Supplementary Information

Cyclopalladation of dimesityl selenide: Synthesis, reactivity, structural characterization, isolation of an intermediate complex with C-H···Pd intra-molecular interaction and computational studies

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Preparation of Bis (2,4,6-trimethylphenyl)selenide[Mes_2Se]

To a freshly prepared Na_2Se (prepared by reacting Se powder with $NaBH_4$ in water under argon flow) was treated with 2,4,6-trimethylphenyl diazonium chloride (prepared by using 2,4,6-trimethylaniline at 0-5°C) and allowed to stire for 2 h. The reaction mixture was allowed to warm to at 40°C and stire for additional 3 h. The crude product was extracted with dichloromethane and the solvent was evaporeted under reduced pressure and the residue was. colum chromatographed using hexane as the eluent and the ligand was crystallized from hexane (yield 60%, mp: 105°C). Analysis Calcd. for $C_{18}H_{22}Se$: C, 68.13; H, 6.99. Found: C, 68.3; H, 6.8%. ^{1}H NMR ($CDCl_3$) δ: 2.24 (s, 3H, 4-Me); 2.26(s, 6H, 2,6 -Me); 6.85 (s, 2H ,3,5 –H). ^{77}Se {^{1}H} NMR ($CDCl_3$) δ: 234 ppm.

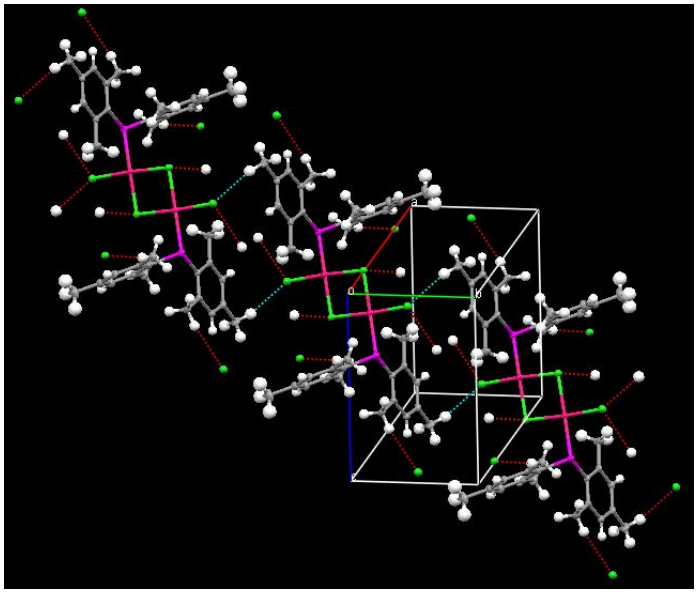
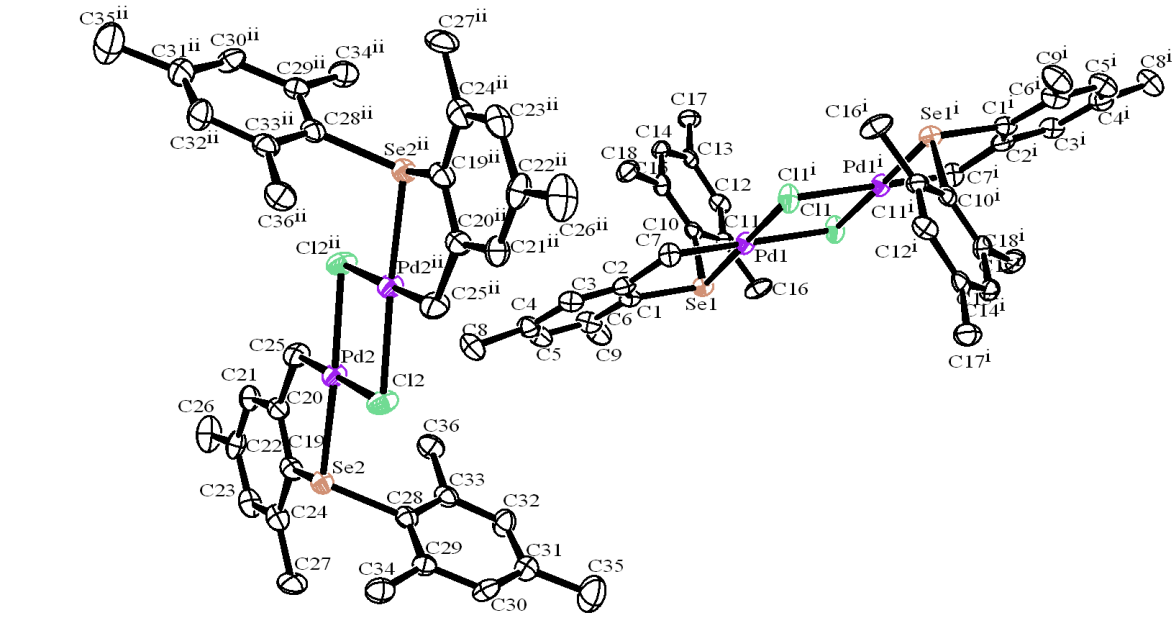


Fig. S-1 Crystal packing of $[Pd_2Cl_2(\mu\text{-}Cl)_2(Mes_2Se)_2]$



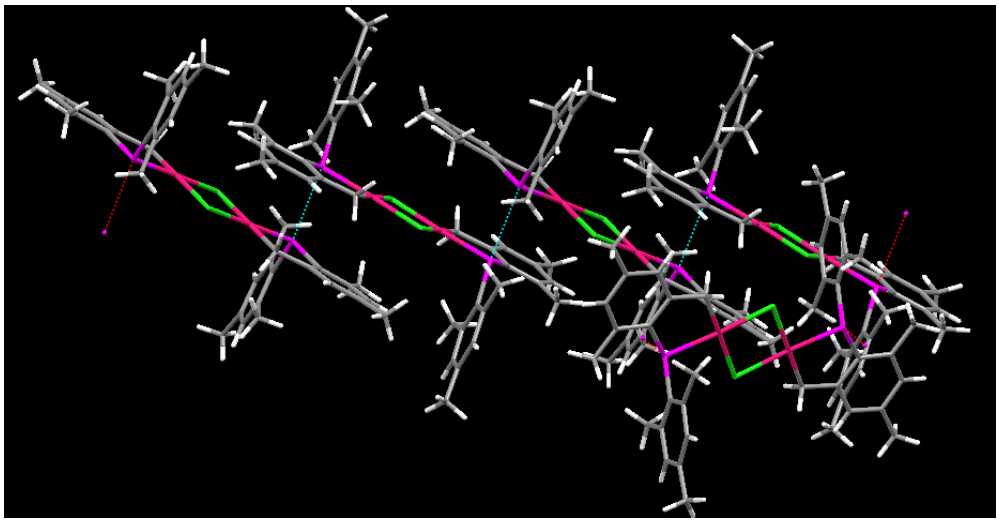


Fig. S-2 ORTEP drawing showing both the molecules of $[Pd_2(\mu\text{-}Cl)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ and crystal packing diagram

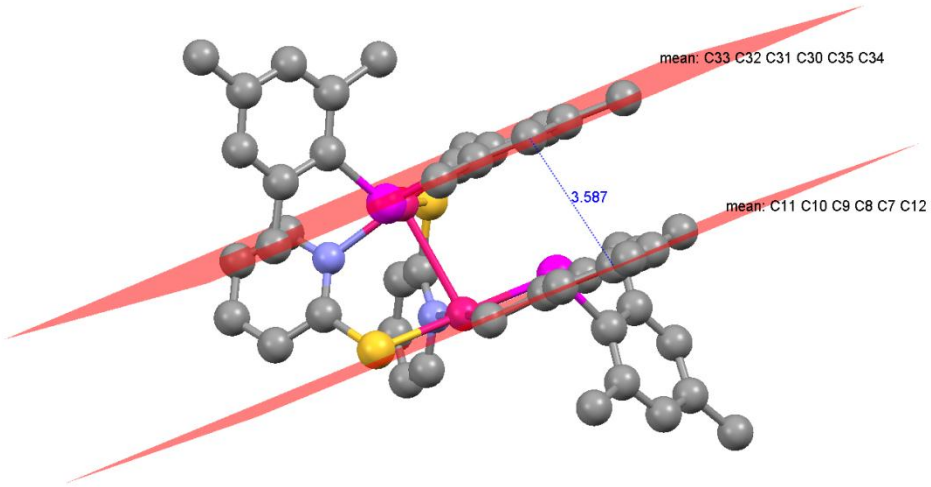


Fig. S-3 Molecular representation of $[Pd_2(\mu\text{-}Spy)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (**3a**) showing π-π staking.

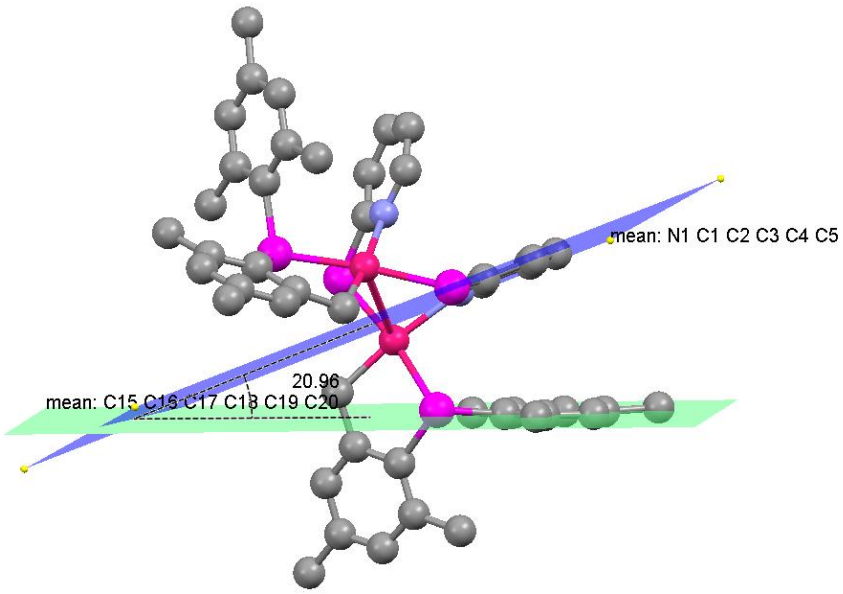
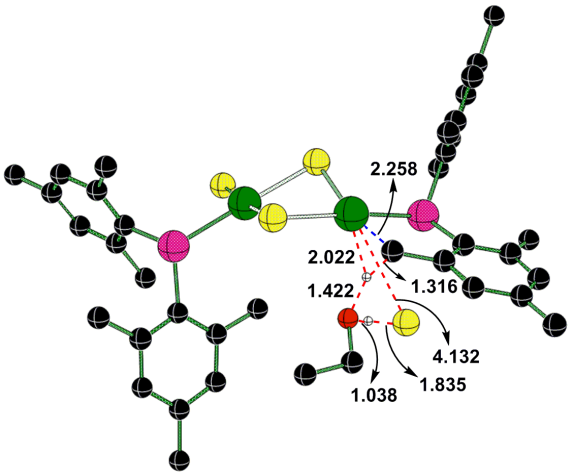
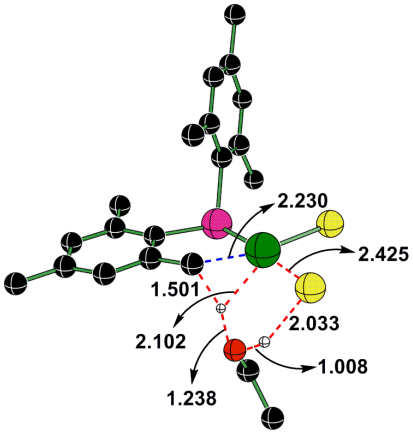


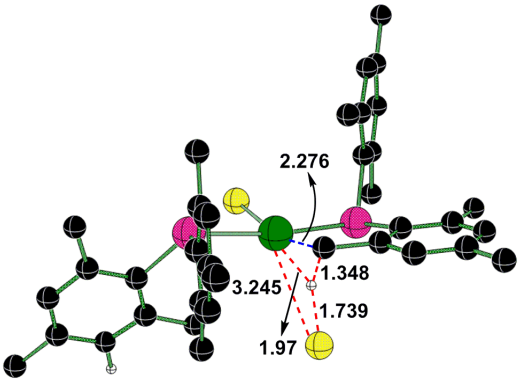
Fig. S-4 Molecular representation of $[Pd_2(\mu\text{-Sepy})_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (**3b**) almost parallel mesityl and Sepy rings



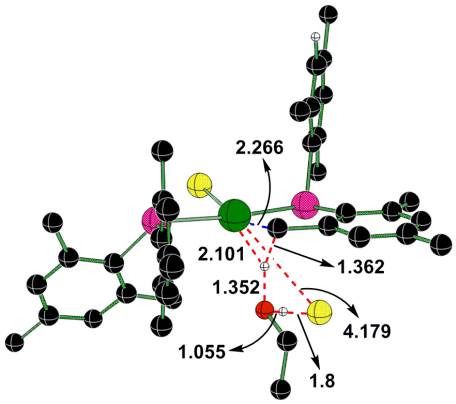
TS(1-4)'



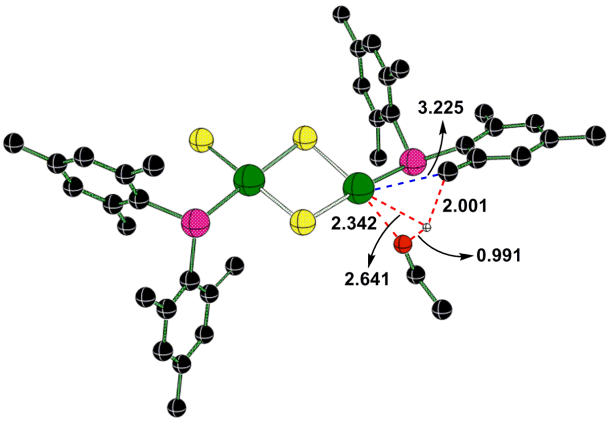
TS(5-6)



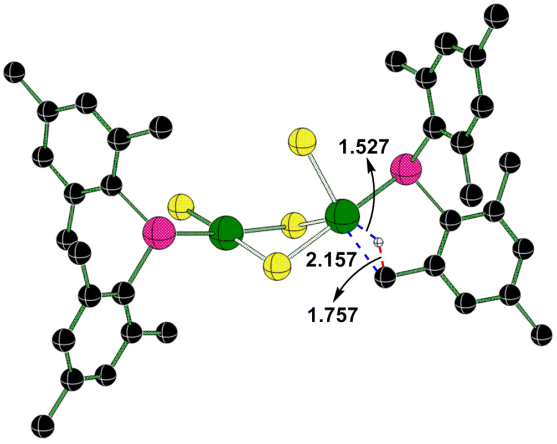
TS(10-11)



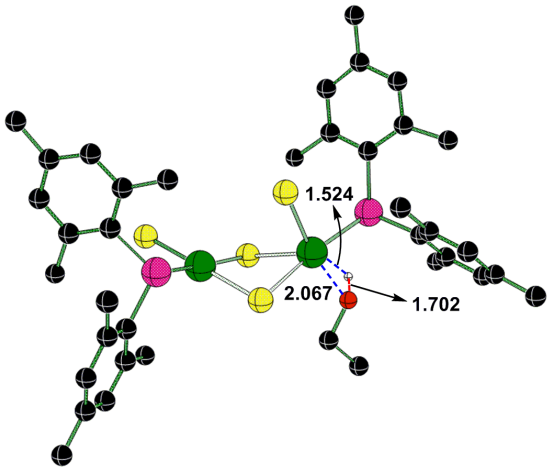
TS(10-11)'



TS(7-4)



TS(1-8)



TS(1-9)

Figure S5. Optimized geometries of transition states (B3LYP/6-31G**, LANL2DZ(Pd) level of theory) involved in different mechanistic pathways. Distances are in Å. Only select hydrogens are shown. Atom colors: C, black; H, ivory; O, red; Cl, yellow; Pd, green; Se, pink.

