Supporting information

Neutral Pd° complex $Ph_3P–Pd–PPh_3$

Gas phase energy (Lacvp*): -2199.38081922563au
Gas phase energy (Lacv3p**+): -2199.81290423026au
Solvation energy: -0.015460774au
Total Gibbs free energy: -2199.43665au
Dispersion energy: -0.08457658au
ZPE: 1447.96 kJ/mol

P1	-1.7376620000	1.8720360000	-0.0220080000
C2	-5.6223490000	-0.2622300000	1.4343910000
C3	-4.3819820000	-0.8232160000	1.7453120000
C4	-3.2030130000	-0.2033980000	1.3256970000
C5	-3.2476990000	0.9915790000	0.5906370000
C6	-4.5002240000	1.5560240000	0.2982150000
C7	-5.6774730000	0.9300010000	0.7090740000
H8	-6.5390390000	-0.7459640000	1.7622120000
H9	-4.3296240000	-1.7460940000	2.3180270000
H10	-2.2454710000	-0.6507790000	1.5763850000
H11	-4.5427740000	2.4962890000	-0.2466650000
H12	-6.6383230000	1.3797790000	0.4705070000
C13	1.6264870000	0.2603130000	2.7771120000
C14	1.3703080000	-0.4060670000	1.5778470000
C15	0.3690960000	0.0496690000	0.7157440000
C16	-0.3883670000	1.1842000000	1.0420760000
C17	-0.1113330000	1.8569220000	2.2441290000
C18	0.8805090000	1.3944980000	3.1082680000
H19	2.4070790000	-0.0955830000	3.4445960000
H20	1.9515270000	-1.2846400000	1.3084170000
H21	0.1825840000	-0.4803690000	-0.2137930000
H22	-0.6707060000	2.7568920000	2.4896800000
H23	1.0789200000	1.9272440000	4.0350240000
C24	-0.8445110000	0.0097830000	-4.2009310000
C25	-1.6425230000	-0.7011250000	-3.3016490000
C26	-1.9323210000	-0.1694480000	-2.0426780000
C27	-1.4281420000	1.0853660000	-1.6671060000
C28	-0.6407560000	1.7991730000	-2.5845710000
C29	-0.3448150000	1.2625280000	-3.8378400000
H30	-0.6215420000	-0.4052030000	-5.1806110000
H31	-2.0437490000	-1.6729180000	-3.5793890000
H32	-2.5556320000	-0.7341990000	-1.3552350000
H33	-0.2725350000	2.7855060000	-2.3110980000
H34	0.2681420000	1.8292380000	-4.5344910000
Pd35	-1.8080690000	4.1959780000	-0.0241960000
P36	-1.7009700000	6.5204730000	0.0003280000
C37	-0.7384110000	8.3199110000	4.1874030000
C38	-0.2006170000	8.9263620000	3.0512190000
C39	-0.4648050000	8.4053460000	1.7822470000
C40	-1.2696140000	7.2663330000	1.6351310000
C41	-1.7913650000	6.6522690000	2.7856970000
C42	-1.5361060000	7.1803380000	4.0506990000
H43	-0.5318800000	8.7276400000	5.1737150000
H44	0.4270610000	9.8089480000	3.1504390000
H45	-0.0397340000	8.8861160000	0.9051950000
H46	-2.3922760000	5.7514170000	2.6793030000
H47	-1.9521950000	6.6963940000	4.9310600000
C48	1.6058880000	8.2007540000	-2.8244630000
C49	1.7952590000	7.0216080000	-2.0990180000
C50	0.7839840000	6.5380990000	-1.2695640000

C51	-0.4277000000	7.2359270000	-1.1368160000
C52	-0.6102430000	8.4177550000	-1.8702230000
C53	0.4000260000	8.8936550000	-2.7105330000
H54	2.3897610000	8.5722010000	-3.4796150000
H55	2.7285290000	6.4711070000	-2.1872770000
H56	0.9218880000	5.6073430000	-0.7237310000
H57	-1.5440280000	8.9671380000	-1.7916310000
H58	0.2412840000	9.8081060000	-3.2772740000
C59	-5.6302850000	8.6739190000	-1.2705800000
C60	-4.7710000000	9.3114490000	-0.3735470000
C61	-3.5862430000	8.6908930000	0.0270180000
C62	-3.2479450000	7.4201300000	-0.4657670000
C63	-4.1253150000	6.7835220000	-1.3569480000
C64	-5.3043220000	7.4084190000	-1.7620840000
H65	-6.5543190000	9.1575250000	-1.5781030000
H66	-5.0245700000	10.2930060000	0.0197950000
H67	-2.9303520000	9.1929960000	0.7320250000
H68	-3.8775100000	5.7886420000	-1.7209720000
H69	-5.9728860000	6.9021160000	-2.4540020000

PhCl

Gas phase energy(Lacvp*): -691.8367583 au
Gas phase energy (Lacv3p**+): -691.93368487914au
Solvation energy: -0.004091739 au
Total Gibbs free energy: -691.8833882au
Dispersion energy: -0.00707780 au
ZPE: 239.57 kJ/mol

C1	5.1016010000	-1.4295500000	-1.2960500000
C2	4.4065730000	-0.2186400000	-1.2960510000
C3	3.0103850000	-0.2221970000	-1.2960480000
C4	2.3050270000	-1.4269780000	-1.2960480000
C5	3.0167210000	-2.6259250000	-1.2960460000
C6	4.4108980000	-2.6427820000	-1.2960460000
H7	6.1882170000	-1.4362610000	-1.2960520000
H8	4.9496550000	0.7219740000	-1.2960530000
H9	2.4612600000	0.7154780000	-1.2960470000
H10	1.2201370000	-1.4387230000	-1.2960500000
Cl11	2.1366120000	-4.1502330000	-1.2960570000
H12	4.9431910000	-3.5881890000	-1.2960450000

Neutral square planar complex ClPdPh(PPh_3)$_2$

Gas phase energy (Lacvp*): -2891.21999899793 au
Gas phase energy (Lacv3p**+): -2891.74908698664au
Solvation energy: -0.025561002 au
Total Gibbs free energy -2891.338957au
Dispersion energy: -0.12752798 au
ZPE: 1691.45 kJ/mol

Pd1	1.2314610000	0.9356940000	0.3705200000
Cl2	1.3189780000	3.2933580000	0.8980100000
P3	1.3891270000	-1.4121010000	0.5610430000
P4	-1.2239440000	1.3484790000	-0.3252620000
C5	4.8730860000	-2.9994060000	3.2299050000
C6	5.1106010000	-2.6108290000	1.9097430000
C7	4.0658530000	-2.1503030000	1.1100020000
C8	2.7564620000	-2.0793470000	1.6155410000
C9	2.5273720000	-2.4702590000	2.9434790000
C10	3.5787920000	-2.9237920000	3.7430490000
H11	5.6902200000	-3.3533710000	3.8530620000
H12	6.1160000000	-2.6536170000	1.4993280000
H13	4.2784420000	-1.8307330000	0.0954770000

H14	1.5282520000	-2.4260020000	3.3636420000
H15	3.3784430000	-3.2219740000	4.7692260000
C16	-2.3224040000	-3.0517610000	2.8483670000
C17	-1.8223970000	-1.7735250000	3.1061560000
C18	-0.7220410000	-1.2949540000	2.3916960000
C19	-0.1042420000	-2.0894760000	1.4122590000
C20	-0.6117840000	-3.3726960000	1.1610000000
C21	-1.7137800000	-3.8479040000	1.8745920000
H22	-3.1821060000	-3.4239870000	3.3994230000
H23	-2.2925950000	-1.1395420000	3.8529770000
H24	-0.3485710000	-0.2927680000	2.5863490000
H25	-0.1551240000	-4.0009490000	0.4023930000
H26	-2.0987930000	-4.8432600000	1.6665400000
C27	1.6710280000	-3.7635050000	-3.4443400000
C28	2.1521340000	-4.3504230000	-2.2717280000
C29	2.0877490000	-3.6597330000	-1.0609470000
C30	1.5391370000	-2.3673890000	-1.0083230000
C31	1.0658480000	-1.7835990000	-2.1926910000
C32	1.1268290000	-2.4790840000	-3.4008800000
H33	1.7256890000	-4.3029980000	-4.3862870000
H34	2.5832390000	-5.3481170000	-2.2978360000
H35	2.4768640000	-4.1227800000	-0.1590770000
H36	0.6468930000	-0.7822200000	-2.1663880000
H37	0.7504110000	-2.0123340000	-4.3071580000
C38	-3.3233360000	-1.8443720000	-3.0147670000
C39	-2.8226410000	-0.6728790000	-3.5817810000
C40	-2.2246880000	0.3000180000	-2.7784050000
C41	-2.1127530000	0.1153150000	-1.3907340000
C42	-2.6175280000	-1.0717180000	-0.8318820000
C43	-3.2204080000	-2.0380990000	-1.6361420000
H44	-3.7924870000	-2.5994790000	-3.6405270000
H45	-2.9033500000	-0.5063720000	-4.6533750000
H46	-1.8521780000	1.2105800000	-3.2361270000
H47	-2.5518950000	-1.2409870000	0.2373030000
H48	-3.6082760000	-2.9455900000	-1.1801110000
C49	-1.2771080000	5.0908120000	-3.0875500000
C50	-0.1478910000	4.2736710000	-3.0157910000
C51	-0.1365400000	3.1677520000	-2.1658690000
C52	-1.2621190000	2.8559910000	-1.3894200000
C53	-2.3923510000	3.6817730000	-1.4679000000
C54	-2.3972380000	4.7942770000	-2.3098610000
H55	-1.2799860000	5.9613150000	-3.7389920000
H56	0.7355670000	4.5078410000	-3.6040780000
H57	0.7614680000	2.5630560000	-2.0821800000
H58	-3.2685220000	3.4656030000	-0.8638800000
H59	-3.2766300000	5.4321960000	-2.3533440000
C60	-4.1734320000	2.4063390000	3.1168910000
C61	-4.6661900000	1.7731570000	1.9750550000
C62	-3.8031710000	1.4374300000	0.9302090000
C63	-2.4329790000	1.7284190000	1.0193140000
C64	-1.9437800000	2.3678440000	2.1713360000
C65	-2.8125910000	2.7049840000	3.2099010000
H66	-4.8475910000	2.6687610000	3.9286850000
H67	-5.7255180000	1.5416620000	1.8926390000
H68	-4.2007960000	0.9454970000	0.0479370000
H69	-0.8887610000	2.6225320000	2.2366030000
H70	-2.4222490000	3.2059390000	4.0924050000
C71	6.0548820000	1.2455340000	0.3170380000
C72	5.3306020000	0.9282880000	-0.8328950000
C73	3.9365200000	0.7932860000	-0.7749220000

