	-0.48613200
Cl	0.13136000	1.35238200	-1.76597800
H	0.92770100	2.68165300	1.52035500
P	-0.14562900	1.79957800	1.83531600
H	-1.17053700	2.62777800	1.29966300
H	-0.29614500	2.24839700	3.18822000
C	-2.02060600	-1.47091600	-1.44607000
C	-0.91028000	-2.01308700	-2.01533700
H	-0.62494000	-3.03623500	-1.79180400
H	-0.50690100	-1.57203100	-2.92186100
C	-3.25510200	-1.15476900	-1.18610200
H	-3.98865100	-1.63111300	-1.84257000
Sn	-4.10244200	0.25213400	0.21681500
C	-3.58061400	2.23421900	-0.40949600
H	-4.23809600	2.53830700	-1.22637300
H	-2.55087500	2.25084000	-0.77035400
H	-3.69582400	2.94785200	0.40906200
C	-3.46933100	-0.24383400	2.21085400
H	-3.87245100	0.47610300	2.92671500
H	-2.38198600	-0.24273900	2.29036600
H	-3.83783200	-1.23656500	2.47693100
C	-6.22502500	-0.06039900	0.05990500
H	-6.76119600	0.61123300	0.73390200
H	-6.48794300	-1.08758000	0.32187200

H	-6.56928600	0.13536300	-0.95798600
3a			
C	5.48987600	-0.92861800	-1.93563800
C	5.32133800	-1.77597800	-0.86986900
C	4.37099000	-1.49158500	0.14546400
C	3.58890500	-0.29414100	0.06236600
C	3.76838200	0.53869300	-1.07213100
C	4.69630400	0.23400000	-2.03927000
H	4.77405600	-3.28473600	1.28094000
H	6.21649900	-1.15694900	-2.70712300
H	5.90930600	-2.68423700	-0.78905800
C	4.17839300	-2.37932500	1.23289600
C	2.65144000	-0.00022900	1.11501200
H	3.13383900	1.40239900	-1.21087400
H	4.80354000	0.88169100	-2.90178800
C	2.50171100	-0.91236800	2.14937300
C	3.25326700	-2.09943200	2.20811300
H	1.81212700	-0.70451600	2.95819500
H	3.10782300	-2.78073700	3.03853000
C	1.93920300	1.28317200	1.13176800
H	2.43475700	2.09865200	0.61348200
C	0.92639800	1.65348200	2.03820200
H	0.51820200	0.92487600	2.72899900
C	0.25788900	2.88260300	1.86763000
H	-0.60000300	3.10918000	2.49015700
H	0.78631000	3.74157000	1.46435900
Pd	-0.05447800	1.68910700	0.08246300
Cl	0.14472700	0.24311800	-1.88294900
C	-2.52514400	1.92087300	-0.61202500
C	-1.73733000	2.99525200	-0.75759000
H	-1.32076100	3.21156900	-1.73694300
H	-1.77509600	3.80251600	-0.03449700
C	-3.36853700	0.94491400	-0.55755400
H	-4.37711800	1.18381900	-0.90160500
Sn	-3.07640400	-1.15369800	-0.07029900
C	-2.80041400	-2.22179200	-1.90291600
H	-2.70857700	-3.29179800	-1.70375900
H	-1.89027100	-1.86192000	-2.38201200
H	-3.64960500	-2.06269700	-2.57009100
C	-4.95951400	-1.69753400	0.82903700
H	-4.95715000	-2.75453900	1.10535000
H	-5.78550700	-1.53179600	0.13361700
H	-5.14485400	-1.10929300	1.73031400
C	-1.50550400	-1.44631200	1.35392200
H	-1.54290200	-2.47248400	1.72728000
H	-1.62428100	-0.76603600	2.19928500
H	-0.54043000	-1.27559700	0.87830000

3b

C	-5.02725100	3.15884700	-0.50612200
C	-5.44078200	2.20029700	0.38369600
C	-4.76620900	0.95554000	0.48772600
C	-3.63067400	0.69623500	-0.34906700
C	-3.24096800	1.71134800	-1.26360000
C	-3.91512700	2.90685400	-1.33821900
H	-6.05822700	0.18023900	2.03459700
H	-5.54997500	4.10601200	-0.57451900
H	-6.29590800	2.37907500	1.02705100
C	-5.20129500	-0.03279100	1.40452600
C	-2.95746100	-0.57008100	-0.22918500
H	-2.39911300	1.55205800	-1.92396500
H	-3.58969200	3.66366600	-2.04305500
C	-3.42332100	-1.49253800	0.69431400
C	-4.54180800	-1.23298000	1.50408200
H	-2.88414100	-2.42189100	0.83243700
H	-4.86478600	-1.97859500	2.22119600
C	-1.79793600	-0.88605600	-1.07263400
H	-1.32313600	-0.05632900	-1.58382400
C	-1.48973200	-2.17200400	-1.55766100
H	-2.10578900	-3.01719100	-1.26837800
C	-0.25354000	-2.39395700	-2.19839500
H	0.02773700	-3.40498900	-2.46992300
H	0.20285700	-1.60790500	-2.79324500
Pd	0.16435600	-1.67590700	-0.19682600
Cl	0.20221800	-0.45174200	1.92319100
C	2.67348600	-1.93358100	0.15464500
C	1.93926800	-3.05418500	0.21464000
H	1.90563200	-3.73189300	-0.63117600
H	1.65397100	-3.44701800	1.18592800
C	3.48917400	-0.93200500	0.15511800
H	4.53668900	-1.19288200	0.32260400
Sn	3.13410800	1.21127100	0.06175600
C	1.35144800	1.72884100	-1.00657000
H	1.37219300	2.79517000	-1.24413600
H	0.48693900	1.51469300	-0.37965200
H	1.28084800	1.16802200	-1.94048200
C	4.84816700	1.91759800	-1.04090900
H	4.81957800	3.00589200	-1.13264200
H	4.86788700	1.49058800	-2.04591400
H	5.77647600	1.64545200	-0.53336000
C	3.19162700	1.96907900	2.06203200
H	2.36383600	1.53602600	2.62261200
H	3.09576100	3.05705700	2.05424100
H	4.13448000	1.70576100	2.54508400

TS(3/4)

C	5.66824500	-2.35292100	-1.48952100
C	5.46737100	-2.42319300	-0.13423300
C	4.61225300	-1.50502900	0.53016200
C	3.94099900	-0.49104200	-0.23015500
C	4.18667500	-0.44419500	-1.62878800
C	5.02120100	-1.34847800	-2.24152300
H	4.93005100	-2.34786300	2.49386800
H	6.32357400	-3.06074700	-1.98421500
H	5.96376400	-3.18615700	0.45630300
C	4.41832300	-1.57373600	1.93210000
C	3.07244000	0.43173500	0.45381700
H	3.71984200	0.32243900	-2.23289000
H	5.18674800	-1.28813900	-3.31134900
C	2.91625200	0.30757300	1.82629500
C	3.58823500	-0.68170100	2.56515300
H	2.22363800	0.96280700	2.34094600
H	3.42911000	-0.74618200	3.63547600
C	2.36406100	1.48445400	-0.28423000
H	2.25403000	1.35053100	-1.35467900
C	2.05298700	2.74229700	0.22706300
H	2.33201300	2.98611400	1.24738400
C	1.19071600	3.62600700	-0.49121600
H	0.92205500	4.57197500	-0.03476100
H	1.22963800	3.64087800	-1.57779700
Pd	0.00611800	1.94866600	-0.04521100
Cl	-0.81735900	-0.42525400	0.38873800
C	-2.91437200	2.16929600	-0.12575100
C	-1.84468200	3.06777500	-0.12364100
H	-1.77174700	3.66245000	-1.03428400
H	-1.79525000	3.68527200	0.77414000
C	-3.78251300	1.28769100	-0.12038200
H	-4.84873400	1.18230900	-0.13101100
Sn	-3.18556400	-1.34704900	-0.07197000
C	-4.55111000	-1.24244100	1.58788200
H	-4.66820100	-2.23510900	2.02642400
H	-5.52429100	-0.87168100	1.26160700
H	-4.15677800	-0.56001600	2.34108400
C	-2.31724400	-3.31964400	0.07078500
H	-3.10136400	-4.06753300	-0.08353200
H	-1.87174200	-3.47727400	1.05392400
H	-1.54349900	-3.46052600	-0.68496800
C	-3.84103500	-1.18011000	-2.11240800
H	-4.80268300	-0.66993900	-2.17296400
H	-3.92158100	-2.17660300	-2.55166000
H	-3.10951600	-0.59989500	-2.67582900
4			
C	-3.91418100	-2.13735300	0.41281100