Table S1. Relative Energies (kcal/mol) with respect to intermediate 1 for transition states involved in Pd catalyzed C−H activation

Transition States	B3LYP/6-31G**			ΔG_{gas}(R^1=Me) M06/6-31G**
	ΔG_{gas}		ΔG_{EtOH}(R^1=Et)	
TS(1−4)	32.0		25.7	32.1
	R^1=Me	R^1=Et		
TS(1−4)′	38.5	37.3	33.25	35.4
TS(5−6)	59.8	59.9	49.61	
TS(1−9)	69.7	70.1	-	
TS(7−4)	52.3	52.5	55.52	
TS(4−2)	31.4		26.0	
TS(10−11)	32.8		51.0	
TS(10−11)'	41.9		59.9	
TS(1−7)	42.9		36.5	

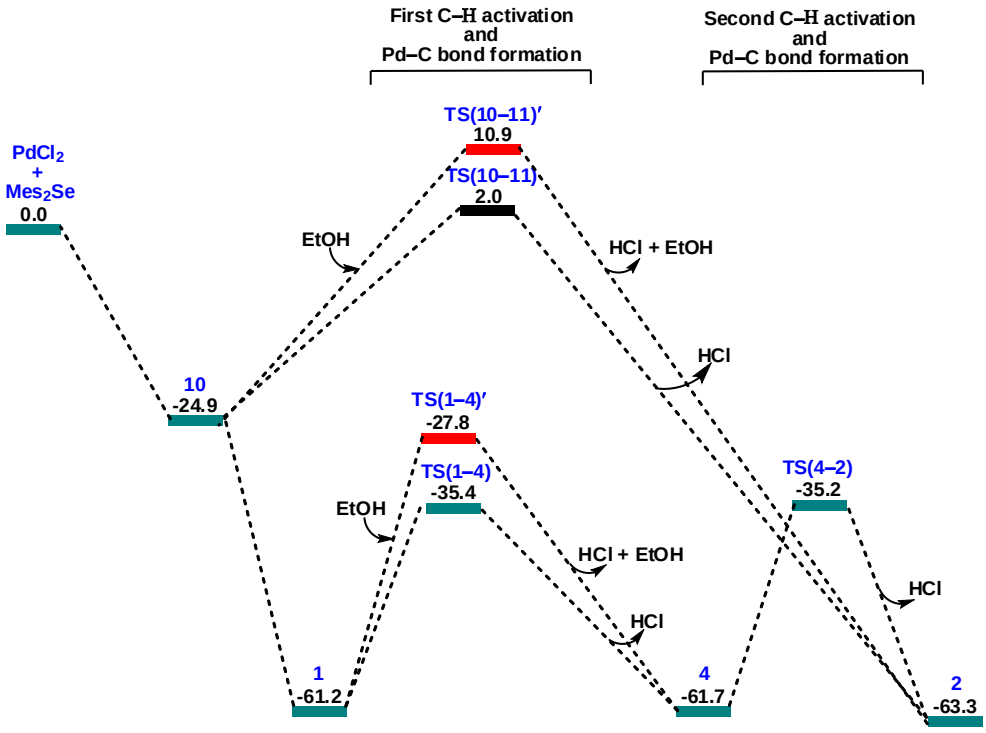
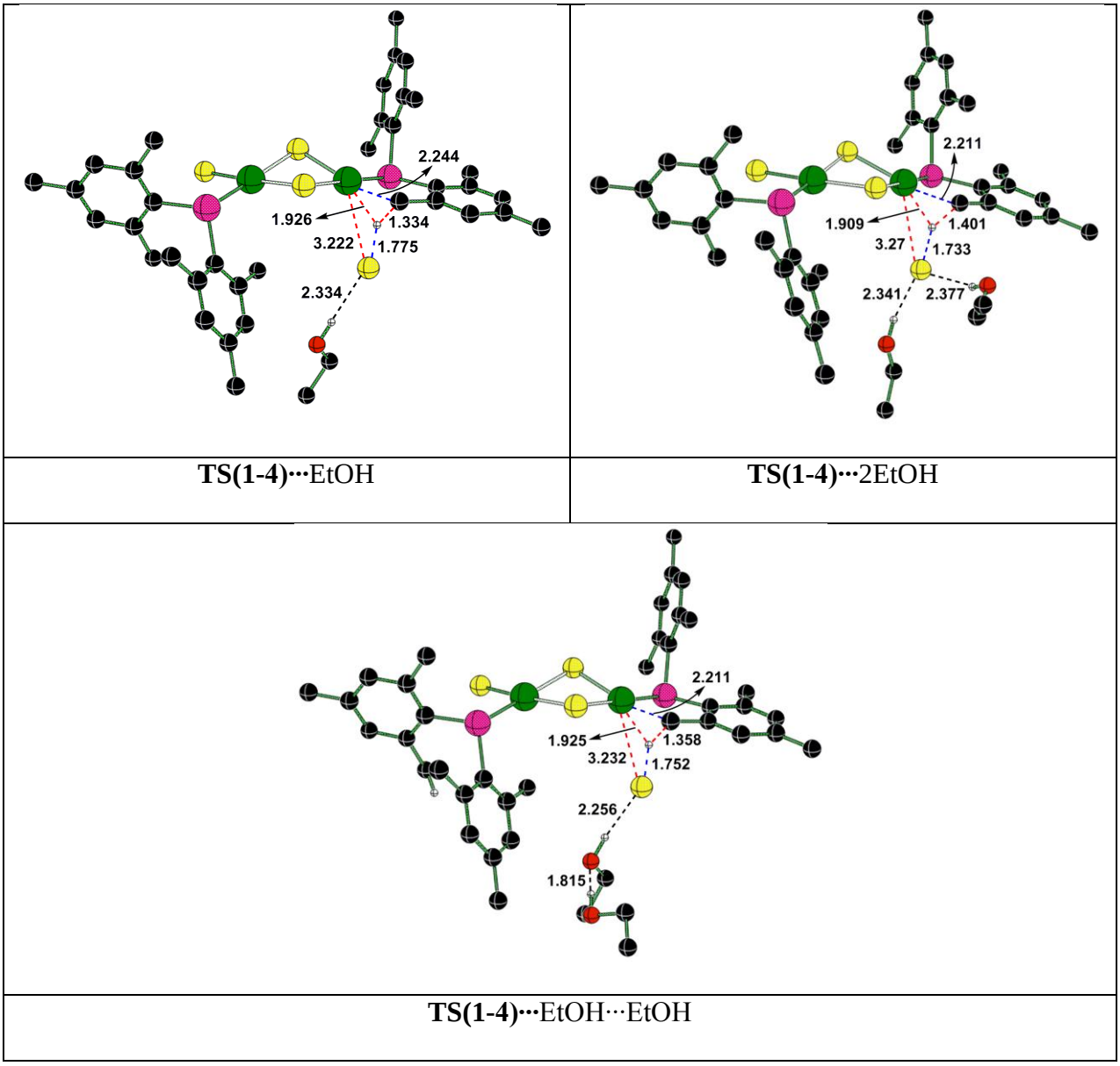


Figure S6. Gibbs free energy profile (in kcal/mol) for the formation of [Pd_2(μ-Cl)$_2${$MesSeC_6H_2(Me_2)CH_2$}$_2$] (**2**) from $PdCl_2$ and Mes_2Se obtained at the $SMD_{(EtOH)}$/B3LYP/6-31G**//B3LYP/6-31G** level of theory

Transition states with explicit treatment of one and two molecule of EtOH:



TS(1-4)···EtOH

TS(1-4)···2EtOH

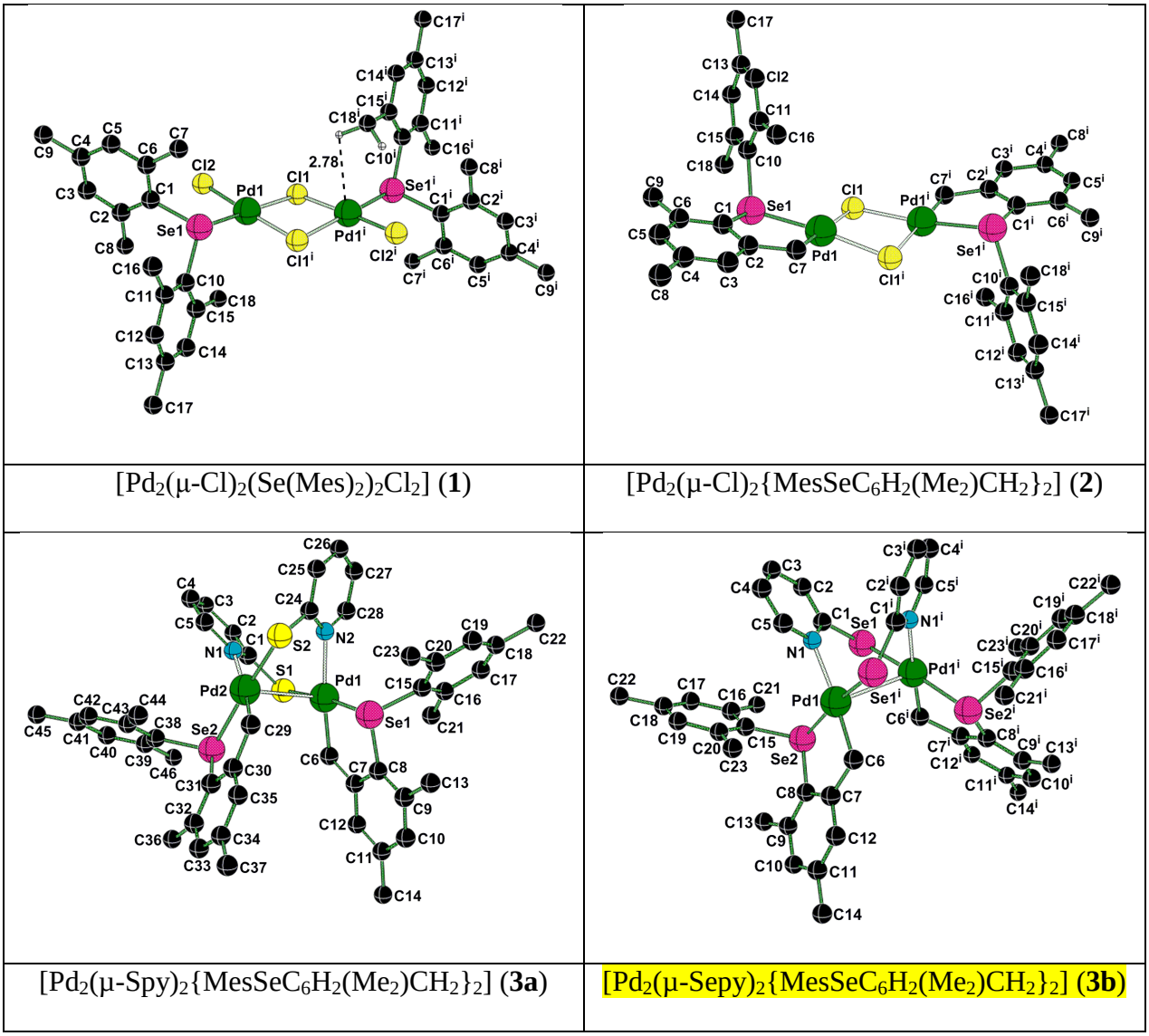
TS(1-4)···EtOH···EtOH

Figure S7. Optimized geometries of important transition states with explicit solvent treatment. Distances are in Å. Only select hydrogens are shown. Atom colors: C, black; H, ivory; O, red; Cl, yellow; Pd, green; Se, pink.

Table S2. Relative Energies (kcal/mol) with respect to intermediate 1 for transition states involved in Pd catalyzed C−H activation

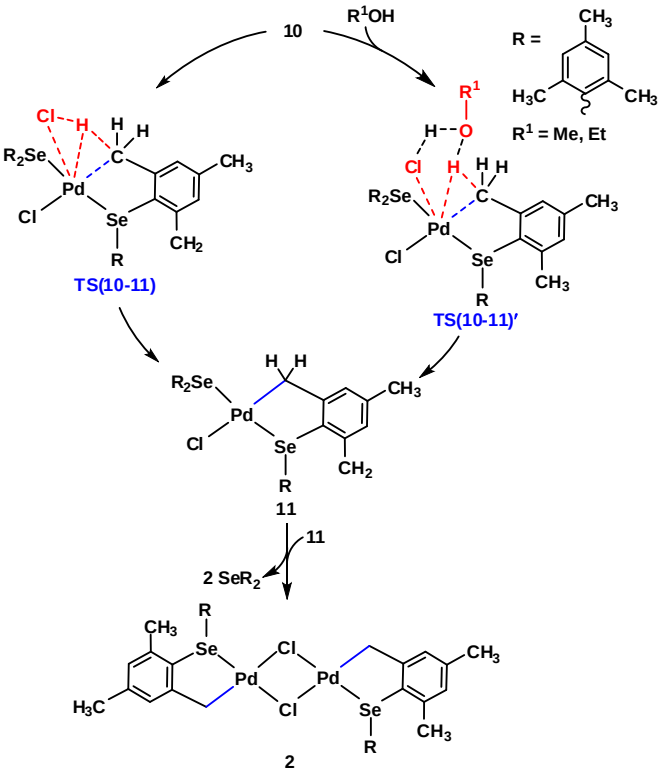
Transition States	B3LYP/6-31G**	
	ΔG_{gas}	$\Delta G_{EtOH}(R^1=Et)$
TS(1−4)1EtOH	34.1	34.1
TS(1−4)2EtOH	34.5	41.9
TS(1−4)EtOH−EtOH	34.3	39.7

Optimized structure of intermediate crystal structure:

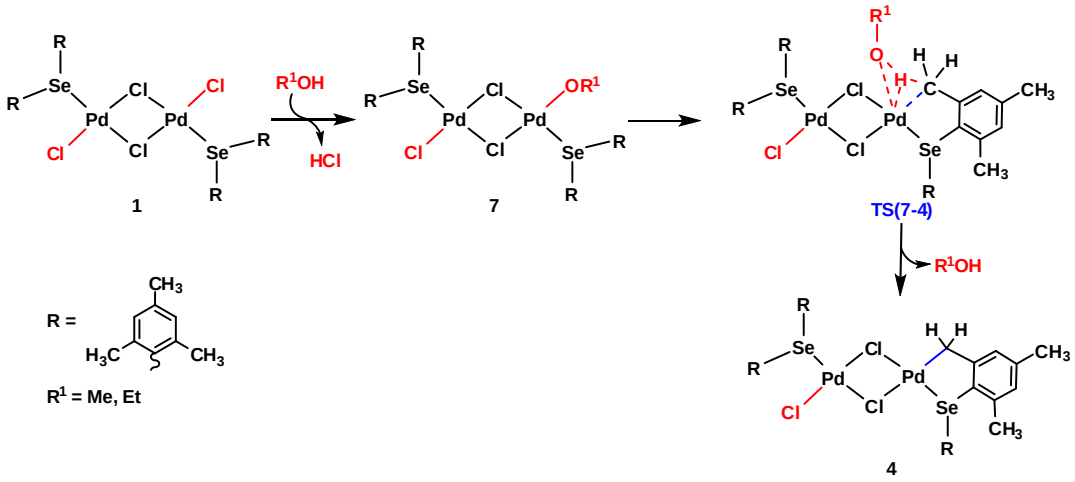


$[Pd_2(\mu\text{-}Cl)_2(Se(Mes)_2)_2Cl_2]$ (**1**)	$[Pd_2(\mu\text{-}Cl)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (**2**)
$[Pd_2(\mu\text{-}Spy)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (**3a**)	$[Pd_2(\mu\text{-}Sepy)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (**3b**)

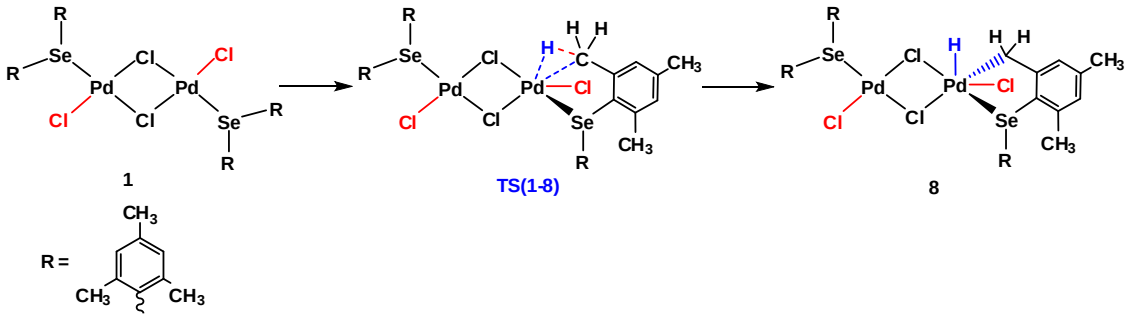
Figure S8. Optimized geometries of important crystal structure. Only select hydrogens are shown.



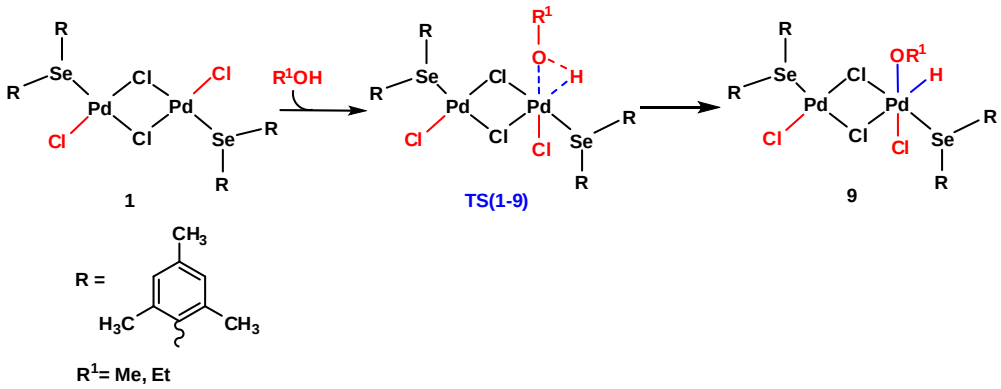
Scheme S1. Mechanistic pathways for Formation of $[Pd_2(\mu\text{-}Cl)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ from *trans*-$[PdCl_2Se(Mes)_2]$ (**10**).



Scheme S2. C−H activation by ligand –OR[1].



Scheme S3. Oxidative addition on one of the palladium centers.



Scheme S4. Oxidative addition of MeOH/EtOH on palladium of $[Pd_2(\mu\text{-}Cl)_2(Se(Mes)_2)_2Cl_2]$ complex.

$[Pd_2(\mu\text{-}Cl)_2(Se(Mes)_2)_2Cl_2]$ (1)

E = -8290.7284936
G = -8290.126928
Nimag = 0

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6	4.468177	3.885506	1.055854
1	4.013135	4.511395	1.819440
6	5.563392	4.374291	0.341351
6	6.113912	3.559243	-0.648950
1	6.954759	3.924451	-1.233384
6	5.610316	2.284582	-0.929708
6	2.724928	2.207104	1.656795
1	2.525582	2.959012	2.424504
1	2.867765	1.244925	2.156349
6	6.141398	5.735894	0.642174
1	5.360434	6.447627	0.925981
1	6.676720	6.142901	-0.220330
1	6.853029	5.685104	1.475692
6	6.251931	1.481999	-2.038430
1	6.742296	0.578913	-1.660892
1	7.006199	2.082437	-2.552333
1	5.513465	1.162013	-2.781467
6	5.234383	-1.214640	-0.190755
6	5.390371	-2.270698	-1.116112
6	6.392143	-3.215018	-0.874664
1	6.513442	-4.034650	-1.578626
6	7.230264	-3.139644	0.239884
6	7.027216	-2.094014	1.142200
1	7.648222	-2.034738	2.032755
6	6.033554	-1.123238	0.966009
6	4.505291	-2.442211	-2.330477
1	4.812644	-3.321247	-2.901926
1	4.544744	-1.575226	-2.998072
1	3.455500	-2.582869	-2.048003
6	8.328196	-4.152162	0.457894
1	9.267105	-3.820706	-0.003451
1	8.072689	-5.120011	0.016887
1	8.525319	-4.304335	1.523061
6	5.865096	-0.069623	2.031506
1	6.445027	-0.341296	2.916970
1	4.817645	0.009993	2.330793
1	6.203356	0.915625	1.698203
34	3.841451	0.058681	-0.686143
46	1.674615	-0.567472	0.308952
6	-4.620953	-1.741248	0.274554
6	-4.208188	-2.610496	-0.755593
6	-4.867743	-3.842489	-0.864461
1	-4.558624	-4.520040	-1.656346
6	-5.894326	-4.230156	-0.002731
6	-6.257856	-3.349219	1.017732
1	-7.042244	-3.633848	1.714888
6	-5.635509	-2.108627	1.186989
6	-3.098354	-2.319865	-1.736094
1	-3.111982	-3.053281	-2.546411

$[Pd_2(\mu\text{-}Cl)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (2)

E = -7369.0942766
G = -7368.512822
Nimag = 0

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6	-4.187246	-2.416210	0.353471
6	-4.878851	-3.554058	0.802222
1	-4.312189	-4.367227	1.250437
6	-6.265979	-3.655417	0.700960
6	-6.975058	-2.592805	0.118668
1	-8.056667	-2.663625	0.025906
6	-6.334166	-1.453067	-0.367792
6	-2.691143	-2.326225	0.542064
1	-2.190515	-3.223049	0.163409
1	-2.443787	-2.225952	1.606197
6	-6.999448	-4.875063	1.207382
1	-6.303601	-5.653149	1.531947
1	-7.645036	-5.301925	0.431772
1	-7.643169	-4.626110	2.059464
6	-7.127886	-0.350576	-1.024081
1	-7.046572	0.591833	-0.472290
1	-8.185899	-0.617262	-1.085367
1	-6.769402	-0.157764	-2.042128
6	-4.390053	1.661880	-0.080750
6	-4.705686	2.767234	-0.900341
6	-5.073760	3.965596	-0.280655
1	-5.313847	4.821893	-0.906407
6	-5.134135	4.095830	1.108855
6	-4.793145	2.987918	1.886496
1	-4.811255	3.074570	2.970306
6	-4.410190	1.763325	1.324900
6	-4.637330	2.722135	-2.411161
1	-4.946255	3.682212	-2.832035
1	-5.284891	1.945175	-2.829967
1	-3.620385	2.516528	-2.762246
6	-5.569299	5.392137	1.748813
1	-6.661306	5.435595	1.847944
1	-5.263553	6.255765	1.150617
1	-5.146486	5.505187	2.751272
6	-4.015966	0.638014	2.246320
1	-3.999951	0.983163	3.283008
1	-3.019526	0.258817	1.993285
1	-4.706697	-0.207832	2.179823
17	-0.413262	1.239971	-1.275299
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46	-1.707794	-0.741795	-0.290605
6	4.689745	1.485034	0.498561
6	3.966737	2.453995	-0.200772
6	4.593748	3.687753	-0.444851
1	4.042682	4.457515	-0.980629
6	5.902183	3.938459	-0.033081
6	6.593250	2.929261	0.656310
1	7.611535	3.116018	0.990634
6	6.007532	1.697288	0.948414
6	2.570585	2.205765	-0.721348

1	-3.179385	-1.324976	-2.180454
6	-6.602221	-5.551623	-0.179021
1	-5.946694	-6.298654	-0.635571
1	-6.955683	-5.946809	0.777886
1	-7.478254	-5.443566	-0.830710
6	-6.073143	-1.232850	2.338670
1	-6.512615	-0.290768	1.995698
1	-6.820952	-1.750276	2.944133
1	-5.229871	-0.979556	2.990247
6	-5.120349	1.316703	0.227123
6	-5.197772	2.369708	1.165445
6	-6.178890	3.347916	0.978472
1	-6.240453	4.163592	1.694766
6	-7.069371	3.310446	-0.096658
6	-6.939213	2.269993	-1.018377
1	-7.599636	2.241299	-1.881633
6	-5.970285	1.266864	-0.895701
6	-4.252984	2.504296	2.339297
1	-4.497296	3.397369	2.919489
1	-4.300611	1.642009	3.012256
1	-3.211926	2.598936	2.010345
6	-8.144574	4.357938	-0.253595
1	-9.069288	4.051441	0.251563
1	-7.838087	5.314058	0.180484
1	-8.389193	4.524356	-1.306692
6	-5.867617	0.231014	-1.985180
1	-6.531264	0.491827	-2.813156
1	-4.846793	0.194526	-2.374731
1	-6.140212	-0.768938	-1.637867
17	-0.579621	-1.211275	0.997448
34	-3.763941	-0.021302	0.650982
46	-1.646220	0.348205	-0.553466
1	1.825399	2.120574	1.038015
1	-2.118100	-2.379815	-1.251792
17	-2.562466	1.872963	-2.055802
17	2.619187	-1.803479	2.042887
17	0.586658	0.705266	-1.467804
1	1.890844	3.014083	-0.433797
1	2.575957	2.143774	-1.816833
6	6.571791	5.262253	-0.318081
1	5.883533	5.962996	-0.797874
1	6.939322	5.728361	0.603090
1	7.436199	5.135587	-0.980511
6	6.768730	0.653361	1.727371
1	6.938355	-0.251874	1.134776
1	7.741170	1.037677	2.044971
1	6.216599	0.349865	2.624583
6	4.572767	-1.593937	0.133767
6	4.834288	-2.703384	0.966873
6	5.473106	-3.814180	0.407080
1	5.672693	-4.673788	1.042426
6	5.851776	-3.854547	-0.936919
6	5.555097	-2.748475	-1.735041
1	5.819114	-2.769268	-2.789727
6	4.910607	-1.610149	-1.234515
6	4.430676	-2.756082	2.424312
1	4.749290	-3.701641	2.870069
1	4.875844	-1.941794	3.005053
1	3.344619	-2.680346	2.544458
6	6.571607	-5.053920	-1.504901
1	7.655688	-4.969523	-1.357025
1	6.249515	-5.980201	-1.019708
1	6.396120	-5.153486	-2.579919
6	4.587566	-0.486671	-2.185354
1	4.844355	-0.769345	-3.209160
1	3.519249	-0.244537	-2.152234
1	5.131380	0.429961	-1.938679
17	0.428264	-1.717928	0.390296
34	3.672891	-0.087875	0.996310
46	1.637067	0.468548	-0.190223

$[Pd_2(\mu\text{-}Spy)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (3a)

E = -7740.4467997
G = -7739.713517
Nimag = 0

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6	-1.798809	-4.027986	2.065729
1	-1.543444	-4.221765	3.101334
6	-2.569103	-4.918564	1.339085
1	-2.939858	-5.827088	1.806102
6	-2.844919	-4.643248	-0.006315
1	-3.429588	-5.317563	-0.622094
6	-2.341981	-3.468372	-0.541488
1	-2.515979	-3.203193	-1.579556
6	0.974385	1.005990	2.116646
1	-0.092936	1.240077	2.172104
1	1.278820	0.668435	3.116804
6	1.762052	2.245415	1.750176

$PdCl_2$

E = -1047.1182173
G = -1047.143751
Nimag = 0

46	0.000000	0.000000	0.000000
17	0.000000	0.000000	2.312625
17	0.000000	0.000000	-2.312625