C74	3.2601720000	0.9850200000	0.4361850000
C75	3.9856650000	1.3108110000	1.5849950000
C76	5.3766560000	1.4361240000	1.5239660000
H77	7.1363650000	1.3505370000	0.2728040000
H78	5.8451240000	0.7833560000	-1.7811170000
H79	3.3900590000	0.5391440000	-1.6808180000
H80	3.4709370000	1.4923940000	2.5236840000
H81	5.9301520000	1.6959820000	2.4242490000

Triphenyl phosphine PPh_3

Gas phase energy (Lacvp*): -1036.280921 au
Gas phase energy (Lacv3p**+): -1036.49765481998au
Solvation energy: -0.009649431 au
Total Gibbs free energy: -1036.309845au
Dispersion energy: -0.03110061 au
ZPE: 721.28 kJ/mol

P1	-1.7474322983	1.8933568296	-0.0158068355
C5	-5.6073816216	-0.2789097895	1.4475767054
C6	-4.3660757010	-0.7920983362	1.8258914220
C7	-3.1887444869	-0.1719201690	1.4025273254
C8	-3.2366679080	0.9758392934	0.5968852379
C9	-4.4926904666	1.4913147425	0.2361931762
C10	-5.6681007186	0.8651020026	0.6494421192
H11	-6.5225453826	-0.7640406252	1.7773302170
H12	-4.3118060316	-1.6805030558	2.4505157662
H13	-2.2290935452	-0.5833203957	1.7008683558
H14	-4.5483076015	2.3918847691	-0.3715126356
H15	-6.6310398159	1.2751512399	0.3554741441
C15	1.6389869954	0.2654691329	2.7483031601
C16	1.4049135527	-0.3724781536	1.5295140406
C17	0.3961094099	0.0832219259	0.6782732643
C18	-0.3914806075	1.1889586513	1.0329946957
C19	-0.1349595557	1.8319519899	2.2553777274
C20	0.8648291685	1.3695424943	3.1104463370
H21	2.4239306164	-0.0918610483	3.4099230395
H22	2.0068392949	-1.2303944992	1.2396905981
H23	0.2214691220	-0.4242845861	-0.2657176624
H24	-0.7228414395	2.7029219638	2.5367545072
H25	1.0450325778	1.8762182129	4.0552002540
C25	-0.8632747437	0.0169180415	-4.1942480322
C26	-1.7365489438	-0.6481441472	-3.3326564620
C27	-2.0205475253	-0.1196977074	-2.0717199025
C28	-1.4373070482	1.0867894001	-1.6555974155
C29	-0.5723551784	1.7542262363	-2.5387231260
C30	-0.2798990169	1.2203833620	-3.7933553826
H31	-0.6427205151	-0.3970504472	-5.1748533591
H32	-2.1973350547	-1.5837729242	-3.6402773693
H33	-2.6991855422	-0.6488466072	-1.4094381512
H34	-0.1272945824	2.7008782372	-2.2401755026
H35	0.3964081329	1.7480966125	-4.4611023490

T-shaped cationic complex $PhPd(PPh_3)_2$

Gas phase energy (Lacvp*): -2430.80588378064 au
Gas phase energy (Lacv3p**+): -2431.29006657570au
Solvation energy: -0.047626219 au
Total Gibbs free energy: -2430.88945au
Dispersion energy: -0.11354057 au
ZPE: 1689.11 kJ/mol

Pd1	0.9759453342	0.4560671834	-0.2154337175
P2	1.4186954098	-1.6342545224	0.6688095610

P3	-1.3791950990	1.1720452441	-0.1469940455
C4	3.9989497737	-1.7602847263	4.5371994483
C5	4.3688761863	-0.9377798973	3.4690907916
C6	3.5854954578	-0.8842605755	2.3152366900
C7	2.4190062235	-1.6617226589	2.2118566858
C8	2.0571622026	-2.4945619270	3.2864257627
C9	2.8434184848	-2.5382577304	4.4402357868
H10	4.6066523044	-1.7927647116	5.4383254664
H11	5.2681276328	-0.3297753331	3.5349922853
H12	3.8830124845	-0.2363005303	1.4976007279
H13	1.1680821179	-3.1124856709	3.2306724451
H14	2.5484814448	-3.1852833259	5.2628594197
C15	-2.5685995002	-3.7023675171	1.8811874600
C16	-2.2029727452	-2.4705036243	2.4349562135
C17	-1.0118273346	-1.8548086811	2.0520796811
C18	-0.1604421588	-2.4679878692	1.1145950894
C19	-0.5284676238	-3.7092050152	0.5691425620
C20	-1.7292262151	-4.3171722943	0.9503667548
H21	-3.5003915934	-4.1788330518	2.1759584709
H22	-2.8475369966	-1.9873373147	3.1646495909
H23	-0.7451479069	-0.8968013276	2.4895971546
H24	0.1152981169	-4.2106578456	-0.1463535508
H25	-2.0020498753	-5.2775080881	0.5193207593
C26	3.4103413378	-4.4355678489	-2.4344181304
C27	3.9425438216	-4.3502392099	-1.1468273725
C28	3.3588987211	-3.5086603156	-0.1965453033
C29	2.2365006905	-2.7403207263	-0.5378780556
C30	1.7084256150	-2.8241749463	-1.8388600742
C31	2.2893767200	-3.6731992522	-2.7795575916
H32	3.8680178117	-5.0921040205	-3.1699959224
H33	4.8144997634	-4.9406597144	-0.8756588323
H34	3.7801921506	-3.4568670617	0.8026327403
H35	0.8421005307	-2.2267424457	-2.1160437618
H36	1.8720755133	-3.7341011339	-3.7815166960
C37	-4.5475499269	-0.5543140616	-3.0566775708
C38	-4.4067107279	0.8315351519	-2.9382415734
C39	-3.4574654894	1.3683377960	-2.0670878542
C40	-2.6379415060	0.5176076057	-1.3048131083
C41	-2.7825774740	-0.8740170879	-1.4314988783
C42	-3.7361462380	-1.4054513205	-2.3023059214
H43	-5.2856023506	-0.9694444862	-3.7388939367
H44	-5.0348706205	1.4970510703	-3.5257235177
H45	-3.3542795570	2.4472660807	-1.9869837041
H46	-2.1516290458	-1.5420514819	-0.8513938119
H47	-3.8422334059	-2.4835737500	-2.3950919820
C48	0.3335877323	5.0472109391	-2.0605795680
C49	0.3575578150	3.8329406299	-2.7503087691
C50	-0.2023557629	2.6909927617	-2.1731790143
C51	-0.8029993242	2.7546766685	-0.8962415195
C52	-0.8198652979	3.9826106789	-0.2118333035
C53	-0.2578841066	5.1192040762	-0.7944754338
H54	0.7688403985	5.9368370444	-2.5092415348
H55	0.8062475607	3.7729635427	-3.7390363002
H56	-0.2030232563	1.7572801626	-2.7332553724
H57	-1.2794096100	4.0556950619	0.7699127526
H58	-0.2874196872	6.0661605091	-0.2605685627
C59	-3.4859742683	2.3467930309	3.8164802227
C60	-4.2590353638	2.0857420488	2.6828492533
C61	-3.6470853324	1.7308822659	1.4783583387
C62	-2.2494534254	1.6303555085	1.3999636220

C63	-1.4786688366	1.8823875779	2.5491451842
C64	-2.0931150786	2.2473412092	3.7479660653
H65	-3.9669063550	2.6232663234	4.7518977019
H66	-5.3428907256	2.1581743662	2.7332164334
H67	-4.2622168758	1.5323693538	0.6056469874
H68	-0.3939836156	1.7986822800	2.5052625045
H69	-1.4866091425	2.4473059230	4.6282328516
C70	5.2322780598	1.9367850191	-1.7081316082
C71	4.6685755488	0.8309756239	-2.3514035382
C72	3.5184320926	0.2181729377	-1.8361201402
C73	2.9170573297	0.7406563268	-0.6865106848
C74	3.4975872164	1.8302350678	-0.0179831082
C75	4.6484073588	2.4343947271	-0.5398288119
H76	6.1294315112	2.4018891914	-2.1091605540
H77	5.1241788545	0.4373604568	-3.2577696884
H78	3.1018690041	-0.6481909695	-2.3418454264
H79	3.0624889150	2.2205967444	0.9010438210
H80	5.0889462474	3.2851363959	-0.0235039748