C	-4.24887800	-0.96035900	-0.20920300
C	-3.33030700	0.11955000	-0.28062400
C	-2.03553900	-0.02044300	0.31618400
C	-1.71979500	-1.25943200	0.93411900
C	-2.63245900	-2.28731000	0.98516000
H	-4.65619400	1.42329600	-1.38553700
H	-4.62617800	-2.95364200	0.45981900
H	-5.22758600	-0.83715500	-0.66136500
C	-3.67280400	1.32892400	-0.93755500
C	-1.10721700	1.07900000	0.25169900
H	-0.73437400	-1.40940800	1.35414400
H	-2.36352100	-3.22292500	1.46283200
C	-1.50368600	2.23765500	-0.39703900
C	-2.77261800	2.36251800	-0.99566500
H	-0.83616700	3.09033600	-0.42887100
H	-3.03664200	3.29102200	-1.48948000
C	0.20937200	0.97975400	0.90607300
H	0.23648400	0.40280600	1.82589800
C	1.28623400	1.86495000	0.68911700
H	1.21355300	2.60884200	-0.09815400
C	2.54569100	1.64048200	1.28270400
H	3.37894700	2.27515000	1.01001600
H	2.61908400	1.15721000	2.25189900
Pd	2.02157800	-0.04522900	-0.02186200
H	4.45967700	-0.57247400	-1.48167000
C	3.90347700	-1.12617400	-0.73314600
H	4.48831000	-1.52777000	0.08706400
C	2.73767600	-1.77238600	-1.10777700
C	1.49742300	-1.91365900	-1.18246300
H	0.63768000	-2.45909400	-1.50731300
TS(4/8)			
C	5.00522900	1.49564200	-0.11881800
C	4.88302900	0.23572900	-0.64788200
C	3.69745300	-0.52558200	-0.47071600
C	2.60365500	0.03703300	0.26827400
C	2.77695200	1.33889700	0.81130600
C	3.93904400	2.04896300	0.62303200
H	4.42045600	-2.24608400	-1.56123700
H	5.91714200	2.06435400	-0.26177400
H	5.69865200	-0.20423400	-1.21240600
C	3.58511100	-1.83250200	-1.00648500
C	1.39795000	-0.73564100	0.43486600
H	1.98705300	1.78504400	1.40070900
H	4.04019000	3.03970000	1.05203200
C	1.34830200	-2.00688000	-0.12204700
C	2.43201800	-2.55724400	-0.82770700
H	0.43193800	-2.58008900	-0.04503700

H	2.34249100	-3.55396700	-1.24532500
C	0.24784900	-0.19497000	1.16918700
H	0.24481400	0.86798100	1.37463400
C	-0.68875200	-0.96731800	1.86244200
H	-0.58700600	-2.04799000	1.87356600
C	-1.87417700	-0.37986600	2.39111300
H	-2.59962300	-1.01860400	2.87975200
H	-1.85043500	0.64507300	2.75017700
Pd	-1.98439900	-0.18791800	0.26382100
H	-4.49018200	-1.34907500	0.19336900
C	-4.05623400	-0.45648700	-0.24849900
H	-4.67248100	0.42930200	-0.11442400
C	-3.44389300	-0.61276600	-1.51094700
C	-2.63413900	-0.68034500	-2.42493000
H	-2.09857900	-0.78924700	-3.33659500
H	-3.09521300	2.97341200	-1.35252800
P	-1.80645900	2.58023100	-0.88010500
H	-1.13514900	2.83124500	-2.11584900
H	-1.49122000	3.85395000	-0.30640300
8			
C	5.34933600	1.82511400	-0.20408300
C	5.48031600	0.51858200	-0.60230400
C	4.42867000	-0.41775500	-0.41749600
C	3.20811200	0.00922100	0.20418000
C	3.10962800	1.37350800	0.59008300
C	4.14648100	2.25562400	0.39674000
H	5.49477900	-2.07329000	-1.31044300
H	6.16222000	2.52732500	-0.35144900
H	6.39801200	0.17722200	-1.07029000
C	4.56678900	-1.76237700	-0.84266100
C	2.14010400	-0.94186400	0.39412500
H	2.19712300	1.73383600	1.04599800
H	4.04038700	3.28961600	0.70615000
C	2.34564600	-2.24726100	-0.03276600
C	3.54014600	-2.65450600	-0.65355400
H	1.57297100	-2.98625500	0.14222500
H	3.64958300	-3.68697200	-0.96705400
C	0.88079600	-0.54717700	1.03647200
H	0.92362900	0.29918100	1.71608400
C	-0.31759200	-1.15344200	0.87867500
H	-0.38310300	-1.99791800	0.19541500
C	-1.57278500	-0.76140700	1.52437600
H	-2.13693700	-1.61391600	1.89840200
H	-1.44461500	-0.01934100	2.31547400
Pd	-2.82262800	0.11241600	0.05276800
P	-1.41756200	2.08701300	-0.23099900
H	-0.51382100	2.11278300	-1.32469900

H	-1.98044800	3.37929400	-0.40953500
H	-0.49398600	2.41083000	0.79611500
H	-5.09552200	1.12159900	-2.31482700
C	-4.77040200	0.40939300	-1.59341900
C	-4.72715200	-0.59582400	-0.88531100
C	-4.24865700	-1.49914400	0.07939500
H	-4.80058500	-1.57307000	1.01191700
H	-3.84197400	-2.44134800	-0.27654100
TS(4/5)			
C	3.63768600	2.37031000	0.30537000
C	4.02825900	1.13064100	-0.13606600
C	3.12842000	0.03343400	-0.13371400
C	1.79060900	0.21970100	0.34567100
C	1.42298800	1.51863600	0.78384200
C	2.31855800	2.56331700	0.76571600
H	4.55459200	-1.36630000	-0.96086400
H	4.33539600	3.20006600	0.29731300
H	5.03828400	0.96913400	-0.49812800
C	3.53944600	-1.24170700	-0.59974700
C	0.88299400	-0.90445600	0.35711700
H	0.41395200	1.70697200	1.12263800
H	2.00524600	3.54447200	1.10442000
C	1.35219100	-2.12834700	-0.10655200
C	2.66389100	-2.29757200	-0.58669400
H	0.70070600	-2.99274200	-0.10339800
H	2.97785900	-3.27400600	-0.93825300
C	-0.50537300	-0.75489400	0.86230500
H	-0.65321100	0.10983900	1.49955200
C	-1.23319100	-1.93347000	1.37526300
H	-1.02380500	-2.90011400	0.92565000
C	-2.13290700	-1.89174000	2.36918600
H	-2.64502200	-2.78581800	2.70401900
H	-2.38130300	-0.96285000	2.87183900
Pd	-1.67335000	-0.44904400	-0.82509100
H	-4.87451400	2.71637400	-0.21552200
C	-3.94797400	2.61277000	0.34018500
H	-3.94342700	2.96901800	1.36576000
C	-2.87397300	2.08563900	-0.20689400
C	-1.82166300	1.55271400	-0.73450200
H	-1.03043300	2.11214200	-1.22376600
5			
C	4.27084300	0.11177400	-1.16527400
C	3.83879200	-0.76946600	-0.19774300
C	2.58120100	-0.61107900	0.42693000
C	1.74308600	0.47363700	0.03426600
C	2.22313200	1.37231800	-0.94124400
C	3.45772600	1.19601400	-1.53429200

H	2.81629000	-2.32695100	1.73526400
H	5.23890600	-0.02434700	-1.63400400
H	4.46608000	-1.60223500	0.10235400
C	2.15506200	-1.51466300	1.45402600
C	0.44630100	0.64687700	0.68741800
H	1.62086200	2.22496900	-1.22645300
H	3.80202500	1.90123300	-2.28208900
C	0.07990400	-0.28324400	1.70265300
C	0.95579300	-1.34901000	2.07300500
H	-0.75594600	-0.06643700	2.35715400
H	0.64756300	-2.02006500	2.86663500
C	-0.55456900	1.58300800	0.22301100
H	-0.32404500	2.12799100	-0.68479200
C	-1.48290300	2.28024100	1.11381400
H	-1.60860400	1.87679400	2.11483100
C	-2.16351900	3.38665300	0.78777400
H	-2.83032300	3.86701800	1.49316400
H	-2.07724600	3.84010200	-0.19467300
Pd	-1.31766600	-0.41666000	-0.14589100
H	-3.69855900	0.29563800	-1.52192400
C	-2.84666000	-0.31847900	-1.79328100
H	-2.42088700	-0.12571400	-2.77215400
C	-2.74673500	-1.60011100	-1.26506500
C	-2.29277200	-2.48897100	-0.51929800
H	-2.25155200	-3.49462900	-0.16250600
TS(5/6)			
C	4.57279100	-0.11978200	-0.88862600
C	4.10734100	-0.60854000	0.31236100
C	2.82203300	-0.26809400	0.79322000
C	1.99064600	0.58677600	0.00947100
C	2.50583200	1.09167400	-1.20373900
C	3.76555600	0.74397700	-1.64886300
H	3.01261200	-1.40116600	2.63237600
H	5.56082300	-0.39118500	-1.24291100
H	4.72784900	-1.26586300	0.91260300
C	2.35770400	-0.75829500	2.05420900
C	0.66200500	0.93573700	0.50457300
H	1.90894500	1.77356800	-1.79557200
H	4.13579900	1.14556600	-2.58541300
C	0.26394100	0.42940200	1.77439500
C	1.12787100	-0.41285600	2.52931400
H	-0.61208400	0.83231900	2.26509000
H	0.79312800	-0.76841200	3.49729200
C	-0.32501100	1.64580600	-0.28372700
H	-0.05943800	1.86362000	-1.31208400
C	-1.27781800	2.59324500	0.28745300
H	-1.43015200	2.55306400	1.36312800