$(Mes)_2Se$

E = -3098.1397274
G = -3097.844511
Nimag = 0

6	2.695238	2.280805	0.709713
6	3.443706	3.435048	0.401359
6	3.240024	4.566122	1.191927
1	3.812361	5.465760	0.975406
6	2.307707	4.581732	2.240861
6	1.578326	3.422076	2.498093
1	0.851916	3.414590	3.307949
6	4.430726	3.472432	-0.739231
1	5.282691	2.807104	-0.561914
1	4.816614	4.484507	-0.885780
1	3.962956	3.147803	-1.675792
6	2.095887	5.836641	3.054917
1	3.044525	6.230967	3.435877
1	1.440102	5.652305	3.910147
1	1.638827	6.629066	2.449913
6	4.569524	0.027207	-0.291621
6	5.232838	-0.180751	0.934744
6	6.535081	-0.696364	0.897735
1	7.052804	-0.859404	1.840348
6	7.180405	-1.016114	-0.297993
6	6.483450	-0.818670	-1.492771
1	6.959814	-1.077552	-2.435609
6	5.184854	-0.299666	-1.520240
6	4.606900	0.109801	2.275190
1	4.500792	1.185158	2.450144
1	5.220149	-0.304659	3.079734
1	3.601808	-0.321410	2.343947
6	4.498461	-0.124425	-2.857565
1	3.556134	-0.678904	-2.915703
1	5.146829	-0.477471	-3.663661
1	4.258134	0.926013	-3.054425
6	1.310855	-2.846624	-1.457718
6	1.799317	-4.027891	-2.065336
1	1.544015	-4.221708	-3.100949
6	2.569691	-4.918372	-1.338658
1	2.940580	-5.826850	-1.805656
6	2.845416	-4.643019	0.006753
1	3.430138	-5.317263	0.622557
6	2.342315	-3.468203	0.541903
1	2.516227	-3.203002	1.579981
6	-0.974303	1.005802	-2.116484
1	0.093015	1.239839	-2.172113
1	-1.278920	0.668212	-3.116579
6	-1.761886	2.245259	-1.749953
6	-2.695296	2.280573	-0.709688
6	-3.443732	3.434844	-0.401327
6	-3.239779	4.566013	-1.191684
1	-3.812077	5.465673	-0.975157
6	-2.307217	4.581701	-2.240402
6	-1.577876	3.422026	-2.497641
1	-0.851277	3.414604	-3.307327
6	-4.430925	3.472194	0.739114
1	-3.963198	3.147843	1.675799
1	-5.282713	2.806643	0.561809
1	-4.817059	4.484207	0.885435
6	-2.095136	5.836709	-3.054236
1	-3.043622	6.230881	-3.435741
6	-1.525696	-0.404975	-0.143510
6	-2.612787	-0.618316	0.732159
6	-3.744624	0.195489	0.607239
1	-4.582007	0.029301	1.281322
6	-3.830061	1.210087	-0.348640
6	-2.748801	1.381140	-1.215590
1	-2.802308	2.147585	-1.985925
6	-1.598328	0.586269	-1.145184
6	-2.608812	-1.701346	1.786139
1	-3.505969	-1.635539	2.407636
1	-1.730089	-1.630196	2.434164
6	-5.045273	2.102782	-0.433706
1	-5.947101	1.586388	-0.091223
1	-5.218782	2.446012	-1.458248
1	-4.925204	2.996617	0.191666
6	-0.501263	0.808849	-2.156536
1	0.396625	1.238834	-1.702006
1	-0.839102	1.485839	-2.945663
1	-0.199831	-0.137407	-2.617655
6	1.525714	-0.405054	0.143512
6	2.612779	-0.618229	-0.732252
6	3.744590	0.195573	-0.607261
1	4.581944	0.029518	-1.281416
6	3.830045	1.210035	0.348786
6	2.748839	1.380913	1.215811
1	2.802357	2.147249	1.986252
6	1.598371	0.586012	1.145338
6	2.608747	-1.701079	-1.786419
1	3.505933	-1.635244	-2.407870
1	1.730058	-1.629741	-2.434469
1	2.586437	-2.702380	-1.341148
6	5.045257	2.102732	0.433852
1	4.926401	2.995121	-0.193813
1	5.947585	1.585412	0.094068
1	5.217096	2.448279	1.457888
6	0.501355	0.808405	2.156784
1	0.839181	1.485369	2.945939
1	0.200064	-0.137921	2.617854
1	-0.396615	1.238327	1.702357
34	-0.000011	-1.598958	-0.000104
1	-2.586611	-2.702574	1.340697

1	-1.438810	5.652556	-3.909090
1	-1.638595	6.629179	-2.448903
6	-4.569851	0.027059	0.291162
6	-5.185464	-0.299909	1.519665
6	-6.484120	-0.818610	1.491928
1	-6.960703	-1.077520	2.434660
6	-7.181004	-1.015696	0.296996
6	-6.535410	-0.695898	-0.898549
1	-7.053078	-0.858637	-1.841248
6	-5.233015	-0.180590	-0.935298
6	-4.499162	-0.125061	2.857089
1	-3.557161	-0.680102	2.915299
1	-5.147826	-0.477756	3.663096
1	-4.258196	0.925217	3.053988
6	-8.596266	-1.542459	0.301957
1	-9.319362	-0.729764	0.446277
1	-8.753107	-2.261802	1.111665
1	-8.843904	-2.034391	-0.643187
6	-4.606851	0.110063	-2.275621
1	-4.501292	1.185465	-2.450709
1	-5.219683	-0.304836	-3.080258
1	-3.601540	-0.320651	-2.344052
7	-1.610421	-2.579703	0.163244
7	1.610688	-2.579618	-0.162863
16	-0.355392	-1.739768	2.432964
16	0.355644	-1.739849	-2.432639
34	2.739470	0.704527	-0.414852
34	-2.739784	0.704221	0.414771
46	1.190217	-0.673566	0.940257
46	-1.190127	-0.673708	-0.940035
6	8.595598	-1.543107	-0.303080
1	8.754514	-2.256493	-1.117617
1	9.319220	-0.729470	-0.439326
1	8.840666	-2.042031	0.639103

***trans*-[$PdCl_2(Se(Mes)_2)_2$] (10)**

E = -7243.5095118
G = -7242.898490
Nimag = 0

6	-3.450908	1.563668	0.271555
6	-3.024221	2.517143	-0.674920
6	-3.865375	3.611521	-0.920170
1	-3.544617	4.350514	-1.650353
6	-5.085379	3.788388	-0.267392
6	-5.461851	2.834951	0.680328
1	-6.398887	2.957985	1.218252
6	-4.665161	1.724502	0.976492
6	-1.716888	2.454532	-1.424415
1	-1.712774	3.189436	-2.234096
1	-1.534285	1.468539	-1.858864
6	-5.978998	4.962123	-0.588033
1	-5.401639	5.816854	-0.951992
1	-6.547480	5.283635	0.289886
1	-6.705345	4.702091	-1.368285
6	-5.140128	0.762819	2.041348

***trans*-[$PdCl_2Se(Mes)_2(EtOH)$] (5)**

E = -4261.0963891
G = -4260.756262
Nimag = 0

6	-0.962450	1.727545	0.167452
6	-0.358364	2.560591	-0.792694
6	-1.010422	3.761629	-1.110424
1	-0.554581	4.409436	-1.854853
6	-2.207138	4.153265	-0.513000
6	-2.764396	3.306673	0.449291
1	-3.691357	3.593713	0.940120
6	-2.163601	2.100145	0.815917
6	-2.884748	5.449673	-0.885860
1	-2.287875	6.022296	-1.600440
1	-3.866329	5.267658	-1.338714
1	-3.049473	6.078514	-0.003916
6	-2.823376	1.260812	1.886230
1	-2.142391	1.072024	2.723295
1	-3.703528	1.774185	2.280265
1	-3.146472	0.287357	1.503875

1	-5.339006	-0.234137	1.635496
1	-6.063101	1.129183	2.497389
1	-4.394070	0.647020	2.834709
6	-3.401514	-1.511529	0.124816
6	-3.558342	-2.567126	1.050265
6	-4.312018	-3.680951	0.665044
1	-4.433442	-4.496679	1.373772
6	-4.904652	-3.776034	-0.595280
6	-4.702024	-2.726679	-1.493602
1	-5.126392	-2.795024	-2.492477
6	-3.947779	-1.592253	-1.172155
6	-2.929191	-2.561867	2.426481
1	-3.182541	-3.480938	2.960881
1	-3.265324	-1.714552	3.032328
1	-1.836487	-2.501624	2.372278
6	-5.745256	-4.971059	-0.975140
1	-6.811326	-4.774033	-0.805121
1	-5.477932	-5.852580	-0.385361
1	-5.627437	-5.221202	-2.033910
6	-3.725687	-0.551949	-2.238894
1	-4.160424	-0.883478	-3.185174
1	-2.653587	-0.403659	-2.396219
1	-4.172753	0.411541	-1.981190
34	-2.380321	0.011853	0.803335
6	3.451137	-1.563662	-0.271558
6	3.024459	-2.517300	0.674760
6	3.865679	-3.611652	0.919900
1	3.544928	-4.350784	1.649947
6	5.085740	-3.788327	0.267175
6	5.462200	-2.834720	-0.680377
1	6.399282	-2.957602	-1.218254
6	4.665439	-1.724294	-0.976444
6	1.717067	-2.454910	1.424174
1	1.712981	-3.189900	2.233776
1	1.534348	-1.468978	1.858710
6	5.979417	-4.962054	0.587688
1	5.402047	-5.817013	0.951099
1	6.548267	-5.283139	-0.290147
1	6.705436	-4.702228	1.368315
6	5.140346	-0.762458	-2.041185
1	5.338993	0.234509	-1.635258
1	6.063425	-1.128630	-2.497164
1	4.394338	-0.646745	-2.834609
6	3.401391	1.511521	-0.124798
6	3.558104	2.567130	-1.050212
6	4.311619	3.681070	-0.664941
1	4.432956	4.496819	-1.373658
6	4.904204	3.776206	0.595382
6	4.701738	2.726769	1.493676
1	5.126103	2.795139	2.492554
6	3.947660	1.592267	1.172192
6	2.929010	2.561808	-2.426456
1	3.182533	3.480768	-2.960964
1	3.265007	1.714354	-3.032181
1	1.836291	2.501757	-2.372268
6	5.744573	4.971351	0.975388
1	6.810946	4.773416	0.808370
6	-1.369192	-1.345155	0.174469
6	-1.948292	-1.381244	-1.109190
6	-2.832867	-2.429297	-1.391720
1	-3.288881	-2.463805	-2.378162
6	-3.129748	-3.434713	-0.470432
6	-2.511290	-3.380323	0.780598
1	-2.716209	-4.159302	1.511026
6	-1.628301	-2.354276	1.129156
6	-1.645514	-0.386022	-2.199472
1	-2.091255	-0.715880	-3.141018
1	-2.033894	0.610772	-1.974538
1	-0.565763	-0.308812	-2.351041
6	-4.056214	-4.570732	-0.830013
1	-4.783204	-4.269804	-1.589885
1	-3.492747	-5.420420	-1.235067
1	-4.605235	-4.932571	0.044561
6	-0.978573	-2.389459	2.495053
1	-1.326858	-3.260096	3.055742
1	0.112603	-2.459184	2.421541
1	-1.204370	-1.495630	3.085494
34	-0.173143	0.058609	0.820622
46	2.121183	-0.338046	0.114423
17	2.835509	1.336519	1.657176
17	1.630157	-1.966449	-1.508581
8	4.240888	-0.689194	-0.079380
1	4.566203	0.034079	0.486822
6	4.886476	-0.661416	-1.368145
1	5.935540	-0.948628	-1.248167
1	4.364195	-1.390216	-1.985641
1	4.816282	0.330661	-1.825909
6	0.946980	2.267116	-1.489736
1	1.788981	2.392813	-0.801291
1	0.994247	1.246191	-1.877369
1	1.087533	2.955528	-2.327270

1	5.479213	5.852079	0.383555
1	5.624281	5.223257	2.033472
6	3.725733	0.551844	2.238850
1	4.160351	0.883397	3.185176
1	2.653659	0.403323	2.396111
1	4.173012	-0.411535	1.981096
17	-0.299185	-1.750130	-1.581226
34	2.380345	-0.011960	-0.803290
46	0.000020	-0.000034	0.000006
1	-0.878592	2.675197	-0.755968
1	0.878819	-2.675571	0.755664
17	0.299046	1.750114	1.581319

[$Pd_2(\mu\text{-}Cl)_2$(metalated-Se)($Se(Mes)_2$)Cl] (4)

E = -7829.9112559
G = -7829.318274
Nimag = 0

6	-4.820590	-1.558586	-0.272017
6	-5.010057	-1.820812	1.099591
6	-5.599245	-3.040723	1.454721
1	-5.754358	-3.250169	2.510340
6	-5.977777	-3.994481	0.508520
6	-5.753581	-3.706907	-0.840249
1	-6.031029	-4.440026	-1.593793
6	-5.175966	-2.504480	-1.258635
6	-4.592679	-0.874447	2.195462
1	-4.736658	-1.338978	3.173872
1	-5.164559	0.057934	2.173826
6	-6.575151	-5.315120	0.930174
1	-5.800144	-6.087701	1.006583
1	-7.315149	-5.669356	0.205999
1	-7.061025	-5.241678	1.907276
6	-4.942819	-2.285723	-2.737608
1	-5.463813	-1.397846	-3.110726
1	-5.298051	-3.147970	-3.306928
1	-3.879351	-2.154574	-2.963643
6	-4.969295	1.537822	-0.072522
6	-4.171775	2.380024	0.704040
6	-4.765375	3.537045	1.235299
1	-4.157777	4.209011	1.837413
6	-6.111618	3.832240	1.020960
6	-6.875229	2.951333	0.238693
1	-7.923863	3.176173	0.056535
6	-6.327831	1.802159	-0.332532
6	-2.723195	2.071292	1.001996
1	-2.587012	1.861814	2.070584
1	-2.077128	2.915743	0.737884
6	-6.745548	5.067554	1.615770
1	-7.502927	4.803348	2.363263
1	-7.247899	5.665758	0.847572
1	-6.002159	5.702453	2.104766
6	-7.172388	0.898961	-1.196846
1	-8.169542	1.321668	-1.341790
1	-7.286753	-0.095638	-0.752897
1	-6.719034	0.758497	-2.185217

[Pd(metalated-Se)Cl] (6)

E = -3684.5224381
G = -3684.241081
Nimag = 0

6	-0.832207	1.347075	-0.274331
6	-2.020837	0.983347	0.368275
6	-2.931532	1.999138	0.702979
1	-3.868449	1.726628	1.182732
6	-2.646271	3.341671	0.456280
6	-1.427017	3.664790	-0.160010
1	-1.196392	4.708111	-0.363548
6	-0.509997	2.689037	-0.553374
6	-2.322781	-0.428958	0.781346
1	-3.380197	-0.679126	0.686842
6	-3.624120	4.430271	0.829365
1	-4.497410	4.024085	1.345882
1	-3.159089	5.173842	1.486167
1	-3.978875	4.963952	-0.059941
6	0.758676	3.078904	-1.269647
1	0.811224	2.607348	-2.258123
1	0.808383	4.161130	-1.411215
1	1.650510	2.767425	-0.716031
6	1.943933	-0.066393	-0.113907
6	2.097961	-0.045855	1.286962
6	3.399199	-0.003200	1.802601
1	3.525753	0.020791	2.882233
6	4.530253	-0.000753	0.984162
6	4.338831	-0.042196	-0.399129
1	5.205544	-0.046743	-1.055750
6	3.064327	-0.076886	-0.974229
6	0.939656	-0.089923	2.249878
1	1.300526	-0.111897	3.280830
1	0.281208	0.776609	2.139127
1	0.329811	-0.984420	2.082282
6	5.919061	0.010660	1.575466
1	5.929400	0.478135	2.564133
1	6.303219	-1.010249	1.692364
1	6.622636	0.550397	0.934577
6	2.952705	-0.134973	-2.482469
1	3.947164	-0.125443	-2.935054
1	2.444537	-1.044314	-2.820931
1	2.389897	0.712210	-2.886763