Styrene

Gas phase energy (Lacvp*): -309.6414579 au
Gas phase energy (Lacv3p**+): -309.73031765162
Solvation energy: -0.006102132au
Total Gibbs free energy: -309.6429208au
Dispersion energy: -0.00903992 au
ZPE: 351.64 kJ/mol

C1	-1.0954740000	2.8700110000	0.3389630000
C2	0.2157350000	2.9570520000	0.0804690000
H3	-1.8485220000	2.8014240000	-0.4415230000
H4	0.9003980000	3.0252860000	0.9262960000
H5	-1.4631270000	2.8645620000	1.3605090000
X6	-0.6757010000	2.8409580000	0.0000000000
C7	2.2379370000	3.0312840000	-3.7062100000
C8	2.9502620000	3.1255300000	-2.5110290000
C9	2.2739360000	3.0985330000	-1.2921520000
C10	0.8747090000	2.9782900000	-1.2365230000
C11	0.1717290000	2.8834860000	-2.4518210000
C12	0.8453760000	2.9100360000	-3.6691210000
H13	2.7602960000	3.0513660000	-4.6590630000
H14	4.0331430000	3.2196890000	-2.5258950000
H15	2.8357170000	3.1723380000	-0.3632560000
H16	-0.9102500000	2.7871760000	-2.4450580000
H17	0.2828560000	2.8347740000	-4.5962700000

Cationic square planar pre-insertion complex

Gas phase energy (Lacvp*): -2740.45662925826 au
Gas phase energy (Lacv3p**+): -2741.02447399979au
Solvation energy: -0.0509727au
Total Gibbs free energy: -2740.533244
Dispersion energy: -0.15468795au
ZPE: 2049.06 kJ/mol

Pd1	14.6027162322	0.2638853364	-0.5482527793
P2	14.5718136872	-2.1311273347	-0.6682806963
P3	12.1532883083	0.7937945451	-1.2612877731
C4	17.9993658049	-4.6483247567	1.2285000583
C5	18.1795737182	-4.0197068552	-0.0058558677
C6	17.1522278257	-3.2656488122	-0.5689438819
C7	15.9211826122	-3.1314712210	0.0947411737

C8	15.7470974902	-3.7655399683	1.3341482782
C9	16.7812529793	-4.5174897364	1.8945660616
H10	18.8007072626	-5.2388972400	1.6635713181
H11	19.1232890044	-4.1170915786	-0.5355695913
H12	17.3117482280	-2.7867072073	-1.5294490292
H13	14.8037724502	-3.6891566511	1.8644154579
H14	16.6258652980	-5.0083675092	2.8516054343
C15	10.8961532413	-3.9375873552	1.5349276565
C16	11.5194776741	-2.7809754892	2.0074076013
C17	12.5985648298	-2.2332657696	1.3105813143
C18	13.0692700684	-2.8344144475	0.1330664450
C19	12.4372932740	-3.9966390794	-0.3352233740
C20	11.3593277877	-4.5419002330	0.3635099156
H21	10.0554812892	-4.3648631675	2.0743198286
H22	11.1644023109	-2.2985179318	2.9137514624
H23	13.0719336931	-1.3289256408	1.6825556624
H24	12.7723523129	-4.4736064806	-1.2500974436
H25	10.8789923614	-5.4416921900	-0.0118778180
C26	14.5764267173	-3.4837327167	-5.1105047828
C27	14.8226192228	-4.4168166355	-4.1008957805
C28	14.8331927606	-4.0193714330	-2.7650958851
C29	14.5831732266	-2.6779010533	-2.4225621868
C30	14.3476914248	-1.7487948327	-3.4447793114
C31	14.3433224621	-2.1491059407	-4.7809804878
H32	14.5751415118	-3.7963015418	-6.1511741114
H33	15.0166161362	-5.4555981775	-4.3537545893
H34	15.0559486627	-4.7495885658	-1.9930322749
H35	14.1739651939	-0.7073755458	-3.1908478518
H36	14.1601603013	-1.4174984800	-5.5631143466
C37	9.5930421957	-2.0442914454	-3.9392199100
C38	10.1750303590	-0.9073076292	-4.4977149914
C39	10.9328530314	-0.0422781043	-3.7076927441
C40	11.1251661654	-0.3065733392	-2.3430084150
C41	10.5345868217	-1.4547033917	-1.7891096430
C42	9.7728615055	-2.3120917898	-2.5818240734
H43	8.9966429854	-2.7120829046	-4.5549557880
H44	10.0299893847	-0.6799931311	-5.5506403239
H45	11.3496859406	0.8497235520	-4.1615317364
H46	10.6493913843	-1.6745894176	-0.7337710905
H47	9.3157854037	-3.1892210831	-2.1317720548
C48	12.0691170883	4.8493749399	-3.5623316560
C49	12.8766471113	3.7956774539	-3.9952589839
C50	12.8928787741	2.5935486006	-3.2887320009
C51	12.0886337868	2.4153594165	-2.1473030992
C52	11.2815393883	3.4816057106	-1.7242284130
C53	11.2767618105	4.6892630379	-2.4263358757
H54	12.0613471906	5.7896991683	-4.1063166307
H55	13.4996279612	3.9111137315	-4.8781165195
H56	13.5368871109	1.7868464645	-3.6343050584
H57	10.6507609691	3.3753282932	-0.8478075129
H58	10.6471590639	5.5053288535	-2.0818980820
C59	9.5301484180	1.5045433785	2.5132920623
C60	8.9159091690	1.3095175644	1.2743608173
C61	9.6875674735	1.0822118262	0.1351490588
C62	11.0893774741	1.0449788593	0.2219451624
C63	11.6956410013	1.2368532429	1.4728110332
C64	10.9215415194	1.4684516429	2.6113238813
H65	8.9252088148	1.6805020607	3.3986986543
H66	7.8325484511	1.3350000841	1.1933005859
H67	9.1972343590	0.9291733471	-0.8215323697

H68	12.7785584186	1.1994706376	1.5605425607
H69	11.4062463801	1.6134047481	3.5733497545
C70	14.7304154258	2.9478434490	0.2082586145
C71	15.3787365947	2.5388207390	-0.9235719433
H72	16.4562329018	2.4390808734	-0.9562874451
C73	19.1349463325	-0.1167084628	1.0941008884
C74	18.0516970238	-0.2043118571	1.9695700377
C75	16.7400046296	-0.1431701605	1.4824846139
C76	16.5109218479	0.0066974728	0.1118934722
C77	17.5949896195	0.0800535911	-0.7710327750
C78	18.9036828526	0.0271515935	-0.2764158765
H79	20.1514361773	-0.1668283360	1.4746135999
H80	18.2204862094	-0.3225733255	3.0373175299
H81	15.9111173409	-0.2201685650	2.1819313893
H82	17.4348596875	0.1880323005	-1.8417184322
H83	19.7410085961	0.0948956495	-0.9673403121
H84	13.6629094179	3.1449658572	0.1233630767
H85	14.8633881675	2.5796922669	-1.8763984029
C86	16.3143631496	3.9739748288	4.0398286174
C87	17.1877940903	3.5819951250	3.0206576794
C88	16.6945646302	3.2288057276	1.7697234580
C89	15.3098129644	3.2628293442	1.5134393016
C90	14.4435148814	3.6660072365	2.5487657755
C91	14.9393615067	4.0159872572	3.8012212416
H92	18.2582909543	3.5535280741	3.2035616947
H93	17.3868692793	2.9292239733	0.9904585966
H94	13.3735728587	3.7105047165	2.3598137403
H95	14.2575125486	4.3283441181	4.5873342106
H96	16.7063611683	4.2511979422	5.0147378917

Carbopalladation step: TS for linear product (Stilbene)

Gas phase energy(Lacvp*): -2740.42852 au
Gas phase energy (Lacv3p**+): -2740.99372528539au
Solvation energy: -0.0517406au
Total Gibbs free energy: -2740.504545au
Dispersion energy: -0.15431073au
ZPE: 2042.89 kJ/mol
Neg freq: -332.71 cm^{-1}

Pd1	14.7759920000	0.4293470000	-0.4875180000
P2	14.6134020000	-2.1118960000	-0.6205960000
P3	12.3013250000	0.9550710000	-0.9597390000
C4	18.0117190000	-4.6094280000	1.4724940000
C5	18.0918030000	-4.3346240000	0.1035910000
C6	17.0901870000	-3.5869180000	-0.5277250000
C7	15.9904860000	-3.1191940000	0.2073480000
C8	15.9164510000	-3.3912400000	1.5838810000
C9	16.9236770000	-4.1311670000	2.2122190000
H10	18.7864070000	-5.1935190000	1.9581340000
H11	18.9316640000	-4.7013030000	-0.4776010000
H12	17.1726910000	-3.3757170000	-1.5866130000
H13	15.0682070000	-3.0506790000	2.1667800000
H14	16.8500210000	-4.3435540000	3.2738200000
C15	10.8959350000	-3.8944450000	1.6391600000
C16	11.5457360000	-2.7480600000	2.1104280000
C17	12.6366480000	-2.2224470000	1.4066670000
C18	13.0877370000	-2.8404630000	0.2287560000
C19	12.4298130000	-3.9864060000	-0.2426410000
C20	11.3391470000	-4.5100140000	0.4619050000
H21	10.0508170000	-4.3036080000	2.1825440000
H22	11.2026780000	-2.2567670000	3.0146530000