C	-1.95687100	3.51444700	-0.41095100
H	-2.64322100	4.19779400	0.07420300
H	-1.84277000	3.61284600	-1.48595000
Pd	-1.01206100	-0.42471500	-0.07294100
H	-4.26650900	-0.26182800	1.60672500
P	-3.63695100	-0.20182500	0.32599900
H	-4.32492900	0.96490100	-0.12199700
H	-4.49712700	-1.15272300	-0.29933100
C	-1.12261000	-2.68252400	-0.09800800
H	-1.10624500	-3.51060900	0.58143900
C	-1.09615700	-2.34531300	-1.30908600
C	-1.08223000	-1.51588600	-2.38833900
H	-1.99220500	-1.32850300	-2.94717500
H	-0.14553700	-1.27777300	-2.87906600
6			
C	4.24553600	-0.70070400	1.30252000
C	3.90104400	0.23910200	0.35357100
C	2.67665000	0.15979900	-0.34482600
C	1.77611500	-0.90283000	-0.04572100
C	2.16755000	-1.86402600	0.90845800
C	3.37406800	-1.76641400	1.57519600
H	3.06141300	1.91283100	-1.56769700
H	5.19069500	-0.62399700	1.82814500
H	4.57461200	1.05872400	0.12672800
C	2.34967300	1.12240900	-1.35860600
C	0.50638100	-0.99278500	-0.77399300
H	1.52135500	-2.70693900	1.11644100
H	3.65013300	-2.51991700	2.30408000
C	0.23673500	0.00621300	-1.76730100
C	1.18842000	1.03140400	-2.05565600
H	-0.55764800	-0.15563100	-2.48654000
H	0.95265600	1.74963800	-2.83158700
C	-0.54045500	-1.88629000	-0.39180700
H	-0.37938200	-2.48170000	0.49953100
C	-1.55998900	-2.41113100	-1.28937500
H	-1.65282000	-1.94605000	-2.26678800
C	-2.37522900	-3.43760500	-1.00049700
H	-3.10830900	-3.79380400	-1.71342500
H	-2.32369000	-3.95541900	-0.04761100
Pd	-1.21176700	0.27242700	-0.02737100
H	-3.46324600	-1.15982200	2.06673900
P	-2.82284500	0.07132900	1.75659900
H	-2.38995500	0.41748000	3.06281300
H	-3.97630700	0.89564400	1.70099600
C	-1.53530600	2.33858900	-0.12124700
H	-2.53847700	2.68844500	-0.35917900
C	-0.57289500	3.16737400	0.10976900

C	0.45243800	3.96247900	0.33574700
H	0.69497200	4.31153800	1.33499400
H	1.08356900	4.31388700	-0.47492200
TS(6/7)			
C	3.58060800	2.70862400	-0.36020100
C	4.08016300	1.44255500	-0.11956400
C	3.22492500	0.36777900	0.19065700
C	1.82074500	0.58765400	0.28034700
C	1.33925900	1.88486600	0.00961500
C	2.19704800	2.92488400	-0.30283600
H	4.83101000	-1.08186300	0.44999500
H	4.25145900	3.52447900	-0.60432300
H	5.14837900	1.25834500	-0.17398300
C	3.75390000	-0.95160200	0.43324200
C	0.94527900	-0.51930600	0.66612400
H	0.27071900	2.06049200	0.00383500
H	1.79371500	3.90812000	-0.51901100
C	1.48473600	-1.84883900	0.56829300
C	2.92915300	-2.00366200	0.62301500
H	0.92269600	-2.62314900	1.07307500
H	3.33057900	-2.99970900	0.77804200
C	-0.35711200	-0.27671500	1.15141000
H	-0.52562400	0.74067200	1.49257100
C	-1.16604300	-1.27108400	1.86511600
H	-1.08604700	-2.30519800	1.54772500
C	-1.98613800	-0.98111200	2.88570900
H	-2.55656800	-1.75222200	3.38904400
H	-2.10938100	0.03550300	3.24659300
Pd	-1.85524600	-0.04159200	-0.59675700
H	1.97983300	-2.25250900	-1.83990700
C	1.12426300	-2.64366200	-1.29568900
H	1.23544800	-3.68274600	-0.99608300
C	-0.11635700	-2.22624000	-1.70557500
C	-1.20007800	-1.60483400	-1.80120100
H	-2.03083100	-1.61534000	-2.50210200
H	-2.90942000	2.64573600	1.29811600
P	-3.26475600	1.86307200	0.16163700
H	-4.60959200	1.61237500	0.55402400
H	-3.54981500	2.95833600	-0.70212700
7			
C	3.84356500	2.24842000	-0.19643200
C	4.07686000	0.89514200	0.01957200
C	3.01655200	0.00134700	0.21471600
C	1.68576800	0.48789700	0.20610300
C	1.46955100	1.85161700	-0.01268500
C	2.53415400	2.72625400	-0.21358300
H	4.28282300	-1.72870300	0.66321200

H	4.67557700	2.92552200	-0.35344300
H	5.09379900	0.51613300	0.03796300
C	3.26229400	-1.42189300	0.45484000
C	0.58782500	-0.47615200	0.51379900
H	0.44995800	2.21847100	-0.04906700
H	2.34018600	3.77813100	-0.39152300
C	0.86825600	-1.90713300	0.03594800
C	2.27601300	-2.32426100	0.40352900
H	0.15193900	-2.58862700	0.49697600
H	2.47669100	-3.37853700	0.56540200
C	-0.31790600	-0.14665100	1.52479500
H	-0.20054700	0.83427500	1.97734800
C	-1.17639900	-1.06245100	2.26692500
H	-1.30235000	-2.06585700	1.87265600
C	-1.80650300	-0.74101800	3.40591800
H	-2.42710200	-1.45740900	3.93016800
H	-1.71633500	0.24698200	3.84662700
Pd	-1.41275600	0.05943700	-0.51033500
H	1.47586700	-1.44436400	-1.99684300
C	0.66950300	-1.99794900	-1.50475900
H	0.73921100	-3.03649300	-1.84869300
C	-0.62163600	-1.39689100	-1.89942600
C	-1.66824600	-1.04837000	-2.46087100
H	-2.45302900	-1.01589200	-3.18327900
H	-3.27519900	2.91885800	-0.36815500
P	-3.28613100	1.55549500	0.04639000
H	-3.61442400	1.80404200	1.41102900
H	-4.61624900	1.27951000	-0.38115700
TS(8/9)			
C	-4.63214100	2.29604000	0.58618800
C	-4.98890700	0.97095800	0.57449700
C	-4.08471000	-0.03067800	0.13251200
C	-2.78027000	0.35194600	-0.32351500
C	-2.44313700	1.73030800	-0.27499400
C	-3.34081900	2.67626800	0.16227300
H	-5.44049700	-1.67548000	0.49466300
H	-5.33337000	3.04931200	0.92754600
H	-5.97437200	0.66471300	0.91026600
C	-4.45071400	-1.39988100	0.14688100
C	-1.86478900	-0.66661500	-0.78542500
H	-1.45270000	2.04886000	-0.57088900
H	-3.05222000	3.72118800	0.18865000
C	-2.28984800	-1.99212100	-0.74866700
C	-3.56267500	-2.35780600	-0.27964900
H	-1.63601700	-2.76768100	-1.12891600
H	-3.84632700	-3.40458100	-0.27696500
C	-0.54840500	-0.31269400	-1.29714000

H	-0.40713800	0.70699400	-1.63906500
C	0.52853000	-1.15128500	-1.40376800
H	0.43228800	-2.16882500	-1.03407900
C	1.83388200	-0.76443800	-1.87412100
H	2.50476200	-1.57297400	-2.15468000
H	1.86620300	0.07265200	-2.57023200
Pd	2.30628800	-0.05741700	0.09681100
P	3.98890100	1.43630100	-0.60880100
H	3.92461900	2.79538800	-0.20506400
H	5.31677900	1.16524500	-0.18877100
H	4.24964200	1.64719600	-1.98906400
H	2.58451600	1.13673700	2.90834100
C	2.33328200	0.35057800	2.21833300
C	1.86944100	-0.82939300	2.29894200
C	1.40891200	-2.06337100	2.03764800
H	2.06791400	-2.92377600	2.07415800
H	0.34738100	-2.24518200	1.91281700
9			
C	-5.02460900	-0.79445400	-1.26015200
C	-4.83831500	0.27763500	-0.42503400
C	-3.60005300	0.48963400	0.23678900
C	-2.52086300	-0.43305200	0.02629500
C	-2.75979500	-1.53516500	-0.83914900
C	-3.97061800	-1.71098600	-1.46551100
H	-4.24479700	2.28462800	1.25256300
H	-5.97542900	-0.94223600	-1.75974800
H	-5.64118400	0.98766700	-0.25533500
C	-3.41983800	1.59637900	1.10259500
C	-1.26660400	-0.20611100	0.69650100
H	-1.97911000	-2.26353400	-1.01298100
H	-4.11834800	-2.56184500	-2.12129100
C	-1.14761900	0.90521000	1.51699100
C	-2.21517300	1.79542000	1.73005700
H	-0.19179800	1.12153700	1.97895300
H	-2.07092800	2.65107200	2.38025400
C	-0.13220100	-1.13150900	0.52306700
H	-0.23440700	-1.88141500	-0.25322200
C	0.78043400	-1.44811800	1.57067600
H	0.70291000	-0.90240100	2.50667100
C	1.89689900	-2.25299300	1.36174600
H	2.62026200	-2.38614700	2.15633600
H	1.91112800	-2.99470400	0.56951800
Pd	1.90198400	-0.41723800	-0.04265600
P	4.20946200	0.11401300	-0.56892700
H	5.35290400	-0.55499300	-0.05084900
H	4.57566900	0.10271700	-1.93931900
H	4.59083100	1.44478600	-0.26399300