34	-4.018087	0.091735	-0.944548
46	-1.877265	0.432471	0.120548
6	4.231671	1.810989	-0.061637
6	3.662096	2.404241	-1.206356
6	4.173316	3.643527	-1.616028
1	3.747598	4.105209	-2.503557
6	5.201512	4.298912	-0.937687
6	5.728314	3.684992	0.200436
1	6.526497	4.176519	0.751682
6	5.257063	2.453945	0.667366
6	2.538624	1.802699	-2.014505
1	2.385484	2.377947	-2.931301
1	2.732393	0.764450	-2.295723
6	5.705989	5.644721	-1.399755
1	5.546025	5.784549	-2.472667
1	5.183377	6.458931	-0.882394
1	6.774356	5.763862	-1.195661
6	5.867013	1.876006	1.923633
1	6.392154	0.935439	1.729812
1	6.584156	2.578481	2.355022
1	5.101582	1.668051	2.679044
6	5.069957	-1.124213	0.478347
6	5.290181	-1.961811	1.593543
6	6.356899	-2.864542	1.540736
1	6.527223	-3.516662	2.393943
6	7.197785	-2.955600	0.430082
6	6.930106	-2.128954	-0.662703
1	7.552464	-2.207050	-1.550968
6	5.869872	-1.214759	-0.678223
6	4.410281	-1.949733	2.824087
1	4.763941	-2.688083	3.547813
1	4.400808	-0.971689	3.316221
1	3.371020	-2.197385	2.580162
6	8.365473	-3.912078	0.412881
1	8.192163	-4.766792	1.073134
1	8.554352	-4.293086	-0.595185
1	9.285153	-3.418323	0.751617
6	5.625429	-0.419547	-1.934766
1	6.283051	-0.770684	-2.733776
1	4.592795	-0.552717	-2.268345
1	5.807654	0.648871	-1.793462
17	0.313250	0.954083	1.128733
34	3.590203	0.129717	0.707517
46	1.465245	-0.736553	-0.238918
1	-3.534866	-0.604685	2.095455
1	1.598059	1.813312	-1.453981
17	2.523956	-2.342556	-1.553877
17	-0.702913	-1.592367	-0.866579

34	0.198412	-0.124618	-0.995269
46	-1.308170	-1.890990	-0.190127
1	-1.996533	-0.627073	1.808020
17	-2.813065	-3.573728	0.361521

[Pd(metalated-Se)(Se(Mes)$_2$)Cl] (11)

E = -6782.6788314
G = -6782.078180
Nimag = 0

6	3.536761	-1.419997	-0.221617
6	3.365031	-1.927949	-1.525731

6	4.449847	-2.595058	-2.112371
1	4.324884	-2.988998	-3.118114
6	5.668383	-2.777448	-1.458469
6	5.790932	-2.283394	-0.158300
1	6.722532	-2.431177	0.383021
6	4.744442	-1.615759	0.485920
6	2.086274	-1.834110	-2.318582
1	2.264844	-2.120222	-3.358734
1	1.660645	-0.826399	-2.309897
6	6.822777	-3.473341	-2.138685
1	6.472633	-4.197824	-2.879677
1	7.452044	-4.002410	-1.416648
1	7.464259	-2.753996	-2.663414
6	4.956134	-1.152565	1.908678
1	4.940827	-0.061136	1.994128
1	5.921499	-1.503463	2.281857
1	4.174909	-1.539665	2.571174
6	2.774661	1.291655	1.001874
6	2.593144	1.838708	2.292753
6	3.041834	3.140913	2.536641
1	2.898522	3.562346	3.528968
6	3.665248	3.909324	1.550534
6	3.809115	3.347425	0.281435
1	4.270452	3.935287	-0.508993
6	3.369495	2.052432	-0.025005
6	1.918524	1.081862	3.415759
1	1.896924	1.689651	4.323930
1	2.435504	0.144510	3.644117
1	0.884439	0.816665	3.168055
6	4.178834	5.296534	1.853309
1	5.192513	5.259459	2.271792
1	3.545625	5.807510	2.585073
1	4.222275	5.913392	0.950900
6	3.547952	1.556000	-1.438589
1	3.784898	2.389614	-2.104887
1	2.641314	1.071798	-1.810403
1	4.356062	0.822772	-1.515934
34	2.104298	-0.531351	0.772197
6	-2.721205	1.364113	-1.272883
6	-1.565687	2.119843	-1.053679
6	-1.610563	3.485111	-1.386089
1	-0.719810	4.089676	-1.229594
6	-2.766243	4.082464	-1.888438
6	-3.906820	3.285353	-2.074097
1	-4.813182	3.738154	-2.470427
6	-3.909048	1.920172	-1.786812
6	-0.312207	1.536622	-0.439850
1	0.568986	1.870766	-0.996227
6	-2.798819	5.552061	-2.237188
1	-1.862723	6.047726	-1.966617
1	-2.957506	5.701361	-3.311793
1	-3.615114	6.067185	-1.718374
6	-5.143272	1.087364	-2.031403
1	-5.545580	0.676714	-1.099175
1	-5.927062	1.683273	-2.505644
1	-4.923484	0.235265	-2.685275
6	-3.738569	-1.065402	0.386557

6	-4.444273	-2.265948	0.155555
6	-5.359402	-2.688336	1.124457
1	-5.902793	-3.614944	0.956160
6	-5.584095	-1.967832	2.299978
6	-4.841087	-0.804621	2.507919
1	-4.976773	-0.245814	3.431037
6	-3.905108	-0.333767	1.578381
6	-4.214401	-3.131463	-1.062502
1	-4.881594	-3.996859	-1.044471
1	-4.390907	-2.586842	-1.995973
1	-3.182456	-3.499269	-1.086834
6	-6.604537	-2.431045	3.311633
1	-7.606582	-2.061479	3.059343
1	-6.662020	-3.523057	3.349606
1	-6.366206	-2.067582	4.315458
6	-3.107972	0.899682	1.920343
1	-3.267345	1.173303	2.966491
1	-2.037609	0.724954	1.769006
1	-3.384681	1.758048	1.300944
34	-2.503115	-0.545132	-1.034716
46	-0.228199	-0.521734	-0.205156
1	1.322709	-2.497478	-1.898553
1	-0.200982	1.916679	0.585212
17	-0.285557	-2.967937	0.160799

TS(1-4)

E = -8290.6729404
G = -8290.075928
Nimag = -226.9255

6	4.493884	-1.747779	0.355272
6	4.851650	-2.083142	-0.967564
6	5.420579	-3.341602	-1.190102
1	5.705182	-3.607357	-2.205283
6	5.619227	-4.267384	-0.162557
6	5.226752	-3.909862	1.129363
1	5.360792	-4.619613	1.941744
6	4.658743	-2.665172	1.417466
6	4.618238	-1.177242	-2.149914
1	4.929409	-1.670384	-3.073752
1	5.166426	-0.234779	-2.066674
6	6.202580	-5.629367	-0.448444
1	5.413562	-6.341862	-0.718996
1	6.721520	-6.034379	0.425045
1	6.909887	-5.595248	-1.282287
6	4.236289	-2.371073	2.840779
1	4.741922	-1.491114	3.251549
1	4.469283	-3.221598	3.485558
1	3.158963	-2.187274	2.912870
6	4.823909	1.314436	0.039671
6	4.222085	2.237786	-0.827731
6	4.990094	3.312567	-1.290837
1	4.525109	4.041366	-1.949852
6	6.329675	3.464824	-0.931480
6	6.897142	2.515920	-0.072266
1	7.935935	2.627632	0.229340

TS(4-2)

E = -7829.8574562
G = -7829.268209
Nimag = -371.3218

6	4.296124	-1.614394	0.180415
6	4.900981	-1.567253	-1.092650
6	5.701825	-2.648821	-1.476700
1	6.176783	-2.618394	-2.454362
6	5.898620	-3.763634	-0.658776
6	5.262147	-3.786988	0.584517
1	5.392884	-4.650259	1.232466
6	4.454199	-2.734975	1.026567
6	4.706214	-0.432764	-2.066411
1	5.184074	-0.664978	-3.021083
1	5.125540	0.506993	-1.695914
6	6.740299	-4.927588	-1.122409
1	6.126537	-5.666459	-1.652463
1	7.212357	-5.441481	-0.279858
1	7.526710	-4.604311	-1.810651
6	3.777369	-2.855001	2.374839
1	4.062446	-2.046833	3.056169
1	4.045337	-3.802775	2.847822
1	2.686510	-2.826083	2.281474
6	4.161822	1.441381	0.602564
6	3.560029	2.460756	-0.148759
6	4.209470	3.698141	-0.230497
1	3.737693	4.499140	-0.794079
6	5.440115	3.922679	0.387773
6	6.008876	2.879774	1.128888
1	6.954485	3.046011	1.639675

6	6.167851	1.441070	0.442208	6	5.388439	1.635512	1.266941
6	2.794648	2.100090	-1.280858	6	2.253510	2.263211	-0.868678
1	2.104935	2.149475	-0.232638	1	1.414562	1.964627	0.048838
1	2.707993	1.380373	-2.107162	1	2.408893	1.802982	-1.854523
1	2.375539	3.033778	-1.665087	1	1.731301	3.201302	-1.075252
6	7.139081	4.640938	-1.421876	6	6.147425	5.249938	0.256109
1	8.165967	4.348474	-1.662409	1	6.929582	5.205586	-0.511954
1	7.194898	5.422036	-0.653953	1	6.631385	5.538429	1.194358
1	6.694241	5.089648	-2.314155	1	5.453265	6.045733	-0.027051
6	6.824041	0.488113	1.410922	6	6.027209	0.574721	2.129993
1	7.823027	0.840353	1.677993	1	6.898164	0.978400	2.651741
1	6.920725	-0.519283	0.993762	1	6.355484	-0.289138	1.543045
1	6.242680	0.402764	2.336354	1	5.326047	0.205191	2.887225
34	3.696184	-0.042373	0.865070	34	3.153002	-0.199536	0.892556
46	1.656904	0.286395	-0.438043	46	1.323464	0.195880	-0.693543
6	-3.991631	1.825779	0.033758	6	-4.017680	1.635365	-0.203612
6	-3.213345	2.351039	1.084612	6	-3.590246	1.900723	1.113501
6	-3.501627	3.658697	1.503816	6	-3.712897	3.214058	1.581862
1	-2.907998	4.074079	2.314018	1	-3.381105	3.429599	2.594041
6	-4.504126	4.436190	0.925885	6	-4.215595	4.249633	0.792138
6	-5.251767	3.876118	-0.112979	6	-4.613731	3.949309	-0.512330
1	-6.041690	4.461022	-0.577941	1	-5.003340	4.742110	-1.146351
6	-5.011892	2.583811	-0.586790	6	-4.522182	2.656633	-1.037998
6	-2.087734	1.634395	1.786622	6	-2.970724	0.870382	2.020390
1	-1.942864	2.054700	2.784996	1	-2.870498	1.270029	3.031894
1	-2.265733	0.563152	1.894933	1	-3.558743	-0.048612	2.069588
6	-4.753661	5.851079	1.388757	6	-4.290169	5.659930	1.324859
1	-4.545154	5.964910	2.456572	1	-4.600906	5.674947	2.374183
1	-4.104651	6.556159	0.854843	1	-3.309143	6.147557	1.272006
1	-5.788292	6.156580	1.206682	1	-4.993565	6.269960	0.750822
6	-5.853172	2.067192	-1.732184	6	-4.949026	2.426846	-2.471899
1	-6.439572	1.187073	-1.449133	1	-5.746320	1.681064	-2.553688
1	-6.550456	2.839138	-2.066324	1	-5.316270	3.358959	-2.908386
1	-5.233582	1.782301	-2.589739	1	-4.116712	2.076151	-3.091379
6	-5.203177	-1.027500	-0.277872	6	-4.799110	-1.364766	0.170447
6	-5.698254	-1.839128	-1.323647	6	-3.993242	-2.402406	0.644933
6	-6.822520	-2.629187	-1.068996	6	-4.614889	-3.448613	1.346569
1	-7.205328	-3.259754	-1.867804	1	-4.004737	-4.272080	1.710774
6	-7.458689	-2.636171	0.174657	6	-5.985422	-3.439566	1.604960
6	-6.922494	-1.841227	1.188709	6	-6.750613	-2.361994	1.131123
1	-7.383472	-1.856536	2.173223	1	-7.821784	-2.348212	1.320208
6	-5.791202	-1.037155	1.002481	6	-6.187227	-1.316525	0.398801
6	-5.054080	-1.913814	-2.690573	6	-2.495539	-2.391412	0.479106
1	-5.603516	-2.610635	-3.328067	1	-2.113373	-3.379598	0.205825
1	-5.035103	-0.940890	-3.192339	1	-2.009274	-2.071741	1.409764
1	-4.018430	-2.267119	-2.631062	6	-6.641116	-4.554407	2.385230
6	-8.693219	-3.471725	0.410563	1	-5.947743	-5.381064	2.560849
1	-8.661480	-4.402969	-0.163048	1	-6.992125	-4.200601	3.361973
1	-8.807105	-3.726465	1.468028	1	-7.513666	-4.951378	1.855016
1	-9.598317	-2.932035	0.104401	6	-7.050913	-0.201276	-0.134954
6	-5.253890	-0.270489	2.183008	1	-8.100983	-0.367769	0.117329
1	-5.785932	-0.562217	3.091725	1	-6.752849	0.770902	0.270960
1	-4.193971	-0.492799	2.330204	1	-6.974395	-0.131053	-1.226593
1	-5.362627	0.810402	2.061756	17	-0.453807	0.681979	-2.285515
17	-0.420119	0.656925	-1.703006	34	-3.906110	-0.132473	-1.029080
34	-3.678644	0.076947	-0.789764	46	-1.678916	-1.050715	-0.826382
46	-1.520204	-0.927174	-0.177022	1	3.639831	-0.264427	-2.255546

1	3.553240	-0.933336	-2.242790
1	-1.138286	1.772597	1.256893
17	-2.466637	-2.516151	1.231704
17	1.580786	2.787788	1.448982
17	0.729963	-1.834221	0.188748

1	-1.960449	0.623472	1.673980
17	0.637906	2.137315	1.718285
17	0.569929	-2.093461	-0.637806

TS(1-4)'

E = -8445.723389
G = -8445.055886
Nimag = -985.9202

6	4.384121	-1.938500	0.389882
6	4.908591	-2.316007	-0.864078
6	5.562926	-3.549242	-0.956354
1	5.975154	-3.845074	-1.918093
6	5.692058	-4.412940	0.134114
6	5.139453	-4.017617	1.354260
1	5.220129	-4.678605	2.213663
6	4.477506	-2.795869	1.511522
6	4.763574	-1.487737	-2.115631
1	5.260922	-1.977074	-2.956441
1	5.187925	-0.487125	-2.004371
6	6.374318	-5.751043	-0.011868
1	5.650015	-6.530813	-0.278170
1	6.854740	-6.059243	0.921336
1	7.134450	-5.729909	-0.798150
6	3.883784	-2.461576	2.863900
1	4.284018	-1.530732	3.277498
1	4.095214	-3.263478	3.575061
1	2.796137	-2.345209	2.809869
6	4.585095	1.114178	-0.017164
6	4.070065	1.886499	-1.065460
6	4.837373	2.961653	-1.534577
1	4.447214	3.569926	-2.347256
6	6.087599	3.260213	-0.992267
6	6.559740	2.469054	0.063247
1	7.516738	2.710267	0.519919
6	5.825501	1.401277	0.582261
6	2.739001	1.584125	-1.701774
1	1.802484	1.906684	-0.835419
1	2.815166	0.746133	-2.409360
1	2.382668	2.409305	-2.330690
6	6.912489	4.411960	-1.514163
1	7.152190	5.120159	-0.713356
1	6.385544	4.959260	-2.300206
1	7.864389	4.061838	-1.929910
6	6.328720	0.645849	1.786181
1	7.295337	1.037110	2.111893
1	6.448912	-0.423298	1.583513
1	5.623069	0.756025	2.618609
34	3.452293	-0.251598	0.774512
46	1.572795	-0.101286	-0.754853
6	-3.937092	1.700493	0.128890
6	-3.066629	2.181787	1.127619
6	-3.325423	3.461193	1.642073
1	-2.663896	3.841303	2.416118