H23	13.1245310000	-1.3242050000	1.7700740000
H24	12.7493600000	-4.4654460000	-1.1596070000
H25	10.8382740000	-5.3982860000	0.0908440000
C26	14.5488940000	-3.6013080000	-5.0710300000
C27	14.7453490000	-4.5296080000	-4.0412960000
C28	14.7734650000	-4.1069290000	-2.7076880000
C29	14.5984680000	-2.7463110000	-2.3930740000
C30	14.4095920000	-1.8211230000	-3.4313120000
C31	14.3830500000	-2.2466620000	-4.7646050000
H32	14.5301840000	-3.9322030000	-6.1040350000
H33	14.8815070000	-5.5805030000	-4.2741560000
H34	14.9512120000	-4.8338320000	-1.9227970000
H35	14.2791310000	-0.7706420000	-3.1947510000
H36	14.2328320000	-1.5229200000	-5.5587550000
C37	9.8793980000	-1.8480270000	-3.8726270000
C38	10.5268240000	-0.7141630000	-4.3744060000
C39	11.2433340000	0.1275770000	-3.5154050000
C40	11.3209840000	-0.1616300000	-2.1432990000
C41	10.6693820000	-1.3012430000	-1.6425380000
C42	9.9514910000	-2.1369890000	-2.5057320000
H43	9.3193830000	-2.4959580000	-4.5385560000
H44	10.4664770000	-0.4739890000	-5.4308860000
H45	11.7153730000	1.0142360000	-3.9206430000
H46	10.7060430000	-1.5355800000	-0.5862140000
H47	9.4480740000	-3.0100620000	-2.1044090000
C48	12.0239570000	5.0940670000	-3.1927060000
C49	12.9820610000	4.1419060000	-3.5615660000
C50	13.0581740000	2.9237450000	-2.8764190000
C51	12.1673080000	2.6383550000	-1.8241530000
C52	11.2108960000	3.5977700000	-1.4587820000
C53	11.1438130000	4.8208560000	-2.1404600000
H54	11.9668440000	6.0405660000	-3.7192700000
H55	13.6697460000	4.3472700000	-4.3753680000
H56	13.8154850000	2.1971950000	-3.1600710000
H57	10.5182970000	3.4000240000	-0.6491250000
H58	10.4007620000	5.5555940000	-1.8486160000
C59	9.5082800000	1.3320440000	2.7940780000
C60	8.9413150000	1.2249030000	1.5178680000
C61	9.7621670000	1.1046140000	0.3908270000
C62	11.1612190000	1.0901490000	0.5351020000
C63	11.7240070000	1.1951120000	1.8163400000
C64	10.8995720000	1.3174850000	2.9418040000
H65	8.8691560000	1.4254790000	3.6658040000
H66	7.8630430000	1.2334810000	1.3981050000
H67	9.3121810000	1.0104920000	-0.5912890000
H68	12.8010580000	1.1894250000	1.9376330000
H69	11.3458120000	1.4053180000	3.9267740000
C70	15.1739990000	2.6292420000	-0.1021480000
C71	16.4658240000	2.2587570000	-0.5651290000
H72	17.3259870000	2.4573300000	0.0622130000
C73	19.4697250000	-0.9914720000	-0.4594900000
C74	18.8154910000	-0.7202850000	0.7490870000
C75	17.5583020000	-0.1066490000	0.7476550000
C76	16.9402980000	0.2470930000	-0.4692500000
C77	17.5940360000	-0.0536980000	-1.6817180000
C78	18.8498670000	-0.6722140000	-1.6743940000
H79	20.4532240000	-1.4490610000	-0.4543030000
H80	19.2826230000	-0.9839090000	1.6922100000
H81	17.0705300000	0.1061240000	1.6928000000
H82	17.1411040000	0.2229700000	-2.6291100000

H83	19.3484150000	-0.8859280000	-2.6146650000
H84	14.4958070000	3.0307760000	-0.8477670000
H85	16.6597650000	2.3722180000	-1.6258330000
C86	14.3779630000	4.0588410000	3.8762450000
C87	15.4843040000	3.2291490000	3.6497000000
C88	15.7507760000	2.7438550000	2.3677380000
C89	14.9071810000	3.0677430000	1.2815830000
C90	13.7975880000	3.9073650000	1.5273590000
C91	13.5396780000	4.4006150000	2.8076720000
H92	16.1464600000	2.9720390000	4.4699790000
H93	16.6265930000	2.1245540000	2.2111240000
H94	13.1460560000	4.1819720000	0.7038770000
H95	12.6888920000	5.0535740000	2.9712420000
H96	14.1799550000	4.4436570000	4.8709360000

Cationic post-insertion complex (after TS leading to stilbene)

Gas phase energy (Lacvp*): -2740.467695 au
Gas phase energy (Lacv3p**+): -2741.03266906851au
Solvation energy: -0.0512306 au
Total Gibbs free energy: -2740.543442au
Dispersion energy: -0.15850777 au
ZPE: 1835.132608 kJ/mol

Pd1	14.6199774816	0.2824226801	-0.3107037244
P2	14.5993674481	-2.2194357678	-0.8992965552
P3	12.4221532002	0.9540727603	-0.9064695333
C4	18.5840687177	-4.6311467253	-0.6441619404
C5	18.4027373770	-3.6301288378	-1.6028702382
C6	17.2151912609	-2.9022040320	-1.6409255631
C7	16.1825191317	-3.1657476492	-0.7243634493
C8	16.3731537761	-4.1675039589	0.2364272643
C9	17.5671270414	-4.8942359798	0.2735143247
H10	19.5062107995	-5.2056230223	-0.6204962646
H11	19.1843576739	-3.4214685604	-2.3288952697
H12	17.0839602721	-2.1406558366	-2.4059891639
H13	15.5882060919	-4.3973123027	0.9500718590
H14	17.6937847476	-5.6761845968	1.0178023122
C15	11.7654827879	-4.5110621419	2.0033612998
C16	12.4660294631	-3.3730008304	2.4068094098
C17	13.2886604573	-2.6997375892	1.5019240108
C18	13.4319177820	-3.1560598218	0.1805485016
C19	12.7168953922	-4.2962521956	-0.2163718062
C20	11.8923169688	-4.9663070701	0.6892359186
H21	11.1234336772	-5.0359306701	2.7049947000
H22	12.3700242005	-3.0043402803	3.4248266585
H23	13.8235833489	-1.8102545058	1.8245781554
H24	12.7850013196	-4.6595309224	-1.2357863498
H25	11.3467301005	-5.8481145623	0.3635591109
C26	13.8691539154	-3.1369599835	-5.4010392586
C27	14.1307155217	-4.1862787333	-4.5163186554
C28	14.3290175577	-3.9282357631	-3.1622904710
C29	14.2394607591	-2.6152251935	-2.6636577589
C30	13.9923428279	-1.5722588407	-3.5640753630
C31	13.8092659560	-1.8293465423	-4.9242035725
H32	13.7277019622	-3.3395268238	-6.4592723103
H33	14.2003466928	-5.2060251942	-4.8855066579
H34	14.5915579649	-4.7476238509	-2.5001135827
H35	13.9536305388	-0.5509743938	-3.1992497975
H36	13.6233453887	-1.0060521096	-5.6089319951
C37	9.5994551741	-2.0107515393	-3.1140754591
C38	10.0824189408	-0.8909403006	-3.7897606686

C39	10.9444189535	0.0001669780	-3.1499196200
C40	11.3322626488	-0.2225911655	-1.8202933204
C41	10.8400813824	-1.3517448409	-1.1460031587
C42	9.9806007144	-2.2385126987	-1.7906830830
H43	8.9247878348	-2.7003538246	-3.6139661972
H44	9.7835165422	-0.7016000490	-4.8170033034
H45	11.2977154748	0.8731962327	-3.6878442227
H46	11.1119368794	-1.5333506948	-0.1119653958
H47	9.6060180783	-3.1053787354	-1.2538349767
C48	12.3268247088	4.6331731081	-3.7492467064
C49	13.3047864719	3.6467752332	-3.8861990828
C50	13.3322995441	2.5642392764	-3.0063378918
C51	12.3751632605	2.4470879030	-1.9845680791
C52	11.3945605332	3.4421722327	-1.8575366108
C53	11.3752802117	4.5284672292	-2.7337473492
H54	12.3093375711	5.4814717006	-4.4277257370
H55	14.0514595812	3.7229549519	-4.6720772831
H56	14.1085206405	1.8092031882	-3.1124719355
H57	10.6507313465	3.3809447775	-1.0696986889
H58	10.6136458866	5.2950380914	-2.6195634776
C59	9.8773621986	1.8352171007	2.8791363444
C60	9.2534851777	1.6830255546	1.6389304101
C61	10.0115738146	1.4139949991	0.5009282884
C62	11.4116437443	1.3059788418	0.5893716711
C63	12.0260318534	1.4540478854	1.8398733946
C64	11.2630515401	1.7168081375	2.9779526693
H65	9.2826946612	2.0396289881	3.7653807321
H66	8.1729815795	1.7640082147	1.5575783497
H67	9.5098776704	1.2693130134	-0.4511978806
H68	13.1040778065	1.3714717286	1.9212952467
H69	11.7548974063	1.8323266811	3.9398661690
C70	15.2991379072	2.3653729418	-0.0932348389
C71	16.7669075836	1.9376559001	-0.1037207351
H72	17.3969628322	2.7336685899	0.3232390668
C73	17.8105662268	-1.6321616167	2.1636380079
C74	16.6542478949	-0.9362276279	2.4893327760
C75	16.2744594307	0.1967785817	1.7495336147
C76	17.0443828162	0.6283840955	0.6462853742
C77	18.1964854130	-0.1121731180	0.3178003487
C78	18.5872482520	-1.2067747757	1.0764684032
H79	18.1201910813	-2.4918456853	2.7503540802
H80	16.0527850246	-1.2422353806	3.3410419399
H81	15.4420966260	0.7928255968	2.1067835111
H82	18.8065238012	0.2053626368	-0.5251362341
H83	19.4940685678	-1.7446239247	0.8170468019
H84	14.9744404910	2.7452902936	-1.0596705742
H85	17.1011684538	1.8112115378	-1.1396680503
C86	14.1195877820	5.1559637341	2.9788010852
C87	15.1825956298	4.2810014613	3.2077833639
C88	15.5652992752	3.3650336334	2.2303665570
C89	14.8835329114	3.2817921664	0.9964155336
C90	13.8301433061	4.1955422034	0.7791879093
C91	13.4521291424	5.1139780429	1.7525177192
H92	15.7321365737	4.3249168150	4.1445210083
H93	16.4235185461	2.7309672709	2.4273606875
H94	13.3157879060	4.1931055215	-0.1758417593
H95	12.6412996183	5.8089017002	1.5499772160
H96	13.8283940356	5.8764645495	3.7382978704