H	1.14983400	0.75257400	-2.42104800
C	1.32323100	1.06272800	-1.39207700
C	1.14396000	2.28769600	-1.02321600
C	0.95067200	3.51829500	-0.59706400
H	-0.02087600	3.84035800	-0.23434800
H	1.74311900	4.26105900	-0.61115500
TS(9/10)			
C	-4.89244700	-1.67091900	-0.87817600
C	-4.88501600	-0.35061500	-0.47499500
C	-3.71865400	0.24931400	0.04184500
C	-2.52483000	-0.51981300	0.16977600
C	-2.56517100	-1.86525400	-0.25382000
C	-3.71761900	-2.42900700	-0.76968700
H	-4.67235700	2.16198500	0.45263800
H	-5.79551200	-2.11721300	-1.27878100
H	-5.78528900	0.25019500	-0.55633200
C	-3.72820500	1.62705000	0.46414300
C	-1.33665900	0.10869100	0.74962100
H	-1.67218500	-2.47446800	-0.19795500
H	-3.70858500	-3.46283500	-1.09696800
C	-1.32550100	1.54122600	0.82176200
C	-2.58950700	2.24278400	0.85616600
H	-0.51335200	2.00018500	1.36931600
H	-2.59823100	3.28764800	1.14797400
C	-0.22191900	-0.63893200	1.13339800
H	-0.23976500	-1.70733400	0.94523100
C	0.91464900	-0.18480700	1.86498800
H	0.89122600	0.80644600	2.30642900
C	2.05018500	-0.97113000	2.07771100
H	2.81327400	-0.63445300	2.76879400
H	2.01729700	-2.03987900	1.89069500
Pd	2.15917000	-0.04707100	0.02170600
H	-1.49020000	1.89820900	-1.58301000
C	-0.59333500	2.18982500	-1.04522800
H	-0.55245000	3.24566600	-0.79133200
C	0.58202200	1.60588500	-1.45377700
C	1.63180500	0.98347100	-1.76093100
H	2.25218200	0.93554700	-2.64084200
H	4.84579300	-0.34836800	-2.01713400
P	4.40284600	-0.61122500	-0.68949000
H	4.85814700	-1.95675400	-0.61406200
H	5.50672400	-0.01756300	-0.01754700
10			
C	-5.14732500	-1.47702900	-0.86133900
C	-5.02587200	-0.17423100	-0.39499200
C	-3.80078800	0.31446100	0.07528100
C	-2.66548500	-0.53483600	0.10010500

C	-2.80705200	-1.84050400	-0.39317900
C	-4.02770600	-2.30904400	-0.86531400
H	-4.58850000	2.27365800	0.64631100
H	-6.10129700	-1.83946600	-1.22708500
H	-5.88768700	0.48560600	-0.39671100
C	-3.67646900	1.69332000	0.54278200
C	-1.39980200	-0.01539100	0.65581400
H	-1.94512000	-2.49577300	-0.42711200
H	-4.10344800	-3.32207800	-1.24464400
C	-1.19933800	1.48497400	0.62882900
C	-2.48811200	2.24303700	0.81038500
H	-0.51451600	1.78038600	1.42565600
H	-2.41842500	3.28030600	1.12458700
C	-0.41401100	-0.82936600	1.09851700
H	-0.54707400	-1.90515700	1.02414800
C	0.85007500	-0.39600400	1.68675500
H	0.85151700	0.54922600	2.22077500
C	1.95443900	-1.22008500	1.83779200
H	2.74200900	-0.95549400	2.53285200
H	1.90931900	-2.26177000	1.53640800
Pd	2.23282300	0.05352500	-0.02668400
H	5.55556500	-0.59816000	0.36560200
P	4.48965200	-0.79610600	-0.55806400
H	4.70120300	-2.19168300	-0.74875900
H	5.20317300	-0.36938300	-1.71476500
C	1.90497600	1.40775700	-1.65503800
H	2.56623600	1.64194600	-2.46280600
C	0.84216100	1.49161200	-1.01196000
C	-0.52839100	1.94824100	-0.72005600
H	-1.18460200	1.64179300	-1.54128100
H	-0.52080300	3.04402000	-0.72105700
TS(8/11)			
C	6.43657100	-1.01573200	0.50961100
C	6.17295100	0.29557900	0.20202300
C	4.86128000	0.72202500	-0.13497700
C	3.79277700	-0.23386400	-0.14026500
C	4.11076600	-1.58468600	0.16293600
C	5.39261700	-1.96590100	0.48261000
H	5.41252700	2.78584200	-0.47034000
H	7.44363100	-1.32667000	0.76395500
H	6.97035700	1.03158300	0.20684100
C	4.59549900	2.07230700	-0.47594900
C	2.45808200	0.20105000	-0.46936200
H	3.33353100	-2.33658100	0.12416300
H	5.60580100	-3.00488500	0.70805500
C	2.26279600	1.53876000	-0.78864400
C	3.32146400	2.46572600	-0.80412900

H	1.25991600	1.88767700	-1.00551600
H	3.11817500	3.50007500	-1.05905900
C	1.33117100	-0.73496300	-0.43605700
H	1.41935400	-1.58471600	0.23554700
C	0.19585600	-0.63767800	-1.16632800
H	0.11396200	0.16617900	-1.89460900
C	-0.94889000	-1.53973800	-1.07331500
H	-1.39832200	-1.76206600	-2.03811400
H	-0.75276400	-2.45572900	-0.51272900
Pd	-2.42484300	-0.56396700	0.06579300
P	-1.03855000	0.17038300	2.04579200
H	-0.19434300	1.30378200	1.90919600
H	-1.68723600	0.56412600	3.24911200
H	-0.08178000	-0.70408200	2.62896300
H	-6.73299100	-0.50971300	0.84284800
C	-5.90075100	-0.70000800	0.21149500
C	-4.98397500	-0.94518300	-0.54143500
C	-3.82215200	-1.18758900	-1.33816900
H	-3.68460800	-2.23873400	-1.59178900
H	-3.76465500	-0.56523700	-2.23320300
H	-4.55452000	2.23493100	-0.80948600
P	-3.55605500	2.58848000	0.14463100
H	-4.26178600	3.73454700	0.63886400
H	-2.75878700	3.33857300	-0.77581200
11			
C	6.20639200	-1.15205800	-0.17471700
C	5.98261400	0.02789900	0.48971800
C	4.69137500	0.61744500	0.52649000
C	3.60177300	-0.03998000	-0.13399000
C	3.87842200	-1.24938500	-0.82581300
C	5.14106500	-1.79335400	-0.84372000
H	5.29740500	2.33501500	1.69301200
H	7.19829200	-1.58983800	-0.19380000
H	6.79648800	0.53424400	0.99882900
C	4.46560900	1.84637300	1.19665100
C	2.28715900	0.55034700	-0.09080200
H	3.08161700	-1.74863200	-1.36113400
H	5.32202200	-2.71842800	-1.37981200
C	2.13086500	1.74950200	0.59129300
C	3.20913900	2.39982200	1.21999500
H	1.13993400	2.18021400	0.67360400
H	3.03464800	3.33366700	1.74375600
C	1.14416000	-0.11155100	-0.72698200
H	1.16383600	-1.19539800	-0.77202600
C	0.06559900	0.51343700	-1.24849100
H	0.05993000	1.60335000	-1.24041400
C	-1.10339400	-0.14680800	-1.83589000

H	-1.54248400	0.40282300	-2.67132200
H	-0.90604400	-1.17439900	-2.12917000
Pd	-2.61059000	-0.11754100	-0.34074600
P	-2.90238000	2.37089600	-0.61545800
H	-4.20913500	2.92254400	-0.73417100
H	-2.41484500	3.29648800	0.35096400
H	-2.34027400	2.99674900	-1.76191600
H	0.24096600	-3.07952800	2.16572300
C	-0.52524200	-2.84450200	1.46955000
C	-1.38685000	-2.57133000	0.66742800
C	-2.40360800	-2.22642600	-0.28545400
H	-2.16404300	-2.58760100	-1.28500800
H	-3.37746400	-2.63587500	-0.00130600
H	-5.52971900	-0.82601900	1.40433700
P	-4.21161800	-0.33389500	1.62115500
H	-4.56365200	0.69194200	2.54596300
H	-3.80081500	-1.30605000	2.57116200
TS(11/12)			
C	-5.38910300	1.49921000	0.39327100
C	-5.24738800	0.12726000	0.35242200
C	-4.01687800	-0.47213200	0.01186500
C	-2.89536000	0.34831800	-0.31031400
C	-3.07578800	1.74765500	-0.26272000
C	-4.28837000	2.31269400	0.08552900
H	-4.77866600	-2.50594000	0.12324800
H	-6.34021900	1.94524300	0.66116200
H	-6.08942200	-0.51588100	0.58802000
C	-3.89037200	-1.90402600	-0.03930900
C	-1.63695700	-0.28864600	-0.69897900
H	-2.24725300	2.40621900	-0.48941300
H	-4.38634600	3.39218100	0.12188300
C	-1.50763500	-1.68852300	-0.44869000
C	-2.69220100	-2.48800200	-0.28202900
H	-0.63281300	-2.19320900	-0.83282100
H	-2.59725300	-3.56873400	-0.29564200
C	-0.56729200	0.44991200	-1.22364200
H	-0.65362500	1.53079500	-1.24521800
C	0.59863900	-0.06438000	-1.84019000
H	0.64011900	-1.12214800	-2.07671500
C	1.69078900	0.73242600	-2.19808100
H	2.47100300	0.32389900	-2.82907700
H	1.58055100	1.81138300	-2.23073400
Pd	1.94726900	0.23208700	0.00117800
P	3.52203200	-1.86898600	-0.29630800
H	4.93279900	-1.75971100	-0.49643400
H	3.60626900	-2.85249200	0.73604700
H	3.31420900	-2.80118200	-1.35923000