TS(5-6)

E = -4300.3658708
G = -4300.004204
Nimag = -1208.0375

6	0.045237	1.829601	0.217232
6	1.170054	1.920953	-0.620058
6	1.679839	3.202234	-0.889254
1	2.554761	3.290775	-1.528933
6	1.083004	4.356566	-0.382968
6	-0.055928	4.219485	0.423052
1	-0.530405	5.109823	0.829331
6	-0.589091	2.970613	0.747451
6	1.792751	0.715233	-1.264525
1	2.738733	0.975247	-1.754834
1	2.774479	0.053950	-0.340883
6	1.644726	5.724972	-0.687241
1	2.486265	5.666735	-1.382313
1	0.884532	6.376808	-1.131711
1	1.997601	6.219525	0.225285
6	-1.789370	2.875359	1.657172
1	-1.574312	2.251427	2.532865
1	-2.084163	3.864814	2.014518
1	-2.649487	2.427635	1.149056
6	-2.291840	-0.241666	0.184999
6	-2.699651	-0.004959	-1.141858
6	-4.044466	-0.230267	-1.458551
1	-4.372606	-0.043955	-2.478237
6	-4.966203	-0.701179	-0.521376
6	-4.513255	-0.956906	0.775209
1	-5.209330	-1.342169	1.516231
6	-3.184868	-0.743917	1.155714
6	-1.760767	0.425281	-2.239516
1	-2.303615	0.548936	-3.179451
1	-1.256009	1.367754	-2.012188
1	-0.988277	-0.336318	-2.396512
6	-6.399991	-0.970006	-0.908764
1	-6.710013	-0.349639	-1.754523
1	-6.533632	-2.017741	-1.204939
1	-7.082745	-0.778897	-0.075412
6	-2.762123	-1.094645	2.564547
1	-3.617614	-1.465344	3.134172
1	-1.995894	-1.877159	2.557269
1	-2.348380	-0.234122	3.100746
34	-0.466777	0.052295	0.815328
46	1.133075	-1.254040	-0.452425
1	1.173748	0.356869	-2.097625
17	0.051691	-3.191294	0.380071
17	2.933322	-2.475321	-1.524220
8	3.890709	-0.241145	0.104994

6	-4.388186	4.253290	1.205308
6	-5.212445	3.745267	0.198502
1	-6.037095	4.348939	-0.173083
6	-5.006457	2.482095	-0.364155
6	-1.871358	1.437370	1.667332
1	-1.471276	1.943431	2.548657
1	-2.106643	0.407870	1.947528
6	-4.651307	5.608993	1.814848
1	-5.363220	5.533501	2.646199
1	-3.734292	6.053934	2.210980
1	-5.079214	6.300620	1.082874
6	-5.932166	2.024175	-1.468524
1	-6.519815	1.147770	-1.176970
1	-6.630571	2.822282	-1.730906
1	-5.375935	1.753816	-2.372706
6	-5.213481	-1.112167	-0.254062
6	-5.705609	-1.938591	-1.289522
6	-6.823490	-2.733598	-1.023627
1	-7.206734	-3.372067	-1.815896
6	-7.454959	-2.733070	0.222355
6	-6.928093	-1.914973	1.222609
1	-7.393229	-1.914147	2.205347
6	-5.802622	-1.104721	1.026066
6	-5.065546	-2.019978	-2.657842
1	-5.607824	-2.730699	-3.285931
1	-5.060414	-1.052550	-3.170884
1	-4.025044	-2.359684	-2.598596
6	-8.643621	-3.623654	0.490843
1	-9.285307	-3.210485	1.274379
1	-9.250101	-3.764717	-0.408895
1	-8.319350	-4.617253	0.824192
6	-5.288015	-0.304029	2.195549
1	-5.764682	-0.646810	3.117141
1	-4.210263	-0.436130	2.310410
1	-5.494196	0.764805	2.089832
17	-0.482095	0.146130	-2.080811
34	-3.692596	-0.012411	-0.786883
46	-1.564014	-1.145885	-0.275987
1	3.705296	-1.373141	-2.378130
1	-1.061506	1.411034	0.931159
17	-2.481759	-2.499749	1.376089
17	2.364039	2.320771	2.498174
17	0.637155	-2.167616	0.033269
1	1.459196	2.614058	0.929364
8	1.025986	2.759175	-0.003195
6	1.039099	4.163372	-0.303799
1	1.120540	4.706407	0.644045
1	1.936687	4.404371	-0.892153
6	-0.222016	4.548656	-1.061297
1	-0.204837	5.615401	-1.310809
1	-0.309087	3.979511	-1.992474
1	-1.110937	4.346061	-0.457406

TS(10-11)

E = -7243.4517338
G = -7242.846156

1	3.941974	-1.106390	-0.409238
6	3.902555	-0.539292	1.536063
1	3.709367	0.416792	2.027813
1	3.080218	-1.228267	1.754845
6	5.246954	-1.119178	1.932685
1	6.060333	-0.431428	1.685479
1	5.261663	-1.302166	3.011765
1	5.425495	-2.073767	1.428322

TS(10-11)'

E = -7398.500494
G = -7397.820238

Nimag = -838.0435				**Nimag** = -1231.3318			
6	3.656373	-1.434748	-0.068615	6	-3.404570	-1.876859	1.547647
6	3.561392	-2.001521	-1.355651	6	-4.463176	-2.504197	2.219154
6	4.684742	-2.687963	-1.839668	1	-4.338593	-2.720875	3.277130
1	4.624159	-3.127622	-2.831973	6	-5.656985	-2.858010	1.589054
6	5.861441	-2.829798	-1.104640	6	-5.788971	-2.572578	0.228527
6	5.902883	-2.276226	0.176813	1	-6.707201	-2.842963	-0.287352
1	6.800905	-2.390600	0.779364	6	-4.768835	-1.957185	-0.503946
6	4.816746	-1.586153	0.723882	6	-2.154716	-1.565143	2.330109
6	2.336565	-1.938879	-2.229178	1	-2.325278	-1.729951	3.396718
1	2.563257	-2.337968	-3.221161	1	-1.823133	-0.531845	2.205112
1	1.955363	-0.923406	-2.363802	6	-6.757090	-3.559719	2.348235
6	7.058822	-3.545747	-1.681532	1	-6.597611	-4.645102	2.353809
1	6.758329	-4.299625	-2.414863	1	-7.736558	-3.375968	1.897119
1	7.642983	-4.042350	-0.900874	1	-6.794247	-3.232761	3.391649
1	7.728958	-2.842834	-2.192247	6	-4.984505	-1.712786	-1.979656
6	4.940060	-1.052766	2.132457	1	-4.984959	-0.645702	-2.224869
1	4.890345	0.040318	2.165832	1	-5.943831	-2.129038	-2.296228
1	5.894098	-1.357376	2.569401	1	-4.197964	-2.182570	-2.579964
1	4.138271	-1.434243	2.773713	6	-2.862175	0.951040	-1.461125
6	2.757338	1.334477	0.997926	6	-2.597654	1.305152	-2.804794
6	2.525675	1.905822	2.270369	6	-3.028322	2.554554	-3.262860
6	2.914626	3.232353	2.486242	1	-2.819708	2.829843	-4.294010
1	2.734416	3.674399	3.463299	6	-3.718653	3.449140	-2.441940
6	3.526750	3.996641	1.490643	6	-3.958845	3.068601	-1.120400
6	3.726066	3.404362	0.242021	1	-4.485657	3.753489	-0.459988
1	4.184304	3.987395	-0.553237	6	-3.542527	1.835947	-0.598537
6	3.347617	2.085070	-0.041621	6	-1.864313	0.396393	-3.767272
6	1.865293	1.155027	3.406896	1	-1.785395	0.869164	-4.749286
1	1.804410	1.790517	4.293967	1	-2.377498	-0.562582	-3.891181
1	2.418040	0.249268	3.674885	1	-0.847648	0.165742	-3.429312
1	0.846145	0.837374	3.158216	6	-4.209618	4.773975	-2.973850
6	3.977535	5.412063	1.760146	1	-5.200985	4.670130	-3.432277
1	5.021674	5.434525	2.096593	1	-3.538366	5.171650	-3.740935
1	3.374084	5.883716	2.541286	1	-4.296546	5.518279	-2.177033
1	3.914227	6.030026	0.859557	6	-3.839197	1.536495	0.849618
6	3.565556	1.560590	-1.437714	1	-4.226011	2.430920	1.345040
1	4.023388	2.332345	-2.061286	1	-2.941693	1.216677	1.384570
1	2.619789	1.276938	-1.912610	1	-4.587170	0.746248	0.957227
1	4.220484	0.686260	-1.448510	34	-2.187691	-0.811817	-0.943284
34	2.162792	-0.519241	0.810930	6	2.853454	1.403934	0.478866
6	-2.898722	1.399180	-0.877319	6	1.812805	2.223393	0.020387
6	-1.824833	2.267529	-0.634052	6	2.052505	3.601544	-0.082330
6	-2.054317	3.646675	-0.722655	1	1.251307	4.248329	-0.432622
1	-1.223009	4.326166	-0.552803	6	3.289744	4.158005	0.244975
6	-3.316511	4.162842	-1.016233	6	4.297685	3.305569	0.712464
6	-4.366230	3.262938	-1.239145	1	5.255575	3.727518	1.007506
1	-5.353358	3.649133	-1.482608	6	4.103974	1.929831	0.853903
6	-4.185334	1.878491	-1.192426	6	0.466133	1.666271	-0.360610
6	-0.456000	1.767306	-0.261975	1	0.514880	1.203724	-1.356390
1	-0.419638	1.532606	0.810976	1	0.117988	1.208444	2.716626
1	-0.056213	1.115728	-1.371835	6	3.542586	5.639827	0.101508
6	-3.542163	5.651598	-1.128710	1	2.611268	6.192418	-0.049689
1	-4.503827	5.945229	-0.696034	1	4.037540	6.046096	0.989684
1	-2.754092	6.215262	-0.621901	1	4.195102	5.848868	-0.755000
1	-3.548603	5.967368	-2.179097	6	5.185391	1.071177	1.459453

6	-5.343351	0.961355	-1.500864
1	-5.639297	0.367378	-0.630208
1	-6.212248	1.536593	-1.829223
1	-5.086224	0.257345	-2.300856
6	-3.644675	-1.318305	0.382506
6	-4.385991	-2.440778	-0.044915
6	-5.235869	-3.058921	0.877856
1	-5.813193	-3.921567	0.554454
6	-5.358517	-2.608731	2.194098
6	-4.588178	-1.511811	2.587179
1	-4.654146	-1.157054	3.613005
6	-3.715431	-0.856031	1.712008
6	-4.282916	-3.016552	-1.439831
1	-4.949758	-3.875877	-1.543645
1	-4.550798	-2.287631	-2.211546
1	-3.263920	-3.355999	-1.653955
6	-6.263137	-3.313356	3.175682
1	-5.717722	-4.095909	3.717655
1	-6.663001	-2.619959	3.921569
1	-7.105462	-3.794450	2.670118
6	-2.871192	0.273353	2.244213
1	-3.047438	0.409474	3.314011
1	-1.807663	0.048861	2.101090
1	-3.077787	1.222054	1.741257
17	0.191934	1.011520	-3.089562
34	-2.512644	-0.505109	-0.981795
46	-0.163860	-0.489525	-0.234370
1	1.522617	-2.533850	-1.804128
1	0.319881	2.520702	-0.418120
17	-0.266809	-2.827340	0.189652
1	5.508485	0.274119	0.782107
1	6.060993	1.673598	1.712922
1	4.817814	0.603157	2.380476
6	3.626722	-1.410638	-0.492597
6	4.368919	-2.474237	0.070310
6	5.245691	-3.180015	-0.759891
1	5.823845	-3.994628	-0.330441
6	5.395819	-2.875544	-2.114401
6	4.626960	-1.835912	-2.641515
1	4.716365	-1.593765	-3.697994
6	3.729097	-1.096909	-1.862618
6	4.241262	-2.898607	1.517719
1	4.915324	-3.733256	1.725246
1	4.481155	-2.089684	2.214635
1	3.221804	-3.226612	1.746192
6	6.330358	-3.674165	-2.990394
1	7.212584	-4.006993	-2.435254
1	5.832327	-4.571981	-3.377054
1	6.668612	-3.091466	-3.852138
6	2.889879	-0.045689	-2.542879
1	3.129857	0.003512	-3.607923
1	1.826366	-0.295014	-2.449881
1	3.036340	0.949190	-2.115109
17	1.493510	0.699357	3.759916
34	2.481952	-0.478087	0.801491
46	0.165729	-0.550466	-0.000742
1	-1.327469	-2.210324	2.019960
1	-0.285412	2.454588	-0.487422
17	0.280823	-2.922702	-0.049572
1	-0.121335	1.358667	0.829325
8	-0.608964	1.608579	2.065469
6	-0.754752	3.001256	2.417466
1	0.235750	3.469829	2.437326
1	-1.346557	3.467011	1.621563
6	-1.440306	3.137621	3.769152
1	-0.840230	2.647948	4.540577
1	-1.550435	4.195940	4.030615
1	-2.433386	2.678570	3.751863

TS(7-4)

E = -7984.88851
G = -7984.223066
Nimag = -47.7626

6	-3.959051	1.746277	0.930379
6	-3.818790	2.172529	2.266504
6	-3.817665	3.546888	2.520914
1	-3.712292	3.886497	3.548445
6	-3.938518	4.490725	1.497891
6	-4.051880	4.027743	0.184895
1	-4.124909	4.747618	-0.626638
6	-4.050135	2.665079	-0.134430
6	-3.647625	1.212693	3.421863
1	-3.578334	1.760967	4.364449
1	-2.731557	0.620757	3.315003
6	-3.897607	5.969369	1.797620

TS(1-8)

E = -8290.6579451
G = -8290.058559
Nimag = -795.8431

6	4.704781	1.579661	0.508065
6	4.754423	2.909696	0.030509
6	5.393131	3.865302	0.825376
1	5.438473	4.889977	0.465701
6	5.961476	3.548365	2.061070
6	5.874839	2.226929	2.504287
1	6.300350	1.962494	3.469174
6	5.247265	1.221001	1.760299
6	4.126466	3.348406	-1.273599
1	4.303254	4.414150	-1.435296
1	3.043532	3.183675	-1.258954
6	6.614903	4.610316	2.910775