Agostic cationic complex (leading to stilbene)

Gas phase energy (Lacvp*): -2740.486176 au
Gas phase energy (Lacv3p**+): -2741.05325011595au
Solvation energy: -0.051463915 au
Total Gibbs free energy: -2740.559024au
Dispersion energy: -0.14561895 au
ZPE: 2050.43 kJ/mol

Pd1	0.7271500000	1.0770680000	0.8210680000
P2	1.4974150000	-1.1791960000	0.0470090000
P3	-1.1891250000	1.5365350000	-0.4244300000
C4	5.9745790000	-0.2148110000	-0.7881760000
C5	4.9520900000	0.5814370000	-1.3105870000
C6	3.6176700000	0.2683610000	-1.0493860000
C7	3.2864210000	-0.8596800000	-0.2746050000
C8	4.3186190000	-1.6551400000	0.2425730000
C9	5.6532240000	-1.3292520000	-0.0117150000
H10	7.0138630000	0.0324490000	-0.9851610000
H11	5.1932810000	1.4477560000	-1.9212390000
H12	2.8287650000	0.8950420000	-1.4613620000
H13	4.0865910000	-2.5274680000	0.8458570000
H14	6.4434790000	-1.9529800000	0.3972660000
C15	1.3077350000	-4.3713480000	3.4216910000
C16	1.0540400000	-3.0267050000	3.6967390000
C17	1.1082620000	-2.0817000000	2.6704180000
C18	1.4232900000	-2.4671090000	1.3577040000
C19	1.6692380000	-3.8245340000	1.0890910000
C20	1.6129190000	-4.7667540000	2.1163820000
H21	1.2608470000	-5.1094400000	4.2173110000
H22	0.8068510000	-2.7110360000	4.7067420000
H23	0.8958620000	-1.0380900000	2.8925240000
H24	1.8954920000	-4.1473770000	0.0769300000
H25	1.8048910000	-5.8132010000	1.8955410000
C26	-0.1195310000	-3.3947990000	-3.7160640000
C27	1.1250580000	-2.7668150000	-3.7683970000
C28	1.6315140000	-2.1041940000	-2.6476150000
C29	0.8939800000	-2.0607640000	-1.4558300000
C30	-0.3618740000	-2.6923830000	-1.4113270000
C31	-0.8601140000	-3.3567580000	-2.5312740000
H32	-0.5073880000	-3.9155600000	-4.5871890000
H33	1.7130340000	-2.7959760000	-4.6819220000
H34	2.6061740000	-1.6307040000	-2.7066990000
H35	-0.9518580000	-2.6768020000	-0.4994640000
H36	-1.8281880000	-3.8478410000	-2.4761040000
C37	-4.6321090000	-1.4295920000	0.4942800000
C38	-4.7815780000	-0.4741070000	-0.5146630000
C39	-3.7383530000	0.4000610000	-0.8110960000
C40	-2.5200940000	0.3128380000	-0.1138830000
C41	-2.3820460000	-0.6426080000	0.9021160000
C42	-3.4351930000	-1.5088270000	1.2056770000
H43	-5.4523030000	-2.1017450000	0.7311250000
H44	-5.7174870000	-0.3997370000	-1.0616690000
H45	-3.8784400000	1.1607400000	-1.5742010000
H46	-1.4540750000	-0.7017660000	1.4645450000
H47	-3.3187730000	-2.2400210000	2.0010510000
C48	0.0260580000	1.5034960000	-4.8979480000
C49	-0.9234260000	0.5885940000	-4.4451330000
C50	-1.3119560000	0.5778870000	-3.1039270000
C51	-0.7487180000	1.4901350000	-2.2012490000
C52	0.2245480000	2.3981450000	-2.6594730000
C53	0.6016000000	2.4070900000	-4.0012020000
H54	0.3203140000	1.5119980000	-5.9439520000

H55	-1.3662920000	-0.1244760000	-5.1347660000
H56	-2.0439690000	-0.1483460000	-2.7682810000
H57	0.6810790000	3.1061180000	-1.9726220000
H58	1.3433670000	3.1224640000	-4.3465580000
C59	-3.6714080000	5.3940430000	0.2977260000
C60	-3.0762280000	5.1970320000	-0.9471000000
C61	-2.3001980000	4.0599610000	-1.1875090000
C62	-2.1124130000	3.1088710000	-0.1762690000
C63	-2.7119790000	3.3164110000	1.0786320000
C64	-3.4882300000	4.4488930000	1.3118880000
H65	-4.2796570000	6.2761360000	0.4786860000
H66	-3.2178090000	5.9251740000	-1.7413160000
H67	-1.8530940000	3.9186340000	-2.1657440000
H68	-2.5897910000	2.5807820000	1.8705600000
H69	-3.9553520000	4.5922570000	2.2826140000
C70	0.9630950000	2.9365170000	1.8115420000
H71	0.1151310000	3.0364620000	2.4889770000
C72	2.1729510000	2.2665700000	2.4319370000
H73	3.0954650000	2.7356120000	2.0764690000
H74	2.2967770000	1.1897190000	2.0549080000
C75	1.6477420000	6.4779340000	-0.5301350000
C76	2.5294040000	5.3962860000	-0.6286770000
C77	2.3034360000	4.2383970000	0.1088630000
C78	1.1857870000	4.1287690000	0.9647210000
C79	0.3066420000	5.2241970000	1.0455680000
C80	0.5373580000	6.3854050000	0.3088710000
H81	1.8314590000	7.3858010000	-1.0982480000
H82	3.4006170000	5.4621820000	-1.2754120000
H83	3.0024830000	3.4098060000	0.0211970000
H84	-0.5575500000	5.1680580000	1.7012150000
H85	-0.1507110000	7.2216760000	0.3973880000
C86	2.2091150000	2.0460460000	6.7525310000
C87	2.5456230000	0.9227480000	5.9966930000
C88	2.5193740000	0.9829620000	4.6024660000
C89	2.1558420000	2.1653380000	3.9477970000
C90	1.8250290000	3.2912790000	4.7143070000
C91	1.8515050000	3.2311240000	6.1073160000
H92	2.2294490000	2.0003440000	7.8379070000
H93	2.8327250000	-0.0015210000	6.4911330000
H94	2.7935120000	0.1041090000	4.0220130000
H95	1.5606920000	4.2235220000	4.2205920000
H96	1.5955160000	4.1127240000	6.6889440000

β-elimination TS (leading to stilbene)

Gas phase energy (Lacvp*): -2740.473952 au
Gas phase energy (Lacv3p**+): -2741.04336785175au
Solvation energy: -0.051678056 au
Total Gibbs free energy -2740.554277au
Dispersion energy: -0.051678056 au
ZPE: 2040.3 kJ/mol
Neg Freq: -611.02 cm^{-1}

Pd1	0.8941833706	1.1618849269	0.8634643902
P2	1.6948130520	-0.9587212425	0.0595467329
P3	-1.1785266995	1.5468566327	-0.3803008600
C4	5.9190016131	-0.1179664092	-1.6795768852
C5	4.8786462487	0.7978437363	-1.8496743468
C6	3.6202066184	0.5339136785	-1.3090879331
C7	3.3842696109	-0.6578421406	-0.6033340224
C8	4.4343028035	-1.5721145069	-0.4365029057