H	-1.48969000	-2.27832900	2.04037200
C	-0.70078500	-1.73388300	1.56111800
C	0.34538200	-1.12311000	1.86689100
C	1.47424900	-0.36723000	2.09980300
H	1.30189500	0.57181800	2.62231800
H	2.35964200	-0.89521800	2.44639100
H	2.85408200	3.53291400	-0.00590700
P	3.13155500	2.30511900	0.66288500
H	4.55124900	2.41287100	0.57989000
H	3.01970600	2.82224700	1.98732200
12			
C	4.56344600	-2.51430700	1.25566000
C	4.88316500	-1.50579600	0.35363300
C	3.88474700	-0.75248000	-0.27378200
C	2.52025700	-1.03025000	-0.00771800
C	2.22082800	-2.03474600	0.92467500
C	3.22417100	-2.77225800	1.54492700
H	5.27089600	0.42745100	-1.48607800
H	5.34906700	-3.08601100	1.73662300
H	5.92279500	-1.28816900	0.12945300
C	4.22841300	0.32383800	-1.19999600
C	1.47818500	-0.27458000	-0.72895800
H	1.18656600	-2.22943800	1.18297300
H	2.96005600	-3.54146100	2.26244200
C	1.86359000	1.10459500	-1.26200200
C	3.31523300	1.18357500	-1.65815300
H	1.26573200	1.29417000	-2.16044800
H	3.60422800	2.00361700	-2.30729800
C	0.24342000	-0.79709100	-0.93306300
H	0.06545600	-1.81303900	-0.59047600
C	-0.89369400	-0.17730500	-1.59552400
H	-0.75841200	0.82005800	-2.00205800
C	-2.00640100	-0.91222800	-2.03422300
H	-2.63742800	-0.51213800	-2.82050100
H	-2.01206500	-1.99462000	-1.94005500
Pd	-2.59156300	-0.04783800	-0.13592800
H	-5.91997800	-0.26308100	-0.66912000
P	-4.91777500	-0.83180400	0.16901300
H	-5.22605400	-2.19076800	-0.12755800
H	-5.68283800	-0.76965700	1.37300200
C	1.47495400	2.20444100	-0.26506400
H	0.40642300	2.30459700	-0.08783000
C	2.29465300	2.99077000	0.37496600
C	3.11179600	3.77739900	1.01829600
H	3.52684600	3.49540900	1.98149200
H	3.41286000	4.73863900	0.61202500
H	-2.55345500	2.60911700	2.03735300

P	-2.03744800	1.29005600	1.87627600
H	-2.39514200	0.83123800	3.17756600
H	-0.68589300	1.60940100	2.18977800
TS(9/6)			
C	-4.81296000	-0.32980700	-0.62982600
C	-4.22357200	0.90525400	-0.76179100
C	-2.93167900	1.16366200	-0.23889900
C	-2.22684200	0.11403100	0.43001400
C	-2.87148100	-1.13999400	0.55998100
C	-4.13043700	-1.36098500	0.04455300
H	-2.88702000	3.23358500	-0.87484700
H	-5.80303000	-0.50942800	-1.03358000
H	-4.74545100	1.70943600	-1.26997700
C	-2.33719100	2.45068100	-0.36422300
C	-0.90007100	0.37368600	0.95970400
H	-2.38008600	-1.94293100	1.09425600
H	-4.60140100	-2.32994900	0.16688700
C	-0.38235100	1.67475100	0.82566500
C	-1.09704300	2.69430100	0.16337500
H	0.57721300	1.92595400	1.26036700
H	-0.64834800	3.67725800	0.07681100
C	-0.05790800	-0.68168600	1.48518800
H	-0.45929200	-1.68520900	1.53774300
C	1.05868500	-0.39487400	2.37156700
H	1.16429400	0.62293100	2.73758700
C	2.00383700	-1.28838300	2.73944000
H	2.82475000	-1.00186500	3.38444700
H	1.96137100	-2.32544900	2.42371900
Pd	1.37793700	-0.33900400	-0.15479600
H	1.09084000	-3.60585300	-0.99220400
P	0.87201900	-2.28762900	-1.48025400
H	-0.44702500	-2.48525100	-1.97080700
H	1.56715900	-2.42055500	-2.71058800
C	2.85270800	0.39460900	-1.42427100
H	3.10181700	-0.05603500	-2.38148000
C	3.46074200	1.44149500	-0.97713600
C	4.03547100	2.51017900	-0.45637300
H	3.66453200	3.51008700	-0.66143400
H	4.91485900	2.43035200	0.17569900
TS(6/13)			
C	-4.26804400	-0.84373500	-2.16512000
C	-4.65018400	-0.02286600	-1.13359300
C	-3.77687900	0.25030400	-0.04826300
C	-2.47695300	-0.35359000	-0.02344400
C	-2.11277900	-1.18096700	-1.11910100
C	-2.98034200	-1.42188600	-2.15849200
H	-5.15378400	1.56787400	0.97574000

H	-4.94593100	-1.04150700	-2.98793400
H	-5.63277900	0.43779300	-1.13386100
C	-4.16851300	1.11498900	1.00480500
C	-1.59396200	-0.09810200	1.08786700
H	-1.12012500	-1.60868700	-1.15024000
H	-2.67115900	-2.05339800	-2.98418600
C	-2.03530900	0.76257800	2.08068700
C	-3.30633100	1.36953900	2.04048100
H	-1.40207900	0.96709900	2.93426200
H	-3.60185100	2.03057500	2.84785700
C	-0.27807600	-0.77339400	1.16274600
H	-0.32386000	-1.79022900	0.77661700
C	0.56906500	-0.66156800	2.34481800
H	0.53585300	0.26894900	2.90300400
C	1.45673500	-1.60291900	2.74300300
H	2.11970300	-1.43342800	3.58265100
H	1.50626200	-2.57498600	2.26504200
Pd	1.46481000	-0.02529300	0.12720800
H	3.30412700	-3.50527600	-0.55943400
P	2.24122900	-2.58706800	-0.83440800
H	1.20474300	-3.56804000	-0.79310300
H	2.40205900	-2.61692800	-2.25155400
C	0.44393600	1.60829300	-0.60240700
H	-0.63774600	1.53160800	-0.57850300
C	1.02756200	2.66591500	-1.06227400
C	1.65965200	3.72682300	-1.52144200
H	1.89770900	4.57007500	-0.87853300
H	1.92857500	3.82053700	-2.57033200
H	4.05267700	2.19290300	0.05699100
P	3.70569400	0.93561900	-0.49906300
H	3.96645900	1.24858800	-1.85899400
H	4.92859300	0.25520800	-0.22661700
13			
C	5.15820100	0.70480500	0.03710400
C	4.69050400	-0.04272200	-1.01370400
C	3.37189500	-0.57235300	-1.01507700
C	2.50063100	-0.29681700	0.09449200
C	3.03696400	0.45882100	1.17551300
C	4.32228700	0.94602900	1.15019500
H	3.58374400	-1.58933800	-2.91039800
H	6.16916600	1.09660400	0.02436200
H	5.33023500	-0.25256200	-1.86504100
C	2.91418100	-1.38304300	-2.08204700
C	1.15413100	-0.80911800	0.07884900
H	2.42976500	0.63276400	2.05377800
H	4.70225900	1.50851200	1.99599800
C	0.77466600	-1.61251900	-0.98714900

C	1.64436900	-1.90596400	-2.05377000
H	-0.23798500	-1.99838600	-1.00963800
H	1.29491500	-2.53609100	-2.86454700
C	0.17566200	-0.51913800	1.18518300
H	0.52964500	0.26054000	1.85789000
C	-0.20462300	-1.70666700	1.98426900
H	-0.38017700	-2.62381200	1.42872800
C	-0.33279700	-1.73304000	3.31475100
H	-0.60814400	-2.64138500	3.83813700
H	-0.17130400	-0.84690200	3.92212500
Pd	-1.44863700	0.53336600	0.22419600
H	1.24458000	2.70218100	0.51868700
P	0.04570200	2.51834800	-0.21792500
H	0.59857500	2.65957400	-1.51943100
H	-0.46544800	3.84026500	-0.09191800
C	-2.68729500	-1.06937200	0.62930900
H	-2.83228800	-1.26276200	1.68913700
C	-3.22827500	-1.81927500	-0.27591200
C	-3.75659300	-2.56774600	-1.22073800
H	-4.73328200	-2.35156800	-1.64477600
H	-3.24769900	-3.45078300	-1.59692900
H	-4.05845000	0.68021300	-1.86526900
P	-3.47888700	1.53164900	-0.88983600
H	-3.59724800	2.76212200	-1.60497300
H	-4.61922500	1.69474000	-0.06012100
TS(13/14)			
C	3.43061800	2.95343900	0.31048800
C	4.04881400	1.75417200	0.01142300
C	3.34598500	0.53488600	0.06189400
C	1.97019300	0.52478600	0.43290300
C	1.36485200	1.76815200	0.71833800
C	2.07380800	2.95464900	0.66384000
H	5.07644500	-0.69071800	-0.43664400
H	3.98566300	3.88361300	0.26478000
H	5.09707400	1.73685600	-0.27008500
C	4.01046900	-0.71017300	-0.23372100
C	1.25908600	-0.74852200	0.53918900
H	0.30769500	1.79720700	0.95175800
H	1.57237600	3.89119800	0.88355100
C	1.88663100	-1.92113900	-0.02525600
C	3.32771700	-1.87284600	-0.25145000
H	1.53850900	-2.85548000	0.39769500
H	3.83487600	-2.80492500	-0.48091000
C	0.02478700	-0.84116500	1.23468100
H	-0.12939600	-0.04424600	1.95654100
C	-0.56821300	-2.11817200	1.65911400
H	-0.53636000	-2.93950000	0.95067100