1	-4.276087	6.185954	2.800977	1	7.040917	5.408611	2.296311
1	-4.489896	6.541284	1.077160	1	7.412404	4.192684	3.532148
1	-2.868939	6.346835	1.747191	1	5.883386	5.072567	3.584991
6	-4.113305	2.255087	-1.585433	6	5.176103	-0.161754	2.356669
1	-3.266554	1.610677	-1.843338	1	4.142158	-0.522223	2.393045
1	-4.069128	3.137065	-2.228643	1	5.555844	-0.147579	3.380728
1	-5.028738	1.705861	-1.822349	1	5.757314	-0.894396	1.790783
6	-5.499152	-0.530214	-0.475972	6	4.796498	-1.324032	-0.622257
6	-6.776435	-0.095680	-0.055622	6	6.131342	-1.396022	-1.061835
6	-7.896309	-0.617863	-0.702308	6	6.761921	-2.641272	-1.000734
1	-8.881341	-0.327426	-0.345902	1	7.798786	-2.714941	-1.320007
6	-7.794538	-1.571537	-1.740231	6	6.103508	-3.790237	-0.543291
6	-6.540564	-1.961175	-2.155524	6	4.768959	-3.677978	-0.147424
1	-6.436253	-2.667170	-2.975611	1	4.236589	-4.561557	0.195905
6	-5.339232	-1.410312	-1.599350	6	4.086887	-2.453880	-0.194307
6	-7.000085	0.831158	1.115512	6	6.883141	-0.188598	-1.567739
1	-8.065602	0.893381	1.348667	1	7.847372	-0.483878	-1.987882
1	-6.636626	1.843241	0.918297	1	7.071453	0.537450	-0.769553
1	-6.480722	0.475484	2.012750	1	6.321934	0.331727	-2.352218
6	-9.045698	-2.132424	-2.372465	6	6.813257	-5.122445	-0.514342
1	-9.634843	-1.342941	-2.853682	1	6.847912	-5.567748	-1.516026
1	-9.692221	-2.601043	-1.621399	1	6.305434	-5.832682	0.143488
1	-8.809180	-2.883898	-3.130295	1	7.847124	-5.017490	-0.171019
6	-4.104642	-1.714230	-2.202736	6	2.625829	-2.425628	0.160050
1	-4.088791	-2.408064	-3.038301	1	2.375415	-3.092605	0.986536
1	-3.128108	-2.881669	-0.904346	1	1.986433	-2.676802	-0.691414
1	-3.273397	-1.019613	-2.150805	1	2.527238	-1.158016	1.372407
34	-3.947759	-0.178824	0.628701	34	3.817084	0.351647	-0.715654
46	-1.694203	-0.750621	-0.289429	46	1.751248	-0.456509	0.259545
6	4.402323	-1.720966	0.507616	6	-4.688185	-1.253356	1.030566
6	3.757904	-1.982402	1.733354	6	-4.679389	-2.534787	0.443885
6	4.249677	-3.038983	2.512291	6	-5.606027	-3.472911	0.919119
1	3.760391	-3.246642	3.460798	1	-5.608994	-4.463388	0.470670
6	5.332061	-3.827253	2.120086	6	-6.517530	-3.185812	1.935852
6	5.930499	-3.548872	0.889621	6	-6.479557	-1.912059	2.506953
1	6.765472	-4.158123	0.551916	1	-7.166585	-1.668720	3.314081
6	5.483573	-2.514239	0.061896	6	-5.573669	-0.933813	2.084799
6	2.566405	-1.218207	2.255056	6	-3.736191	-2.964796	-0.653522
1	2.386414	-1.471623	3.303243	1	-4.005469	-3.962541	-1.010045
1	2.699195	-0.136025	2.185346	1	-3.749167	-2.283553	-1.508352
6	5.852638	-4.933373	3.005878	6	-7.525125	-4.212950	2.393349
1	5.063346	-5.338644	3.645503	1	-7.168961	-5.231252	2.212746
1	6.269365	-5.755422	2.416218	1	-7.742714	-4.111985	3.461031
1	6.650940	-4.567892	3.663940	1	-8.475086	-4.099024	1.856230
6	6.173096	-2.303590	-1.266518	6	-5.586712	0.410805	2.774599
1	6.669853	-1.329742	-1.321205	1	-5.899888	1.213595	2.099332
1	6.929694	-3.075307	-1.427435	1	-6.276392	0.396112	3.622009
1	5.461071	-2.350116	-2.097495	1	-4.593195	0.678072	3.150187
6	5.230626	0.971687	-0.778050	6	-4.444122	1.582639	-0.215776
6	5.569179	1.434748	-2.069167	6	-3.999199	2.871967	0.152621
6	6.619139	2.350067	-2.187827	6	-4.708313	3.974898	-0.333211
1	6.884692	2.709384	-3.179187	1	-4.370879	4.970493	-0.055237
6	7.328070	2.814677	-1.077930	6	-5.825685	3.835484	-1.158638
6	6.948997	2.349829	0.182096	6	-6.225463	2.544578	-1.507633
1	7.473970	2.715242	1.061424	1	-7.084143	2.414653	-2.162159
6	5.897502	1.443944	0.369371	6	-5.551134	1.398767	-1.067632
6	4.834462	1.007894	-3.320839	6	-2.787962	3.111570	1.025789

1	5.265237	1.499057	-4.196753
1	4.883217	-0.073876	-3.481990
1	3.773699	1.279448	-3.277929
6	8.439630	3.824049	-1.233780
1	9.162395	3.754188	-0.415631
1	8.976946	3.686185	-2.177047
1	8.042191	4.846617	-1.232291
6	5.521333	1.062873	1.777929
1	6.094171	1.658548	2.492951
1	4.460248	1.263683	1.949536
1	5.711635	0.007618	1.990033
17	0.612714	-1.485096	-1.018694
34	3.799141	-0.356725	-0.760801
46	1.579563	0.625503	-0.272412
1	-4.480715	0.506467	3.501998
1	1.663553	-1.467114	1.688092
17	2.453573	2.662528	0.460693
17	-0.675060	1.479274	-0.082835
8	-2.340668	-3.001832	-0.314467
6	-2.659119	-3.791360	0.840833
1	-1.781375	-3.722976	1.488909
1	-3.509699	-3.350304	1.380246
6	-2.944607	-5.241667	0.472405
1	-3.131886	-5.833812	1.375263
1	-3.828678	-5.318732	-0.169635
1	-2.093827	-5.676958	-0.059375

1	-2.639391	4.183660	1.176650
1	-2.893394	2.644527	2.010953
1	-1.870227	2.711491	0.579824
6	-6.554124	5.045381	-1.692315
1	-6.490295	5.889787	-0.999324
1	-6.121970	5.373126	-2.646001
1	-7.611720	4.829803	-1.871735
6	-6.037709	0.054272	-1.547472
1	-6.766479	0.188571	-2.350871
1	-5.207202	-0.532786	-1.946343
1	-6.518564	-0.522515	-0.752176
17	-0.350811	-1.327932	1.101253
34	-3.394355	0.138157	0.570135
46	-1.529244	-0.521208	-0.945740
1	4.533363	2.807972	-2.134845
1	-2.700034	-3.008529	-0.300730
17	0.467347	-0.922022	-2.219253
17	1.006902	1.857751	0.373943
17	-2.652420	0.136580	-2.874152

TS(1-9)

E = -8445.6777108
G = -8445.003736
Nimag = -897.6477

6	4.386050	2.005367	-0.294815
6	3.537130	2.922930	-0.962614
6	3.754913	4.289554	-0.765748
1	3.094604	4.989582	-1.270976
6	4.786177	4.774285	0.037016
6	5.657199	3.841474	0.601309
1	6.511712	4.196866	1.171964
6	5.502349	2.457890	0.448607
6	2.430506	2.511136	-1.898294
1	2.099761	3.367820	-2.489744
1	1.561884	2.129011	-1.357120
6	4.965955	6.253335	0.271516
1	4.644427	6.837765	-0.595606
1	6.009298	6.502636	0.485947
1	4.366801	6.586668	1.127954
6	6.596787	1.594570	1.037247
1	6.296980	1.103506	1.966079
1	7.462368	2.221225	1.265457
1	6.927749	0.811719	0.352241
6	5.046120	-1.027525	0.438568
6	5.918096	-1.901976	-0.245691
6	6.668864	-2.801952	0.515899
1	7.351076	-3.474461	0.001875
6	6.566972	-2.864564	1.908609

TS(1-4)···EtOH

E = -8445.7326233
G = -8445.062712
Nimag = -751.4686

6	4.573499	-1.873446	0.567634
6	4.920008	-2.461094	-0.666696
6	5.504376	-3.732349	-0.640769
1	5.781434	-4.192294	-1.586049
6	5.727597	-4.431182	0.547829
6	5.345026	-3.827019	1.748219
1	5.498142	-4.358815	2.683914
6	4.762521	-2.557241	1.790133
6	4.663885	-1.812411	-2.003541
1	4.969828	-2.478561	-2.813487
1	5.203433	-0.868456	-2.117815
6	6.325884	-5.816452	0.534657
1	5.538358	-6.580017	0.526042
1	6.940901	-5.995151	1.421669
1	6.946694	-5.977195	-0.351207
6	4.347187	-1.990832	3.130588
1	4.845497	-1.041984	3.354395
1	4.594097	-2.694403	3.928900
1	3.268261	-1.807508	3.173951
6	4.841354	1.072163	-0.374220
6	4.188071	1.784557	-1.388854
6	4.908881	2.765599	-2.080392
1	4.405062	3.335356	-2.857026
6	6.252119	3.019957	-1.800635

6	5.686985	-1.986325	2.544312	6	6.871930	2.277090	-0.787586
1	5.598809	-2.014817	3.627857	1	7.914539	2.472810	-0.548473
6	4.907190	-1.060268	1.839956	6	6.190029	1.309275	-0.045962
6	6.068365	-1.912366	-1.750205	6	2.758544	1.509572	-1.765517
1	6.825202	-2.641199	-2.049834	1	2.065403	1.820828	-0.668881
1	6.369314	-0.935711	-2.143423	1	2.691784	0.670740	-2.471986
1	5.124670	-2.182213	-2.233770	1	2.283055	2.352078	-2.275037
6	7.366908	-3.871024	2.699165	6	7.011593	4.093213	-2.542478
1	8.329728	-4.079828	2.223640	1	8.045752	3.791484	-2.735125
1	6.828085	-4.823544	2.775462	1	7.046590	5.020287	-1.957465
1	7.556409	-3.521519	3.718050	1	6.540233	4.327887	-3.500619
6	3.970734	-0.171741	2.622949	6	6.896468	0.582880	1.072317
1	4.360816	-0.009114	3.631807	1	7.896752	0.993995	1.226246
1	2.982043	-0.632545	2.726279	1	6.998205	-0.487407	0.865906
1	3.801286	0.798214	2.154961	1	6.347005	0.680727	2.016007
34	3.983282	0.131620	-0.712431	34	3.763716	-0.108593	0.736434
46	1.642029	-0.679425	-0.114588	46	1.702469	-0.067820	-0.568325
6	-4.859526	-1.506691	0.572460	6	-3.989029	1.430347	-0.614290
6	-4.925646	-2.429652	-0.491285	6	-3.205185	2.211428	0.257098
6	-5.880871	-3.451253	-0.405479	6	-3.474528	3.588180	0.312019
1	-5.940709	-4.166753	-1.221930	1	-2.851081	4.199390	0.959955
6	-6.751429	-3.583130	0.677419	6	-4.483130	4.183506	-0.445535
6	-6.640750	-2.661575	1.720201	6	-5.241576	3.371557	-1.293967
1	-7.295357	-2.752031	2.583816	1	-6.028097	3.816530	-1.899393
6	-5.701848	-1.624887	1.700825	6	-5.010190	1.998677	-1.410290
6	-4.036452	-2.394778	-1.710756	6	-2.088210	1.689494	1.126045
1	-4.362917	-3.146592	-2.434133	1	-1.808434	2.444385	1.862719
1	-4.043948	-1.420588	-2.206693	1	-2.356793	0.766526	1.645430
6	-7.791839	-4.676580	0.710850	6	-4.758406	5.664109	-0.338046
1	-7.455017	-5.565642	0.169638	1	-5.574634	5.862036	0.368187
1	-8.029877	-4.971539	1.737148	1	-3.877823	6.204248	0.019428
1	-8.726593	-4.344624	0.241861	1	-5.055360	6.087808	-1.302712
6	-5.636806	-0.686180	2.883626	6	-5.852176	1.199630	-2.379101
1	-5.916367	0.336387	2.610140	1	-6.437128	0.423574	-1.874842
1	-6.316087	-1.020832	3.671353	1	-6.550822	1.856852	-2.902308
1	-4.626460	-0.640819	3.303939	1	-5.233838	0.700536	-3.133785
6	-4.519432	1.587326	0.571359	6	-5.166303	-1.434319	-0.216366
6	-4.000434	2.607402	1.399652	6	-5.627555	-2.491128	-1.032418
6	-4.664254	3.837809	1.421238	6	-6.754132	-3.205035	-0.612507
1	-4.269070	4.628354	2.054721	1	-7.115677	-4.018495	-1.236777
6	-5.808418	4.078806	0.657960	6	-7.420898	-2.906534	0.577179
6	-6.282706	3.047765	-0.154263	6	-6.920542	-1.868687	1.366033
1	-7.163344	3.219381	-0.768693	1	-7.412397	-1.633337	2.306807
6	-5.656760	1.797395	-0.233096	6	-5.789819	-1.124828	1.009718
6	-2.756663	2.435917	2.242804	6	-4.949012	-2.899649	-2.321195
1	-2.543919	3.357109	2.790832	1	-5.477759	-3.740900	-2.775739
1	-2.864411	1.627007	2.973424	1	-4.921140	-2.084620	-3.051627
1	-1.874421	2.201277	1.636459	1	-3.913673	-3.214517	-2.148648
6	-6.486532	5.427418	0.677886	6	-8.620189	-3.708071	1.021564
1	-6.369398	5.920880	1.647509	1	-9.109992	-4.199125	0.175904
1	-6.055893	6.093066	-0.080529	1	-8.325574	-4.491485	1.730721
1	-7.556349	5.341651	0.465368	1	-9.359093	-3.077329	1.525392
6	-6.224631	0.772529	-1.182487	6	-5.290143	-0.075493	1.968775
1	-6.964206	1.241752	-1.836086	1	-5.865677	-0.112147	2.896866
1	-5.435666	0.358576	-1.814136	1	-4.241675	-0.259409	2.217982
1	-6.715214	-0.052593	-0.658135	1	-5.370022	0.935754	1.562186
17	-0.511435	-1.710582	0.436976	17	-0.361610	0.011079	-1.893177

34	-3.520146	-0.085974	0.673207
46	-1.723716	-0.146817	-1.053132
1	2.741801	1.732590	-2.602763
1	-2.993208	-2.612886	-1.457210
17	0.208283	-0.138108	-2.468234
1	2.323065	-1.726840	0.759004
8	2.572482	-2.398764	-0.785055
6	1.741374	-3.442795	-1.276267
1	1.157469	-3.895537	-0.465001
1	1.034171	-3.048249	-2.016482
17	1.000951	1.251921	1.114159
17	-2.847514	1.290598	-2.499261
6	2.651834	-4.489132	-1.917551
1	3.206267	-4.059770	-2.757415
1	3.368836	-4.882117	-1.190223
1	2.047022	-5.321529	-2.294897