C9	5.6945000793	-1.2989068858	-0.9709754373
H10	6.9012860110	0.0895428188	-2.0953087380
H11	5.0462708348	1.7201076495	-2.3999663309
H12	2.8173720340	1.2556256371	-1.4390812316
H13	4.2764671522	-2.4941604516	0.1138723374
H14	6.5018821613	-2.0127226643	-0.8317350468
C15	2.2162866560	-4.1742762409	3.3818356166
C16	2.0523839123	-2.8308326264	3.7218671062
C17	1.8784937089	-1.8688490574	2.7247879038
C18	1.8717626165	-2.2368844530	1.3711180345
C19	2.0289565427	-3.5949878031	1.0379740056
C20	2.2024975793	-4.5526001590	2.0367244105
H21	2.3476104942	-4.9233784489	4.1577314144
H22	2.0520493250	-2.5258205022	4.7648420875
H23	1.7394782102	-0.8294379389	3.0067313404
H24	2.0095803903	-3.9083754727	-0.0014050467
H25	2.3246076099	-5.5969679410	1.7620330303
C26	-0.5077972838	-3.2885276348	-3.3082223668
C27	0.6692528553	-2.5994851462	-3.5990309246
C28	1.3370908310	-1.8907567036	-2.5981980634
C29	0.8305854021	-1.8657156204	-1.2906269562
C30	-0.3600948477	-2.5560822140	-1.0077907667
C31	-1.0220402511	-3.2627753451	-2.0095475194
H32	-1.0214585279	-3.8455843471	-4.0873778938
H33	1.0774176795	-2.6161910280	-4.6061094495
H34	2.2570855046	-1.3688916209	-2.8402004676
H35	-0.7668672464	-2.5602503454	-0.0019691108
H36	-1.9366678784	-3.7999184510	-1.7726609635
C37	-4.5718575572	-1.2948358847	1.0230147938
C38	-4.8284647557	-0.3445543614	0.0305552700
C39	-3.8111323485	0.4994214002	-0.4107465855
C40	-2.5148780569	0.3886532634	0.1224186618
C41	-2.2713616087	-0.5583190422	1.1264997314
C42	-3.2950428821	-1.3960980438	1.5751717160
H43	-5.3698008023	-1.9452462753	1.3713713424
H44	-5.8259626555	-0.2520829723	-0.3907937425
H45	-4.0313082125	1.2570224316	-1.1577314988
H46	-1.2804708911	-0.6318592161	1.5678372522
H47	-3.0940074030	-2.1228157561	2.3579774946
C48	-0.4827510824	1.3884808189	-4.9718890758
C49	-1.4851292038	0.5945739130	-4.4138672171
C50	-1.7164321854	0.6077029905	-3.0361137094
C51	-0.9417962356	1.4209777674	-2.1993277742
C52	0.0845737229	2.2002394357	-2.7639552141
C53	0.3050494165	2.1899045024	-4.1412334197
H54	-0.3123588513	1.3803204976	-6.0449634286
H55	-2.0942793759	-0.0409766883	-5.0510966573
H56	-2.4941215415	-0.0249113901	-2.6219999717
H57	0.7034805549	2.8302738093	-2.1279656423
H58	1.0919427498	2.8083775707	-4.5651244819
C59	-3.3810735280	5.5843966099	0.3672216644
C60	-2.8408955428	5.3305525853	-0.8928843750
C61	-2.1716872461	4.1301099157	-1.1486755097
C62	-2.0404289475	3.1658957926	-0.1416901247
C63	-2.5927582298	3.4280899606	1.1250807568
C64	-3.2567000423	4.6266382973	1.3781907718
H65	-3.9024533014	6.5178035332	0.5615062196
H66	-2.9431011527	6.0653997641	-1.6871634440
H67	-1.7645485375	3.9496268569	-2.1378092485
H68	-2.5311629350	2.6802152051	1.9125044444

H69	-3.6842784478	4.8101462457	2.3605224626
C70	1.0198320960	3.1940985085	1.8533281561
H71	-0.0052412410	3.4337952202	2.1189753046
C72	1.7665918155	2.4040504920	2.7602777707
H73	2.8435934955	2.5610349613	2.7611540449
H74	2.1586044890	1.0026681793	1.8688088645
C75	2.8258020133	5.9729131825	-0.8728998451
C76	3.5631163825	4.8754135640	-0.4191121207
C77	2.9879287761	3.9519011046	0.4489607476
C78	1.6562464429	4.1088951411	0.8853728415
C79	0.9240308062	5.2143367751	0.4138359781
C80	1.5051572458	6.1372232524	-0.4532131816
H81	3.2802799697	6.6955860925	-1.5449280919
H82	4.5931822523	4.7416281175	-0.7390100101
H83	3.5774795287	3.1017399804	0.7814306701
H84	-0.1007350640	5.3567256376	0.7438752877
H85	0.9259638429	6.9905503234	-0.7951375588
C86	0.3481494072	1.0337266758	6.5711160029
C87	1.7070000931	1.2573538413	6.3494739037
C88	2.1488497888	1.6782110943	5.0954237817
C89	1.2386920497	1.8898712162	4.0472101012
C90	-0.1266463617	1.6530638113	4.2807026449
C91	-0.5658253273	1.2311879388	5.5319006322
H92	0.0011388030	0.7050108585	7.5467044103
H93	2.4245797328	1.1076979355	7.1513795854
H94	3.2092282666	1.8571755425	4.9293012182
H95	-0.8464498496	1.7870611405	3.4781071533
H96	-1.6246727248	1.0533770946	5.6988791339

Cationic product complex ($HPd(PPh_3)_2$Stilbene)

Gas phase energy (Lacvp*): -2740.478396 au
Gas phase energy (Lacv3p**+): -2741.04610388682au
Solvation energy: -0.051614277au
Total Gibbs free energy: -2740.557333 au
Dispersion energy: -0.14945505au
ZPE: 2044.45 kJ/mol

Pd1	0.8941833706	1.1618849269	0.8634643902
P2	1.6948130520	-0.9587212425	0.0595467329
P3	-1.1785266995	1.5468566327	-0.3803008600
C4	5.9190016131	-0.1179664092	-1.6795768852
C5	4.8786462487	0.7978437363	-1.8496743468
C6	3.6202066184	0.5339136785	-1.3090879331
C7	3.3842696109	-0.6578421406	-0.6033340224
C8	4.4343028035	-1.5721145069	-0.4365029057
C9	5.6945000793	-1.2989068858	-0.9709754373
H10	6.9012860110	0.0895428188	-2.0953087380
H11	5.0462708348	1.7201076495	-2.3999663309
H12	2.8173720340	1.2556256371	-1.4390812316
H13	4.2764671522	-2.4941604516	0.1138723374
H14	6.5018821613	-2.0127226643	-0.8317350468
C15	2.2162866560	-4.1742762409	3.3818356166
C16	2.0523839123	-2.8308326264	3.7218671062
C17	1.8784937089	-1.8688490574	2.7247879038
C18	1.8717626165	-2.2368844530	1.3711180345
C19	2.0289565427	-3.5949878031	1.0379740056
C20	2.2024975793	-4.5526001590	2.0367244105
H21	2.3476104942	-4.9233784489	4.1577314144
H22	2.0520493250	-2.5258205022	4.7648420875
H23	1.7394782102	-0.8294379389	3.0067313404
H24	2.0095803903	-3.9083754727	-0.0014050467

H25	2.3246076099	-5.5969679410	1.7620330303
C26	-0.5077972838	-3.2885276348	-3.3082223668
C27	0.6692528553	-2.5994851462	-3.5990309246
C28	1.3370908310	-1.8907567036	-2.5981980634
C29	0.8305854021	-1.8657156204	-1.2906269562
C30	-0.3600948477	-2.5560822140	-1.0077907667
C31	-1.0220402511	-3.2627753451	-2.0095475194
H32	-1.0214585279	-3.8455843471	-4.0873778938
H33	1.0774176795	-2.6161910280	-4.6061094495
H34	2.2570855046	-1.3688916209	-2.8402004676
H35	-0.7668672464	-2.5602503454	-0.0019691108
H36	-1.9366678784	-3.7999184510	-1.7726609635
C37	-4.5718575572	-1.2948358847	1.0230147938
C38	-4.8284647557	-0.3445543614	0.0305552700
C39	-3.8111323485	0.4994214002	-0.4107465855
C40	-2.5148780569	0.3886532634	0.1224186618
C41	-2.2713616087	-0.5583190422	1.1264997314
C42	-3.2950428821	-1.3960980438	1.5751717160
H43	-5.3698008023	-1.9452462753	1.3713713424
H44	-5.8259626555	-0.2520829723	-0.3907937425
H45	-4.0313082125	1.2570224316	-1.1577314988
H46	-1.2804708911	-0.6318592161	1.5678372522
H47	-3.0940074030	-2.1228157561	2.3579774946
C48	-0.4827510824	1.3884808189	-4.9718890758
C49	-1.4851292038	0.5945739130	-4.4138672171
C50	-1.7164321854	0.6077029905	-3.0361137094
C51	-0.9417962356	1.4209777674	-2.1993277742
C52	0.0845737229	2.2002394357	-2.7639552141
C53	0.3050494165	2.1899045024	-4.1412334197
H54	-0.3123588513	1.3803204976	-6.0449634286
H55	-2.0942793759	-0.0409766883	-5.0510966573
H56	-2.4941215415	-0.0249113901	-2.6219999717
H57	0.7034805549	2.8302738093	-2.1279656423
H58	1.0919427498	2.8083775707	-4.5651244819
C59	-3.3810735280	5.5843966099	0.3672216644
C60	-2.8408955428	5.3305525853	-0.8928843750
C61	-2.1716872461	4.1301099157	-1.1486755097
C62	-2.0404289475	3.1658957926	-0.1416901247
C63	-2.5927582298	3.4280899606	1.1250807568
C64	-3.2567000423	4.6266382973	1.3781907718
H65	-3.9024533014	6.5178035332	0.5615062196
H66	-2.9431011527	6.0653997641	-1.6871634440
H67	-1.7645485375	3.9496268569	-2.1378092485
H68	-2.5311629350	2.6802152051	1.9125044444
H69	-3.6842784478	4.8101462457	2.3605224626
C70	1.0198320960	3.1940985085	1.8533281561
H71	-0.0052412410	3.4337952202	2.1189753046
C72	1.7665918155	2.4040504920	2.7602777707
H73	2.8435934955	2.5610349613	2.7611540449
H74	2.1586044890	1.0026681793	1.8688088645
C75	2.8258020133	5.9729131825	-0.8728998451
C76	3.5631163825	4.8754135640	-0.4191121207
C77	2.9879287761	3.9519011046	0.4489607476
C78	1.6562464429	4.1088951411	0.8853728415
C79	0.9240308062	5.2143367751	0.4138359781
C80	1.5051572458	6.1372232524	-0.4532131816
H81	3.2802799697	6.6955860925	-1.5449280919
H82	4.5931822523	4.7416281175	-0.7390100101
H83	3.5774795287	3.1017399804	0.7814306701
H84	-0.1007350640	5.3567256376	0.7438752877