C	-1.15488500	-2.32726600	2.84560200
H	-1.58406300	-3.28845300	3.10243700
H	-1.22078800	-1.54533700	3.59655500
Pd	-1.56042400	-0.05187000	-0.22477800
H	1.91706500	-1.82987100	-2.49399100
C	1.24056600	-2.37769200	-1.84009200
H	1.49174700	-3.43364700	-1.77455200
C	-0.09668600	-2.06289800	-1.96036000
C	-1.21473700	-1.53202100	-1.75892700
H	-2.18080700	-1.59933000	-2.23724500
H	-2.43148800	1.10320400	3.01989400
P	-2.90275900	1.03790600	1.67433400
H	-4.10950400	0.34115400	1.96663800
H	-3.48467200	2.34159900	1.65135700
H	-1.35071600	2.37964000	-2.59359600
P	-2.40126500	1.53055600	-2.14173900
H	-2.73722900	1.00276000	-3.42416700
H	-3.41059600	2.54424500	-2.12583100
14			
C	3.62444400	-0.08983000	2.55055900
C	3.92553800	-0.51825800	1.26355400
C	2.91746600	-0.72568000	0.31357300
C	1.56470400	-0.49775900	0.66211400
C	1.28275000	-0.07110700	1.96539000
C	2.29330900	0.13040800	2.90131800
H	4.26274500	-1.52325900	-1.21451500
H	4.41715900	0.07082500	3.27266800
H	4.95748600	-0.70041300	0.97975300
C	3.24170800	-1.20410900	-1.02741400
C	0.49481500	-0.80647000	-0.33808800
H	0.24993200	0.12290300	2.23620200
H	2.04073600	0.46577000	3.90143900
C	0.91888100	-0.74696500	-1.81312900
C	2.33260300	-1.24310500	-2.00509100
H	0.25964100	-1.40895400	-2.37821300
H	2.60682000	-1.58590200	-2.99880500
C	-0.54184200	-1.68497800	0.07769300
H	-0.50251400	-2.00353900	1.11749300
C	-1.35166900	-2.55833600	-0.77047100
H	-1.41411700	-2.32161400	-1.82857900
C	-2.03180500	-3.62562600	-0.32612300
H	-2.61861400	-4.24166200	-0.99695500
H	-2.01189600	-3.91819700	0.71921400
Pd	-1.42070900	0.31579300	0.12128100
H	0.03987800	3.30478300	0.76891500
P	-1.11422300	2.78194600	0.12573200
H	-0.99641000	3.54482400	-1.06998900

H	-2.05783000	3.64041200	0.76408500
C	2.27987400	2.62591700	-1.64207300
H	2.90826800	3.40895400	-1.29589900
C	1.58820100	1.71927100	-2.02249200
C	0.74416200	0.63708800	-2.51710500
H	0.94624800	0.50123300	-3.58699000
H	-0.30838500	0.92526200	-2.42212600
H	-4.17843800	-1.48165300	0.81583500
P	-3.79657300	-0.11397900	0.69479400
H	-4.84925400	0.26661400	-0.18911400
H	-4.43574400	0.34488500	1.88545500
15			
C	-4.21573400	-1.89254900	0.30429900
C	-4.42707400	-0.63168500	-0.19607600
C	-3.39044500	0.33790700	-0.20697700
C	-2.10513400	-0.00679700	0.32353800
C	-1.92021200	-1.32635900	0.81649000
C	-2.94531400	-2.24322100	0.81038600
H	-4.57819100	1.88424200	-1.14366200
H	-5.01774300	-2.62216600	0.30548600
H	-5.39710400	-0.35609700	-0.59693300
C	-3.60204500	1.63471700	-0.74168400
C	-1.05464800	0.97809200	0.32337000
H	-0.94840800	-1.62141000	1.19224600
H	-2.77618300	-3.24404100	1.19186100
C	-1.32597500	2.23121800	-0.19982600
C	-2.58615000	2.55674100	-0.74082100
H	-0.55857500	2.99573500	-0.17053500
H	-2.75086800	3.55154700	-1.13989500
C	0.26586900	0.66090600	0.91011100
H	0.25093400	0.06416000	1.81790700
C	1.45895400	1.28613400	0.57961800
H	1.45095600	2.04453400	-0.20127500
C	2.71876900	1.24653000	1.42729100
H	2.90388900	2.22830400	1.88256900
H	2.58877100	0.52950000	2.24178700
Pd	1.58292900	-0.63768300	-0.46986100
H	4.21797600	1.65729100	-0.09742000
C	3.95334500	0.83963300	0.58329000
H	4.82464800	0.66617700	1.22423000
C	3.66416300	-0.36273400	-0.23611300
C	3.66360200	-1.35694900	-0.97796700
H	4.06333400	-2.15386300	-1.56634300
16			
C	-4.44682200	-1.24480000	1.07444100
C	-4.55565200	-0.27482400	0.10950400
C	-3.45001100	0.54551200	-0.23909500

C	-2.19754100	0.35927000	0.43411400
C	-2.12311200	-0.66355900	1.41855800
C	-3.21346900	-1.44081200	1.73298200
H	-4.51897600	1.67129800	-1.74568800
H	-5.30101600	-1.86170400	1.33023900
H	-5.49711500	-0.11800900	-0.40704200
C	-3.56674500	1.53948700	-1.24319600
C	-1.07549000	1.19538400	0.08629600
H	-1.18573900	-0.84863700	1.92579900
H	-3.12502400	-2.21204500	2.49025600
C	-1.25946900	2.15954700	-0.89295000
C	-2.48745600	2.32534100	-1.56124200
H	-0.44248500	2.82488000	-1.14420500
H	-2.57699800	3.09466400	-2.32047500
C	0.21301400	1.05224000	0.79375100
H	0.15355200	0.67092900	1.80807700
C	1.41952400	1.61659300	0.42167800
H	1.47348400	2.17034900	-0.51386900
C	2.58252000	1.86132400	1.36532400
H	2.63903200	2.92277300	1.64305200
H	2.43448100	1.29330800	2.28791100
Pd	1.65933000	-0.52166000	-0.22478400
P	0.21292500	-2.35384200	-1.02588500
H	0.56995500	-3.09799800	-2.18627100
H	-0.07758600	-3.47892900	-0.20262400
H	-1.13030700	-2.08064000	-1.40788600
H	4.31425700	-1.95262100	-0.72703600
C	3.84455300	-1.06129800	-0.37493100
C	3.72689100	0.07034400	0.11206300
C	3.89865800	1.41958700	0.69734100
H	4.73806100	1.43474100	1.40155100
H	4.15300800	2.11561800	-0.11126300
17			
C	6.99866700	-0.82046600	-1.04936500
C	6.66290500	0.50105300	-0.89149000
C	5.38794100	0.88036000	-0.39535600
C	4.44228200	-0.13791900	-0.04428700
C	4.82084700	-1.49358500	-0.23847800
C	6.06332200	-1.82712200	-0.72290200
H	5.75392000	3.00769500	-0.51817500
H	7.97616200	-1.09485300	-1.42994600
H	7.37112800	1.28186300	-1.14926300
C	5.03036600	2.24492800	-0.25037900
C	3.15368500	0.24594900	0.46385700
H	4.11142100	-2.28004800	-0.01523600
H	6.32662700	-2.86988000	-0.86146600
C	2.86318400	1.59378500	0.58963200

C	3.79060200	2.59081100	0.22585300
H	1.90678400	1.88779400	1.00592700
H	3.52182600	3.63480100	0.34315500
C	2.16702000	-0.77207400	0.87189400
H	2.56199100	-1.67034800	1.34165200
C	0.84218400	-0.67313500	0.71512900
H	0.42359900	0.19788400	0.21637900
C	-0.15164500	-1.69608200	1.17893000
H	-0.70736600	-2.08002600	0.31472400
H	0.36845700	-2.54354100	1.63663600
Pd	-3.40495700	0.11519600	0.02196900
P	-3.64275900	-1.96830100	-1.27506400
H	-4.74235500	-2.21048300	-2.15165700
H	-2.63163500	-2.34611900	-2.20581100
H	-3.71036600	-3.22711800	-0.61083800
H	-2.58493000	2.09952400	2.04304900
C	-2.50488000	1.10791200	1.64413100
C	-2.03679800	-0.05731600	1.65607700
C	-1.18204000	-1.14061700	2.19172700
H	-0.64898100	-0.77565100	3.07816600
H	-1.81919600	-1.96874100	2.52027400
H	-5.92103600	2.37570200	-0.34660300
P	-4.94306700	1.68866000	-1.12180600
H	-5.82392900	1.34793600	-2.19302200
H	-4.40256100	2.85030800	-1.74529000
TS(4/15)			
C	-4.19460800	-2.18154500	0.23255600
C	-4.54067800	-0.92401800	-0.19557000
C	-3.59579900	0.13531300	-0.20141800
C	-2.26356800	-0.11327400	0.26228500
C	-1.93644400	-1.43205200	0.67306300
C	-2.87479800	-2.43750500	0.66308400
H	-4.95850400	1.60432800	-1.01613800
H	-4.92676200	-2.98127500	0.22976400
H	-5.54801900	-0.72019800	-0.54382600
C	-3.94676800	1.42829400	-0.66680600
C	-1.30794300	0.96521000	0.27189700
H	-0.92163700	-1.65874300	0.97294300
H	-2.59644700	-3.43715600	0.97763400
C	-1.71277700	2.20878500	-0.19104900
C	-3.01775400	2.43868700	-0.66696600
H	-1.02153900	3.04259100	-0.15519900
H	-3.28800100	3.42967800	-1.01462300
C	0.04123700	0.75717200	0.81332300
H	0.11729500	0.08411400	1.66160100
C	1.15384900	1.54286600	0.51568500
H	1.05908300	2.32958600	-0.22711700

C	2.44972500	1.42650500	1.19571500
H	3.06449600	2.31781400	1.14611600
H	2.43132100	0.96946400	2.17873200
Pd	1.91558500	-0.26386400	-0.33310900
H	4.64340200	1.12039800	-0.04499300
C	4.13666300	0.31459100	0.47608800
H	4.50588700	0.15160400	1.48403400
C	3.94467900	-0.86730500	-0.30321800
C	3.59210000	-1.82810800	-1.00426000
H	3.75981000	-2.71618200	-1.57238700

TS(8/16)