34	-3.647919	-0.464954	-0.963472
46	-1.484268	-1.242022	-0.088022
1	3.596176	-1.599289	-2.131620
1	-1.189424	1.489426	0.534478
17	-2.449310	-2.497053	1.611815
17	1.665467	2.901718	0.680471
17	0.777241	-2.011778	0.507980
1	-0.103413	4.214590	1.451697
8	-0.768524	4.726441	1.946808
6	-0.155317	5.217027	3.130470
1	0.225070	4.390660	3.750877
1	0.706764	5.858345	2.887489
6	-1.189076	6.016589	3.908841
1	-0.755377	6.420116	4.829881
1	-1.560153	6.851171	3.305422
1	-2.041833	5.384214	4.175901

TS(1-4)···2EtOH

E = -8600.7920754
G = -8600.048930
Nimag = -956.5016

6	4.476775	-2.418632	0.314036
6	4.739605	-2.759708	-1.028972
6	5.248745	-4.037043	-1.287359
1	5.460596	-4.308903	-2.318484
6	5.477458	-4.972684	-0.275475
6	5.181267	-4.605321	1.039338
1	5.341156	-5.321790	1.841037
6	4.677645	-3.342278	1.364035
6	4.469509	-1.841082	-2.193303
1	4.716388	-2.337957	-3.134294
1	5.048314	-0.915303	-2.135557
6	5.990968	-6.354392	-0.598416
1	5.158792	-7.044999	-0.782479
1	6.579089	-6.766331	0.226764
1	6.615623	-6.350024	-1.496294
6	4.356361	-3.036691	2.810812
1	4.909380	-2.168901	3.184700
1	4.609692	-3.891998	3.441353
1	3.290498	-2.826795	2.951287
6	4.867105	0.652804	-0.026511
6	4.191388	1.582890	-0.828934
6	4.897339	2.701468	-1.290945
1	4.356792	3.462064	-1.847229
6	6.256965	2.863346	-1.017317
6	6.903601	1.893910	-0.239028
1	7.957920	2.019388	-0.003695
6	6.231827	0.788568	0.289485
6	2.751223	1.410744	-1.225569
1	2.048650	1.562518	-0.022678
1	2.656612	0.754751	-2.100478
1	2.284428	2.359726	-1.512562
6	7.014950	4.052728	-1.555869
1	7.482584	3.816787	-2.519968
1	7.813389	4.361068	-0.874284

TS(1-4)···EtOH···EtOH

E = -8600.7949037
G = -8600.049192
Nimag = -852.4654

6	4.734816	-2.048416	0.507426
6	5.087612	-2.577631	-0.751154
6	5.707693	-3.831895	-0.778275
1	5.989489	-4.247298	-1.742565
6	5.959998	-4.569233	0.380805
6	5.570976	-4.022364	1.606443
1	5.746683	-4.585140	2.519778
6	4.954065	-2.771921	1.701577
6	4.802577	-1.885463	-2.059996
1	5.115900	-2.513303	-2.897217
1	5.318728	-0.925244	-2.143558
6	6.596451	-5.935534	0.309945
1	5.830504	-6.720575	0.293695
1	7.235895	-6.124647	1.177349
1	7.201573	-6.049944	-0.593711
6	4.535644	-2.267977	3.065728
1	5.011789	-1.315824	3.321596
1	4.807405	-2.994572	3.834716
1	3.452753	-2.114934	3.124169
6	4.890736	0.940269	-0.334629
6	4.193226	1.661439	-1.313101
6	4.864212	2.694234	-1.979234
1	4.326420	3.270962	-2.727440
6	6.201438	2.990163	-1.711155
6	6.866966	2.235220	-0.736580
1	7.905710	2.461557	-0.508065
6	6.235092	1.216031	-0.020027
6	2.771191	1.340188	-1.681379
1	2.067682	1.608077	-0.550946
1	2.730005	0.529208	-2.421387
1	2.253437	2.181808	-2.149516
6	6.905758	4.119132	-2.424159
1	7.952528	3.873495	-2.627537
1	6.897775	5.029981	-1.813189

1	6.350435	4.906265	-1.714693	1	6.420075	4.357846	-3.374143
6	6.961656	-0.183840	1.183244	6	6.986989	0.474321	1.057617
1	7.981743	0.158566	1.372033	1	7.974932	0.914536	1.210625
1	7.017060	-1.184159	0.741475	1	7.121954	-0.583130	0.808309
1	6.460133	-0.285570	2.153180	1	6.451397	0.516500	2.013310
34	3.780722	-0.685523	0.868639	34	3.875029	-0.316067	0.749518
46	1.681328	-0.290134	-0.302892	46	1.793288	-0.296758	-0.520042
6	-4.071279	1.251912	-0.475498	6	-4.020031	0.860545	-0.538899
6	-3.317514	2.007290	0.444225	6	-3.309416	1.664141	0.376183
6	-3.582499	3.383293	0.525313	6	-3.681954	3.011465	0.476822
1	-2.969691	3.976764	1.198672	1	-3.123938	3.642250	1.162084
6	-4.562909	4.004002	-0.247943	6	-4.716048	3.567699	-0.279554
6	-5.297254	3.217410	-1.139727	6	-5.393908	2.735202	-1.173354
1	-6.063233	3.681089	-1.757229	1	-6.197638	3.146366	-1.779602
6	-5.064856	1.847705	-1.286880	6	-5.063357	1.385966	-1.333885
6	-2.231737	1.460524	1.338305	6	-2.167334	1.192260	1.242287
1	-2.019275	2.171305	2.138996	1	-1.919435	1.958441	1.978969
1	-2.497950	0.500297	1.785106	1	-2.395690	0.261986	1.768157
6	-4.833249	5.483036	-0.111672	6	-5.084114	5.022302	-0.120199
1	-5.647306	5.670294	0.599982	1	-5.746432	5.161540	0.743999
1	-3.950007	6.013298	0.254402	1	-4.193206	5.636381	0.047819
1	-5.130292	5.926126	-1.067361	1	-5.615322	5.397068	-1.000605
6	-5.874819	1.082428	-2.308642	6	-5.830268	0.567796	-2.348073
1	-6.465997	0.282135	-1.852185	1	-6.372270	-0.262656	-1.883807
1	-6.564893	1.755354	-2.823159	1	-6.560945	1.195493	-2.863647
1	-5.232047	0.620254	-3.066329	1	-5.165253	0.138327	-3.105926
6	-5.260048	-1.609911	-0.193090	6	-5.011598	-2.080839	-0.235836
6	-5.784669	-2.568218	-1.088756	6	-5.426393	-3.117839	-1.100891
6	-6.930455	-3.270524	-0.703621	6	-6.513193	-3.906007	-0.710663
1	-7.338465	-4.011944	-1.386256	1	-6.839488	-4.704192	-1.372994
6	-7.556620	-3.053447	0.525923	6	-7.184316	-3.699634	0.496431
6	-6.987181	-2.122201	1.396118	6	-6.729080	-2.679058	1.333283
1	-7.438433	-1.964032	2.372545	1	-7.224178	-2.515438	2.287390
6	-5.834096	-1.396016	1.075559	6	-5.638886	-1.863768	1.007502
6	-5.150721	-2.889874	-2.423935	6	-4.740171	-3.427622	-2.413053
1	-5.721591	-3.669750	-2.933663	1	-5.225845	-4.276261	-2.900772
1	-5.108459	-2.017436	-3.083851	1	-4.767651	-2.579921	-3.105362
1	-4.124857	-3.255336	-2.304075	1	-3.686691	-3.690216	-2.265256
6	-8.814929	-3.798781	0.899320	6	-8.338298	-4.582205	0.906097
1	-9.707394	-3.263337	0.551418	1	-8.856529	-4.994762	0.035534
1	-8.837810	-4.795546	0.449052	1	-7.987256	-5.428685	1.509259
1	-8.905189	-3.912119	1.983479	1	-9.067327	-4.033621	1.509863
6	-5.244576	-0.481421	2.116471	6	-5.177539	-0.843353	2.014393
1	-5.823788	-0.538256	3.041207	1	-5.750284	-0.942331	2.939575
1	-4.219058	-0.789676	2.341860	1	-4.122994	-1.005514	2.253671
1	-5.225244	0.562488	1.793808	1	-5.291991	0.181871	1.653981
17	-0.394469	0.082958	-1.563510	17	-0.292667	-0.240791	-1.807707
34	-3.717539	-0.631621	-0.878789	34	-3.551377	-0.996767	-0.942119
46	-1.557669	-1.461899	-0.033007	46	-1.345199	-1.657079	-0.079520
1	3.409249	-1.564847	-2.229055	1	3.728891	-1.693472	-2.169887
1	-1.299551	1.319190	0.784414	1	-1.263268	1.024641	0.649127
17	-2.561371	-2.975426	1.415812	17	-2.228537	-3.074095	1.534921
17	1.718318	2.504179	1.394290	17	1.650491	2.653576	0.791272
17	0.670600	-2.354637	0.466589	17	0.955380	-2.312085	0.500690
1	-0.141477	3.888743	1.716935	1	-0.154820	3.809180	1.495545
8	-0.768835	4.608145	1.909090	8	-0.816690	4.351196	1.969352
6	-0.279231	5.328373	3.035184	6	-0.199698	4.881450	3.148097

1	-0.239655	4.683161	3.926641
1	0.744818	5.688032	2.852738
6	-1.204907	6.507481	3.290072
1	-0.860998	7.090698	4.150592
1	-1.237143	7.165397	2.415875
1	-2.222868	6.160205	3.494069
1	2.238602	4.214587	-0.172063
8	2.218361	4.608014	-1.060579
6	1.157893	5.566043	-1.092486
1	1.539516	6.556623	-0.795365
1	0.370520	5.294329	-0.377530
6	0.596200	5.635840	-2.504304
1	-0.181049	6.404489	-2.573152
1	1.386954	5.882817	-3.220491
1	0.160142	4.674709	-2.793993
1	0.157386	4.059435	3.783403
1	0.675256	5.489840	2.877477
6	-1.223168	5.728488	3.887251
1	-0.775274	6.175243	4.780905
1	-1.590846	6.529125	3.238640
1	-2.077117	5.118159	4.197895
1	-1.588911	5.682599	1.007009
8	-2.000012	6.475146	0.603580
6	-1.133185	6.960143	-0.407527
1	-1.010082	6.221812	-1.217730
1	-0.126073	7.158172	-0.004160
6	-1.716490	8.246523	-0.973454
1	-1.068738	8.657995	-1.754944
1	-2.705125	8.061368	-1.405352
1	-1.827506	8.994923	-0.182584

$[Pd_2(\mu\text{-}Sepy)_2\{MesSeC_6H_2(Me_2)CH_2\}_2]$ (3b)

E = -11741.9356845
G = -11741.205678
Nimag = 0

6	-1.338193	-2.589754	1.499253
6	-1.779410	-3.778609	2.116043
1	-1.522278	-3.953898	3.154462
6	-2.511686	-4.706760	1.393454
1	-2.850838	-5.624421	1.866385
6	-2.788246	-4.452552	0.045592
1	-3.344238	-5.153268	-0.567468
6	-2.326452	-3.264221	-0.499789
1	-2.502548	-3.016516	-1.541463
6	0.979955	1.467701	1.875658
1	0.116514	1.903454	1.355933
1	0.677714	1.305332	2.913785
6	2.145339	2.426246	1.816343
6	3.085384	2.397101	0.776284
6	4.085092	3.373959	0.634168
6	4.171879	4.357793	1.625504
1	4.950710	5.113083	1.544868
6	3.290449	4.395607	2.712742
6	2.278372	3.434222	2.782753
1	1.564963	3.466404	3.603460
6	5.054108	3.379526	-0.522774
1	5.767586	2.550928	-0.459017
1	5.622130	4.313229	-0.547098
1	4.530296	3.275175	-1.479303
6	3.441187	5.443956	3.790182
1	4.148196	5.117220	4.563218
1	2.487998	5.647538	4.286818
1	3.820509	6.386039	3.382197
6	4.533706	0.013001	-0.549735
6	5.228891	-0.374616	0.613418
6	6.436236	-1.069372	0.455019
1	6.978862	-1.369741	1.348606
6	6.954483	-1.396564	-0.798458
6	6.224267	-1.018177	-1.928409
1	6.599679	-1.276819	-2.915950

6	5.019374	-0.314692	-1.835545
6	4.740317	-0.089548	2.011326
1	4.863050	0.964967	2.277872
1	5.298193	-0.687294	2.737289
1	3.673178	-0.318430	2.115974
6	4.286620	0.048777	-3.108298
1	3.280019	-0.383121	-3.140663
1	4.838591	-0.314973	-3.978952
1	4.168105	1.132830	-3.211524
6	1.354952	-2.655733	-1.336106
6	1.817144	-3.873051	-1.876825
1	1.569753	-4.115238	-2.904071
6	2.557811	-4.744349	-1.094382
1	2.913143	-5.684208	-1.508177
6	2.821758	-4.403903	0.236817
1	3.383455	-5.057735	0.894852
6	2.339718	-3.191166	0.705570
1	2.504560	-2.877384	1.731084
6	-1.035060	1.311435	-1.990906
1	-0.058353	1.703109	-1.681568
1	-0.944152	1.044510	-3.049343
6	-2.089263	2.386636	-1.830718
6	-3.022292	2.390674	-0.788659
6	-3.938424	3.442843	-0.596083
6	-3.933708	4.481688	-1.528924
1	-4.643559	5.297177	-1.407117
6	-3.040385	4.504766	-2.609911
6	-2.124142	3.460383	-2.736580
1	-1.411142	3.470742	-3.558173
6	-4.903960	3.468159	0.563228
1	-4.379608	3.340022	1.517033
1	-5.641585	2.661629	0.494840
1	-5.442997	4.418430	0.598370
6	-3.079948	5.636400	-3.610074
1	-3.987787	5.592101	-4.224042
1	-2.221326	5.602868	-4.286223
1	-3.078450	6.611234	-3.110124
6	-4.622991	0.039786	0.404484
6	-5.184037	-0.280150	1.660404
6	-6.425587	-0.924627	1.686660
1	-6.859722	-1.176777	2.651438
6	-7.118445	-1.252135	0.518774
6	-6.525069	-0.936501	-0.704820
1	-7.038272	-1.199769	-1.627112
6	-5.280261	-0.299780	-0.796082
6	-4.498288	0.034804	2.972035
1	-3.504727	-0.421129	3.040758
1	-5.097222	-0.333134	3.809227
1	-4.358432	1.113041	3.105431
6	-8.475703	-1.911519	0.578531
1	-9.277271	-1.163025	0.617832
1	-8.576239	-2.540979	1.467833
1	-8.657345	-2.534701	-0.302273
6	-4.710697	-0.022808	-2.164545
1	-4.743467	1.043148	-2.410463
1	-5.277447	-0.562672	-2.927928
1	-3.659537	-0.328066	-2.228004

7	-1.634761	-2.343011	0.202909
7	1.639448	-2.325187	-0.056253
34	2.829075	0.968373	-0.514107
34	-2.875047	0.915453	0.461088
46	1.234777	-0.343191	0.908671
46	-1.262972	-0.421906	-0.888464
6	8.270974	-2.123850	-0.934567
1	8.239895	-2.859321	-1.744807
1	9.086538	-1.426339	-1.163367
1	8.537174	-2.646445	-0.011333
34	-0.362211	-1.331869	2.545549
34	0.364869	-1.478520	-2.458484