H85	0.9259638429	6.9905503234	-0.7951375588
C86	0.3481494072	1.0337266758	6.5711160029
C87	1.7070000931	1.2573538413	6.3494739037
C88	2.1488497888	1.6782110943	5.0954237817
C89	1.2386920497	1.8898712162	4.0472101012
C90	-0.1266463617	1.6530638113	4.2807026449
C91	-0.5658253273	1.2311879388	5.5319006322
H92	0.0011388030	0.7050108585	7.5467044103
H93	2.4245797328	1.1076979355	7.1513795854
H94	3.2092282666	1.8571755425	4.9293012182
H95	-0.8464498496	1.7870611405	3.4781071533
H96	-1.6246727248	1.0533770946	5.6988791339

Stilbene

Gas phase energy (Lacvp*): -540.6981205 au
Gas phase energy (Lacv3p**+): -540.84571110627 au
Solvation energy: -0.007929519 au
Total Gibbs free energy: -540.6953805au
Dispersion energy: -0.01785631 au
ZPE: 566.52 kJ/mol

C1	-0.3809560000	0.9726250000	-0.0677560000
C2	-1.7189840000	0.8081280000	-0.0677420000
H3	0.2550720000	0.0887400000	-0.0677710000
H5	-2.3543420000	1.6924300000	-0.0677470000
C6	1.8914930000	4.6102820000	-0.0679290000
C7	2.5225000000	3.3662590000	-0.0679370000
C8	1.7624510000	2.1989830000	-0.0678630000
C9	0.3554630000	2.2402360000	-0.0677900000
C10	-0.2644230000	3.5056900000	-0.0677860000
C11	0.4945420000	4.6714760000	-0.0678490000
H12	2.4796400000	5.5241080000	-0.0679850000
H13	3.6077330000	3.3034070000	-0.0680000000
H14	2.2611520000	1.2319960000	-0.0678780000
H15	-1.3479830000	3.5804720000	-0.0677440000
H16	-0.0056450000	5.6366610000	-0.0678390000
C16	-3.9959340000	-2.8268380000	-0.0679390000
C17	-4.6251530000	-1.5818650000	-0.0679400000
C18	-3.8637820000	-0.4154630000	-0.0678490000
C19	-2.4569210000	-0.4585080000	-0.0677620000
C20	-1.8393090000	-1.7247930000	-0.0677590000
C21	-2.5991510000	-2.8898270000	-0.0678460000
H22	-4.5851820000	-3.7399150000	-0.0680070000
H23	-5.7102510000	-1.5175780000	-0.0680140000
H24	-4.3611390000	0.5521850000	-0.0678590000
H25	-0.7556620000	-1.8008720000	-0.0677010000
H26	-2.0996350000	-3.8553720000	-0.0678460000

Ammonia

Gas phase energy (Lacvp*): -56.54668002 au
Gas phase energy (Lacv3p**+): -56.58241161268au
Solvation energy: -0.011209985 au
Total Gibbs free energy: -56.578202 au
Dispersion energy: -0.000038 au
ZPE: 90.68 kJ/mol

N1	-0.6167990000	0.3062230000	-0.0549360000
H2	-0.6753210000	1.3237230000	-0.0425390000
H3	-1.3023960000	-0.0045320000	-0.7421080000
H4	-0.9678100000	-0.0046640000	0.8500330000

Ammonium

Gas phase energy (Lacvp*): -56.89263351 au
Gas phase energy (Lacv3p**+): -56.92025806757au
Solvation energy: -0.130386491 au
Total Gibbs free energy: -57.018243au
Dispersion energy: -0.000098 au
ZPE: 130.8 kJ/mol

N1	0.0000000000	0.0000000000	0.0000000000
H2	0.5944970000	0.5944970000	-0.5944970000
H3	-0.5944970000	-0.5944970000	-0.5944970000
H4	-0.5944970000	0.5944970000	0.5944970000
H5	0.5944970000	-0.5944970000	0.5944970000

Carbopalladation step: TS for branched product (α-phenyl styrene)

Gas phase energy (Lacvp*): -2740.430364 au
Gas phase energy (Lacv3p**+): -2740.99697362846au
Solvation energy: -0.0515416 au
Total Gibbs free energy: -2740.504876au
Dispersion energy: -0.14918857 au
ZPE: 2040.11 kJ/mol
Neg freq: -309.43 cm^{-1}

C1	-1.9226060000	0.5202660000	0.9681310000
C2	-0.5898240000	1.0456120000	0.9425780000
H3	-0.0714390000	1.1052370000	1.8936160000
H4	-2.3075400000	0.1983230000	1.9338500000
C5	3.1945290000	-1.4257010000	1.3525640000
C6	2.1129070000	-1.7447260000	2.1860960000
C7	0.8161540000	-1.3669760000	1.8208620000
C8	0.5873900000	-0.7049790000	0.5945020000
C9	1.6770540000	-0.3800590000	-0.2285640000
C10	2.9754910000	-0.7414040000	0.1511760000
H11	4.2031200000	-1.6961240000	1.6466710000
H12	2.2816350000	-2.2602510000	3.1263370000
H13	-0.0084320000	-1.5663570000	2.4998030000
H14	1.5203100000	0.1730530000	-1.1479590000
H15	3.8111050000	-0.4927650000	-0.4937000000
H16	-2.6649770000	0.9986650000	0.3369280000
C17	0.6917960000	4.1163450000	-1.7747220000
C18	1.2795580000	3.9875010000	-0.5108760000
C19	0.8666480000	2.9681640000	0.3505840000
C20	-0.1502500000	2.0705050000	-0.0309930000
C21	-0.7292690000	2.2063980000	-1.3085040000
C22	-0.3117830000	3.2214410000	-2.1715260000
H23	1.0135770000	4.9046330000	-2.4468380000
H24	2.0562630000	4.6770020000	-0.1983300000
H25	1.3284320000	2.8680590000	1.3286060000
H26	-1.5002730000	1.5125350000	-1.6284210000
H27	-0.7647980000	3.3162190000	-3.1528520000
Pd28	-1.3907040000	-1.2286580000	-0.1438380000
P29	-0.4902150000	-3.1259760000	-1.6118150000
P30	-3.8710730000	-1.7758000000	-0.2019260000
C31	4.1494250000	-3.5165740000	-2.2772790000
C32	3.3950100000	-2.6141540000	-3.0377800000
C33	2.0162840000	-2.5017670000	-2.8303370000
C34	1.3781210000	-3.3005030000	-1.8652700000
C35	2.1365610000	-4.2009880000	-1.1040470000
C36	3.5182060000	-4.3057280000	-1.3101200000
H37	5.2177930000	-3.6081840000	-2.4430750000
H38	3.8760720000	-2.0041380000	-3.7956440000
H39	1.4402450000	-1.8083500000	-3.4344410000
H40	1.6593230000	-4.8305210000	-0.3619040000