C	-4.33309700	2.51819900	0.77608800
C	-5.00653700	1.35804200	0.48533800
C	-4.31055300	0.18292600	0.09751200
C	-2.88146800	0.21738900	-0.00502200
C	-2.21916900	1.42978800	0.32575900
C	-2.92328200	2.54958900	0.70135600
H	-6.08420400	-1.03858900	-0.09554000
H	-4.87805000	3.40753100	1.07234700
H	-6.08895700	1.31971100	0.55298300
C	-5.00247400	-1.02408200	-0.17666500
C	-2.17575200	-0.97116300	-0.40846700
H	-1.13761300	1.46827700	0.30335800
H	-2.39253700	3.46158000	0.95125000
C	-2.90919000	-2.11935300	-0.66899800
C	-4.31123800	-2.15233100	-0.54342800
H	-2.39117700	-3.00638800	-1.01471900
H	-4.84307900	-3.07201800	-0.76108800
C	-0.71809000	-0.95871000	-0.57207100
H	-0.26454800	-0.02522000	-0.89411100
C	0.10813500	-2.00043100	-0.34701200
H	-0.31546500	-2.91178000	0.07227400
C	1.55149000	-2.00527400	-0.57255000
H	2.00688400	-2.98787700	-0.56822700
H	1.86393100	-1.46679600	-1.46697400
Pd	2.67148500	0.11061800	0.00810500
P	2.80946200	1.74488000	-1.73798800
H	2.06937000	2.95340300	-1.61399500
H	4.07176400	2.34667300	-1.99563800
H	2.47226900	1.48933200	-3.09933100
H	3.91896600	1.23866800	2.81089000
C	3.46557300	0.47223500	2.22392600
C	2.99130100	-0.64807500	1.99976500
C	2.40886300	-1.80059100	1.40542200
H	3.09718400	-2.63048600	1.28311000
H	1.45793300	-2.09657900	1.83465500

TS(11/17)

C	6.16460000	-1.12282700	0.16479100
C	5.84376100	0.20220900	0.32396300
C	4.51187300	0.66260600	0.15072600
C	3.48306200	-0.27814400	-0.18394800
C	3.85969600	-1.63600900	-0.36031800
C	5.15980000	-2.04973100	-0.18769100
H	4.97576900	2.73808700	0.54388900
H	7.18664100	-1.45886000	0.29973000
H	6.61056300	0.92525500	0.58264400
C	4.18811200	2.03588800	0.29238900
C	2.12660800	0.18579600	-0.34838800
H	3.11248000	-2.36159300	-0.65401700
H	5.41726800	-3.09347700	-0.32980400
C	1.87342200	1.54357600	-0.18544800
C	2.89409500	2.46252500	0.11905500
H	0.85210400	1.89823100	-0.25726300
H	2.64548600	3.51163300	0.23810300
C	1.04277200	-0.74463300	-0.65174700
H	1.16210400	-1.77029600	-0.31379800
C	-0.10940900	-0.43025200	-1.29898100
H	-0.21838200	0.56329400	-1.72136400
C	-1.18244000	-1.39008500	-1.57176700
H	-1.77309600	-1.17896800	-2.45716300
H	-0.80693300	-2.40909300	-1.58192300
Pd	-2.29075900	0.06043600	-0.00042500
P	-3.15741300	2.04844400	-1.16671700
H	-4.56810500	2.13555500	-1.34802700
H	-2.99701500	3.38483100	-0.69225900
H	-2.82278200	2.35364800	-2.52205100
H	-5.84970200	-1.32512800	1.23885200
C	-4.91824600	-1.56750400	0.79075000
C	-3.83951600	-1.80842600	0.29297700
C	-2.61011200	-2.23837100	-0.32408300
H	-1.95800300	-2.77143000	0.36366000
H	-2.83726700	-2.85675500	-1.18978400
H	-1.13945200	-0.85963500	3.17502300
P	-1.50329600	0.27997200	2.39436200
H	-2.30867200	0.88075300	3.40776800
H	-0.32589300	1.02796600	2.68898300
PPh₃			
P	0.00139400	-0.00206500	-1.25732200
C	-0.38469500	1.64719000	-0.41537400
C	0.16127500	2.79875900	-0.99432300
C	-1.20063200	1.77892000	0.71155200
C	-0.08753500	4.05465400	-0.44735600
H	0.78073900	2.71152500	-1.88069900
C	-1.45942600	3.03820000	1.25220400

H	-1.63932600	0.89920600	1.16659600
C	-0.90128100	4.17751700	0.67778200
H	0.34569300	4.93698000	-0.90532500
H	-2.09752200	3.12614700	2.12480100
H	-1.10358800	5.15555400	1.09966400
C	-1.23711500	-1.15947400	-0.41668900
C	-0.94259300	-1.94468400	0.70141600
C	-2.51168600	-1.24860800	-0.98891800
C	-1.90710100	-2.79622600	1.23993500
H	0.04107700	-1.89747000	1.15228500
C	-3.47777300	-2.08999500	-0.44430800
H	-2.74713900	-0.65860800	-1.86843000
C	-3.17655900	-2.86845800	0.67224100
H	-1.66343800	-3.40206700	2.10591600
H	-4.46155500	-2.14486200	-0.89718900
H	-3.92481300	-3.53124000	1.09216500
C	1.62349300	-0.49117700	-0.41394100
C	2.35927800	-1.52566400	-1.00364100
C	2.13602300	0.13837600	0.72426700
C	3.57231300	-1.93596100	-0.45689900
H	1.98252800	-2.00851900	-1.89911600
C	3.35623200	-0.26551100	1.26533300
H	1.58727600	0.94927400	1.18755200
C	4.07493800	-1.30474700	0.67962800
H	4.12894900	-2.74089500	-0.92396900
H	3.74366600	0.23419700	2.14651900
H	5.02360900	-1.61692600	1.10160900
Pd(PPh₃)₂			
P	-2.39024600	-0.00218000	-0.00387100
C	-3.20048500	0.04330300	1.69968500
C	-2.56043200	0.78603400	2.69706000
C	-4.38721100	-0.62788000	2.00292100
C	-3.10974400	0.87184600	3.97334100
H	-1.62162400	1.28000300	2.47028200
C	-4.93125900	-0.54885000	3.28468200
H	-4.88373500	-1.22182700	1.24496100
C	-4.29713500	0.20377800	4.27011700
H	-2.60420800	1.45024100	4.73877900
H	-5.85007700	-1.07877000	3.51111400
H	-4.72062100	0.26268400	5.26661900
C	-3.20289900	-1.49928200	-0.81592500
C	-4.37965700	-1.42455900	-1.56435700
C	-2.57085300	-2.73695700	-0.65810600
C	-4.92117700	-2.57430100	-2.13921900
H	-4.87100000	-0.47033100	-1.71121200
H	-1.63940700	-2.79018200	-0.10495300
C	-4.29484100	-3.80615600	-1.96664700

H	-5.83205700	-2.50373800	-2.72370400
H	-2.61808900	-4.83884000	-1.09513600
H	-4.71631800	-4.69867100	-2.41570600
C	-3.19724800	1.45464900	-0.88994500
C	-2.53193600	1.98173300	-2.00130100
C	-4.40437800	2.02634300	-0.48156300
C	-3.07650100	3.05245200	-2.70560700
H	-1.57789800	1.55830000	-2.29694300
C	-4.94385000	3.10463300	-1.18222300
H	-4.92081100	1.64048500	0.38901400
C	-4.28429100	3.61627500	-2.29711800
H	-2.55127400	3.45349700	-3.56539800
H	-5.87869300	3.54504100	-0.85296400
H	-4.70401200	4.45611400	-2.83968900
Pd	0.00031000	-0.00358300	-0.00315400
H	4.70370600	5.22649300	-0.77082200
C	4.28412900	4.23604300	-0.63364600
C	4.91892600	3.12563100	-1.18446600
C	3.10065200	4.07037100	0.08459400
C	4.37986300	1.85106200	-1.01112000
H	5.83429200	3.24805200	-1.75314600
C	2.55607600	2.79963600	0.25010000
H	2.59421400	4.93163600	0.50617800
C	3.19721000	1.67935200	-0.28791300
H	4.87729500	0.99490200	-1.45110300
H	1.62008300	2.66927200	0.78274300
P	2.39140800	-0.00210200	-0.00092200
C	3.19991200	-0.59102300	1.59872900
C	3.20455600	-1.09002300	-1.30968000
C	2.56200200	-1.61913000	2.29995200
C	4.38080000	-0.04657600	2.10861200
C	2.55974700	-1.19897900	-2.54554800
C	4.39565500	-1.78782000	-1.09577500
C	3.10842800	-2.11019700	3.48254200
H	1.62689000	-2.01788500	1.92166400
C	4.92157600	-0.53272100	3.29899700
H	4.87532300	0.76356100	1.58617500
C	3.10857500	-1.97882700	-3.55973100
H	1.61737200	-0.68380100	-2.69854600
C	4.93931600	-2.57615500	-2.10967100
H	4.89573100	-1.72772300	-0.13651800
C	4.29028900	-1.56746500	3.98471400
H	2.60464200	-2.90766600	4.01753100
H	5.83566300	-0.09889900	3.68957800
C	4.30038300	-2.66943800	-3.34368300
H	2.59910700	-2.05678500	-4.51382600
H	5.86139900	-3.11863200	-1.93148600

H	4.71150800	-1.94293000	4.91071200
H	4.72348500	-3.28436100	-4.13025800
PdPPh₃			
P	-0.00186800	0.00096400	0.34581100
Pd	-0.00121600	0.03154800	2.66618300
C	1.21724300	-1.19799500	-0.45353400
C	1.45563400	-2.41267400	0.19618400
C	1.88356300	-0.92016700	-1.64950400
C	2.33342000	-3.34419800	-0.35124400
H	0.95915700	-2.61451700	1.13940400
C	2.77036100	-1.85008400	-2.19150800
H	1.72170800	0.02410000	-2.15522300
C	2.99350400	-3.06421100	-1.54697600
H	2.50976400	-4.28353900	0.16093800
H	3.28756700	-1.62178100	-3.11696600
H	3.68395900	-3.78563000	-1.96945000
C	0.42488500	1.64341000	-0.48148000
C	-0.19971500	2.09911800	-1.64459900
C	1.41007000	2.43259600	0.11938800
C	0.16356400	3.32485800	-2.20234700
H	-0.97641300	1.50699200	-2.11327600
C	1.77981900	3.65012600	-0.44476900
H	1.87267200	2.09337400	1.04017100
C	1.15584700	4.09990000	-1.60772000
H	-0.33268500	3.67221700	-3.10192500
H	2.54604100	4.25251500	0.03046400
H	1.43554000	5.05303900	-2.04233100
C	-1.64294000	-0.46543700	-0.46031900
C	-2.81509800	-0.01120500	0.15191800
C	-1.73354400	-1.24153600	-1.61808600
C	-4.05891500	-0.31370700	-0.39463200
H	-2.74495000	0.56658900	1.06737700
C	-2.98116900	-1.55270600	-2.15866600
H	-0.83549200	-1.61488700	-2.09514800
C	-4.14459800	-1.08686800	-1.55185300
H	-4.96086400	0.04440100	0.08914800
H	-3.04021000	-2.16244300	-3.05354000
H	-5.11342700	-1.33139900	-1.97275600
TS(PdPPh₃/1a)			
C	-6.09227000	3.16079700	-0.15687600
C	-6.87405800	2.12798500	0.29570400
C	-6.39233300	0.79267900	0.29944500
C	-5.06588400	0.51941200	-0.16940800
C	-4.29401700	1.61211500	-0.64199800
C	-4.79044800	2.89536000	-0.63222500
H	-8.20854800	-0.04983700	1.10889700
H	-6.47119000	4.17631400	-0.15600900

H	-7.87977300	2.31608400	0.65629900
C	-7.20813900	-0.27295200	0.75382500
C	-4.59018800	-0.84510600	-0.16010500
H	-3.29760400	1.44655600	-1.02909800
H	-4.17571800	3.70902600	-0.99991800
C	-5.44296200	-1.84680300	0.30011800
C	-6.74063700	-1.56657500	0.75143600
H	-5.08376800	-2.86691500	0.35108900
H	-7.36585100	-2.37497900	1.11210100
C	-3.24334300	-1.16602600	-0.58677200
H	-2.52012700	-0.35729900	-0.59831400
C	-2.78120400	-2.39287800	-0.96925900
H	-3.44590100	-3.25024800	-0.97845000
C	-1.45156800	-2.60396300	-1.38907400
H	-1.18877600	-3.50261900	-1.92316700
H	-0.79237200	-1.75196600	-1.52171000
Pd	0.89247100	-1.82216300	0.28236000
Cl	-0.48702500	-3.83879200	0.52658300
P	2.24506700	0.07674200	0.07113000
C	1.32385600	1.67579700	-0.32671900
C	1.71568400	2.55785900	-1.33512600
C	0.17933600	1.96404900	0.42590100
C	0.97632900	3.71479900	-1.58501000
H	2.59388900	2.34425300	-1.93168400
C	-0.54906600	3.12570100	0.18567100
H	-0.13962800	1.27179100	1.19791200
C	-0.15215200	4.00426500	-0.82340800
H	1.28869900	4.39001900	-2.37407500
H	-1.42855100	3.34143900	0.78218300
H	-0.72062100	4.90784100	-1.01384200
C	3.56720100	-0.00942200	-1.27205100
C	4.77419400	0.69101400	-1.19837400
C	3.31593600	-0.82319600	-2.37987600
C	5.71093700	0.58554000	-2.22523500
H	4.99283600	1.30876300	-0.33557200
C	4.24900200	-0.92177400	-3.40925200
H	2.39509900	-1.39515900	-2.41653900
C	5.44854900	-0.21671200	-3.33368900
H	6.64767900	1.12743100	-2.15502900
H	4.04457400	-1.55935700	-4.26216200
H	6.18017200	-0.30032000	-4.12960400
C	3.23526600	0.54603400	1.60602800
C	3.72941600	-0.49374300	2.39899100
C	3.48810200	1.86945800	1.97552900
C	4.47897600	-0.21361800	3.53818600
H	3.51166200	-1.52099300	2.12773900
C	4.23268700	2.14780700	3.12133600

H	3.09732300	2.68510300	1.37883200
C	4.73170900	1.10813000	3.90204000
H	4.85592800	-1.02789100	4.14683700
H	4.41880400	3.17840300	3.40313200
H	5.30806100	1.32619200	4.79420800
TS(Pd(PPh₃)₂/1b)			
C	4.88316400	-1.94399200	2.88659200
C	5.64550500	-2.57382600	1.93528200
C	5.13174600	-2.82245200	0.63560200
C	3.79017100	-2.42849700	0.31985700
C	3.04178500	-1.76235600	1.32353300
C	3.57255600	-1.52646800	2.57103600
H	6.94355800	-3.73710700	-0.10151600
H	5.28762800	-1.75168700	3.87374500
H	6.66072700	-2.88448800	2.15854900
C	5.93130500	-3.44148400	-0.35622600
C	3.27780800	-2.69463500	-1.00555000
H	2.04726700	-1.39607000	1.10538800
H	2.98256100	-0.99632300	3.30935200
C	4.12210100	-3.29646300	-1.93851700
C	5.43682300	-3.66476300	-1.62103100
H	3.74370300	-3.52339000	-2.92738700
H	6.05425500	-4.14158200	-2.37346000
C	1.90165700	-2.39514000	-1.34242600
H	1.21442400	-2.21294900	-0.52189700
C	1.35973600	-2.32969100	-2.60137400
H	1.99798100	-2.39505100	-3.47613700
C	-0.01379400	-2.14111400	-2.82176600
H	-0.41853000	-2.24414600	-3.81401900
H	-0.70986300	-2.24060400	-1.99821600
Pd	-0.47561400	-0.00968100	-0.88804300
Cl	-0.26096400	0.27683700	-3.58543600
P	-2.49365300	-0.91977400	0.12884000
P	0.87573900	1.89757500	-0.10696300
C	-0.20421700	3.43826600	-0.26303000
C	-0.91123100	3.59992900	-1.46126400
C	-0.34530000	4.38800800	0.75112600
C	-1.73777600	4.70552100	-1.64094400
H	-0.81839200	2.85654100	-2.24636900
C	-1.18323200	5.48951700	0.56969000
H	0.19182900	4.27201400	1.68463800
C	-1.87795000	5.65207400	-0.62587300
H	-2.27925100	4.82196900	-2.57317400
H	-1.28700900	6.22057400	1.36435200
H	-2.52787500	6.50880200	-0.76589300
C	1.43125100	1.95964200	1.70030500
C	2.62811600	2.55006800	2.11457500

C	0.60001900	1.36593800	2.65667900
C	2.98393300	2.55178400	3.46320000
H	3.28804200	3.00506100	1.38663400
C	0.94921100	1.38051100	4.00510400
H	-0.32353400	0.89328000	2.34273400
C	2.14498700	1.97197800	4.41193800
H	3.91768900	3.01045400	3.76994500
H	0.28723700	0.92702800	4.73473700
H	2.42061100	1.97967500	5.46084700
C	2.43812400	2.42809900	-1.02901100
C	3.29212600	1.42938800	-1.50160000
C	2.76248300	3.76778800	-1.26085700
C	4.46586400	1.76222600	-2.17266900
H	3.02888700	0.38843800	-1.35772000
C	3.93241700	4.10048900	-1.94207100
H	2.10004100	4.55360200	-0.91836800
C	4.78862400	3.09934500	-2.39465300
H	5.11915700	0.97603500	-2.53427000
H	4.17089800	5.14331100	-2.12095000
H	5.69675700	3.35948000	-2.92715700
C	-3.13518100	-0.11495600	1.71514500
C	-3.13735300	1.28338700	1.76494100
C	-3.60168000	-0.83728500	2.81584500
C	-3.61140400	1.94762200	2.89244700
H	-2.75831900	1.85244500	0.92295400
C	-4.06540400	-0.16923000	3.94997500
H	-3.60327200	-1.92028400	2.79456200
C	-4.07524900	1.22245400	3.98974500
H	-3.60818300	3.03155200	2.91520000
H	-4.42308200	-0.74096600	4.79952300
H	-4.43832800	1.73980300	4.87082100
C	-2.42011300	-2.75129700	0.58787700
C	-3.29203200	-3.70879200	0.06423100
C	-1.38639700	-3.16928300	1.43642200
C	-3.13507400	-5.05778800	0.38641200
H	-4.09321700	-3.40680400	-0.59846000
C	-1.23952000	-4.51232700	1.76829100
H	-0.69119200	-2.43747900	1.83407300
C	-2.11420100	-5.46278800	1.24082400
H	-3.81692000	-5.78991500	-0.03229600
H	-0.43690100	-4.81805400	2.43033500
H	-1.99498100	-6.51098400	1.49084100
C	-4.02785000	-0.80903600	-0.97163600
C	-3.84461200	-0.58670900	-2.33882500
C	-5.32575500	-0.92460400	-0.46240500
C	-4.94769400	-0.50167300	-3.18851600
H	-2.84421900	-0.45171200	-2.73731000

C	-6.42479200	-0.83724600	-1.31318500
H	-5.48190500	-1.07140100	0.59998400
C	-6.23719700	-0.62904600	-2.67920700
H	-4.79298600	-0.32262000	-4.24667500
H	-7.42699800	-0.92477200	-0.90783900
H	-7.09397000	-0.55614300	-3.34009500