H41	4.0949290000	-5.0126230000	-0.7225230000
C42	-1.6006710000	-7.2718380000	0.3081820000
C43	-1.3193250000	-6.1566910000	1.1059200000
C44	-1.0027860000	-4.9298100000	0.5094980000
C45	-0.9596790000	-4.8104440000	-0.8905500000
C46	-1.2434620000	-5.9312550000	-1.6860510000
C47	-1.5632410000	-7.1558560000	-1.0867080000
H48	-1.8480360000	-8.2223120000	0.7689630000
H49	-1.3501700000	-6.2380350000	2.1874090000
H50	-0.7926240000	-4.0666210000	1.1328050000
H51	-1.2330140000	-5.8548200000	-2.7665330000
H52	-1.7806010000	-8.0171670000	-1.7100420000
C53	-2.0083660000	-3.0477560000	-6.0573740000
C54	-0.9715100000	-3.9167010000	-5.6951330000
C55	-0.5103240000	-3.9506020000	-4.3748570000
C56	-1.0921020000	-3.1190370000	-3.3999180000
C57	-2.1218250000	-2.2435430000	-3.7731760000
C58	-2.5802470000	-2.2088140000	-5.0957530000
H59	-2.3614820000	-3.0211050000	-7.0828360000
H60	-0.5165830000	-4.5618030000	-6.4395150000
H61	0.3140360000	-4.6054600000	-4.1147500000
H62	-2.5644400000	-1.5916660000	-3.0295030000
H63	-3.3804210000	-1.5299700000	-5.3711080000
C64	-5.9066740000	-4.6782860000	-3.2916950000
C65	-6.1936520000	-3.3104520000	-3.3418380000
C66	-5.6006870000	-2.4296170000	-2.4279920000
C67	-4.7111820000	-2.9171320000	-1.4585000000
C68	-4.4299570000	-4.2928460000	-1.4051430000
C69	-5.0264350000	-5.1672680000	-2.3191380000
H70	-6.3696830000	-5.3582070000	-3.9989860000
H71	-6.8859340000	-2.9252710000	-4.0833860000
H72	-5.8488600000	-1.3759490000	-2.4697450000
H73	-3.7595830000	-4.6875750000	-0.6510800000
H74	-4.8031880000	-6.2275290000	-2.2665390000
C75	-6.3898220000	2.1841350000	-0.4996730000
C76	-5.4310790000	1.8678570000	-1.4706840000
C77	-4.6896700000	0.6862990000	-1.3636090000
C78	-4.9100520000	-0.1990310000	-0.2911230000
C79	-5.8685130000	0.1251230000	0.6799350000
C80	-6.6030060000	1.3142660000	0.5741410000
H81	-6.9614360000	3.1025220000	-0.5790090000
H82	-5.2579470000	2.5397730000	-2.3048450000
H83	-3.9394760000	0.4571870000	-2.1157230000
H84	-6.0476960000	-0.5387370000	1.5172910000
H85	-7.3406610000	1.5560490000	1.3320630000
C86	-5.0592880000	-3.7392570000	3.8957590000
C87	-5.9612790000	-3.7594330000	2.8246750000
C88	-5.6113880000	-3.1847310000	1.5978010000
C89	-4.3524830000	-2.5797930000	1.4350040000
C90	-3.4503740000	-2.5692660000	2.5098670000
C91	-3.8026540000	-3.1453550000	3.7366090000
H92	-5.3333420000	-4.1867180000	4.8452300000
H93	-6.9349430000	-4.2234050000	2.9416480000
H94	-6.3127420000	-3.2175080000	0.7712800000
H95	-2.4696740000	-2.1227050000	2.3833790000
H96	-3.0977990000	-3.1323990000	4.5616000000

Cationic post-insertion complex (after TS branched product)

Gas phase energy (Lacvp*): -2740.474252 au

Gas phase energy (Lacv3p**+): -2741.03742786777au

Solvation energy: -0.0509224 au
Total Gibbs free energy: -2740.543039au
Dispersion energy: -0.15112059 au
ZPE: 2053.92 kJ/mol

C1	-1.9720834609	0.3912661529	0.8275424992
C2	-0.5898330028	0.9879861053	1.1033724871
H3	-0.7313521886	1.7554655523	1.8815666885
H4	-2.4674758434	0.1191663761	1.7607269405
C5	1.7420256623	-2.2764090922	2.7954722559
C6	1.0153519831	-1.4158141394	3.6278307831
C7	0.2926957812	-0.3504283116	3.0884076669
C8	0.2893761325	-0.1140981415	1.7062033458
C9	1.0331243369	-0.9718236086	0.8806487532
C10	1.7486179678	-2.0498897267	1.4208476973
H11	2.3110334832	-3.0982145731	3.2205600256
H12	1.0206532083	-1.5680534458	4.7042325406
H13	-0.2660477671	0.3112856676	3.7483459082
H14	1.1371629540	-0.7499151130	-0.1777525961
H15	2.3291631180	-2.6882970710	0.7601225950
H16	-2.6176268175	1.0528275370	0.2486968274
C17	1.3649790807	2.9560784535	-2.2417660925
C18	1.8630525211	3.0777126361	-0.9404696399
C19	1.2158907163	2.4468099512	0.1182697096
C20	0.0574839045	1.6815658449	-0.0933602855
C21	-0.4381114255	1.5780894044	-1.3995926433
C22	0.2127206173	2.2060556035	-2.4677809858
H23	1.8686495108	3.4497830322	-3.0681468385
H24	2.7568243211	3.6674096077	-0.7512657448
H25	1.6155077620	2.5432515825	1.1262716137
H26	-1.3534710022	1.0219483114	-1.5977449683
H27	-0.1925570795	2.1147838719	-3.4731713912
Pd28	-1.5781562331	-1.2968781784	-0.3689476106
P29	-0.5930845769	-3.0359187780	-1.9597831605
P30	-3.8452541489	-1.6937279812	-0.0444867773
C31	3.9878427926	-2.4617879900	-2.5939617065
C32	3.0866734720	-1.4261839455	-2.8527837095
C33	1.7210851489	-1.6152187024	-2.6458598302
C34	1.2330875561	-2.8466275302	-2.1763034709
C35	2.1431317384	-3.8822355765	-1.9204340593
C36	3.5117597514	-3.6873037228	-2.1293746804
H37	5.0518265159	-2.3148553894	-2.7555828304
H38	3.4454124993	-0.4673926045	-3.2148605453
H39	1.0350678895	-0.7978485915	-2.8560219920
H40	1.7903539576	-4.8450344602	-1.5661744880
H41	4.2036237324	-4.5016265087	-1.9313832861
C42	-1.0127826805	-7.3843310581	-0.3836559735
C43	-0.7510299485	-6.3232881006	0.4868517394
C44	-0.6425343527	-5.0239898017	-0.0091216782
C45	-0.7846688063	-4.7718669724	-1.3853271661
C46	-1.0485351305	-5.8414117716	-2.2520703507
C47	-1.1622914028	-7.1402609081	-1.7501609790
H48	-1.1012347805	-8.3962787159	0.0025547840
H49	-0.6348115110	-6.5064513147	1.5520974222
H50	-0.4406238407	-4.2029689761	0.6755525725
H51	-1.1686511538	-5.6651353134	-3.3168599327
H52	-1.3666089073	-7.9625335051	-2.4310014948
C53	-2.1126057491	-2.9387281394	-6.3491786815
C54	-0.8501839010	-3.4660944795	-6.0664384868
C55	-0.3808901129	-3.4964653780	-4.7544109748
C56	-1.1767360399	-3.0038752888	-3.7053402990

C57	-2.4392259773	-2.4696518199	-4.0010829085
C58	-2.9056075642	-2.4403348023	-5.3152133702
H59	-2.4737903474	-2.9125276947	-7.3735512704
H60	-0.2264339255	-3.8506173324	-6.8693934832
H61	0.6081420014	-3.8966486721	-4.5481463989
H62	-3.0629114219	-2.0837818233	-3.2013472582
H63	-3.8879713202	-2.0263671573	-5.5300448940
C64	-5.8735786721	-4.9867894858	-2.6089727642
C65	-6.2687217133	-3.6588070967	-2.7684855953
C66	-5.6593110827	-2.6471676397	-2.0237741934
C67	-4.6436997084	-2.9621351622	-1.1080553716
C68	-4.2517730106	-4.3028188529	-0.9513901896
C69	-4.8645340571	-5.3061832016	-1.6980540427
H70	-6.3537226937	-5.7716738424	-3.1871322999
H71	-7.0616250496	-3.4048023719	-3.4665625526
H72	-5.9926371713	-1.6223199204	-2.1464197028
H73	-3.4758539792	-4.5681491907	-0.2403022389
H74	-4.5525198750	-6.3381456810	-1.5648709439
C75	-6.3220777178	2.1650424956	-0.7939462892
C76	-5.4015861148	1.7032920449	-1.7393266330
C77	-4.6646688727	0.5471648397	-1.4899589876
C78	-4.8503521224	-0.1762634304	-0.2972341563
C79	-5.7686120073	0.2974501191	0.6495791656
C80	-6.4981832026	1.4631085486	0.3982473330
H81	-6.8907899425	3.0710137235	-0.9839219492
H82	-5.2504655458	2.2490129891	-2.6670764201
H83	-3.9352255388	0.2095386059	-2.2236672225
H84	-5.9173160200	-0.2329780894	1.5846852736
H85	-7.2042296127	1.8213925368	1.1426554528
C86	-4.7649497835	-3.3308206580	4.1970427987
C87	-5.7621176442	-3.2998717302	3.2190793688
C88	-5.4789512220	-2.8096458840	1.9465540484
C89	-4.1922888287	-2.3285306026	1.6419336990
C90	-3.1941168363	-2.3752806870	2.6250119235
C91	-3.4824611230	-2.8739245559	3.8966367556
H92	-4.9875794425	-3.7186846959	5.1874023330
H93	-6.7603288368	-3.6649905164	3.4449824789
H94	-6.2565527568	-2.8108087548	1.1877273729
H95	-2.1882123793	-2.0354688957	2.3969049459
H96	-2.6996311003	-2.9077732563	4.6494720539

Cationic agostic complex (leading to α-phenyl styrene)

Gas phase energy (Lacvp*): -2740.477424 au
Gas phase energy (Lacv3p**+): -2741.04634058791au
Solvation energy: -0.052126236 au
Total Gibbs free energy: -2740.549271au
Dispersion energy: -0.14037907 au
ZPE: 2050.25 kJ/mol

Pd1	0.9127970000	1.0853460000	0.3434390000
P2	1.2804320000	-1.3775050000	0.4195360000
P3	-1.2391560000	1.6271810000	-0.3454400000
C4	5.5599280000	-2.0069210000	2.1408680000
C5	5.3680640000	-1.4613520000	0.8680900000
C6	4.0788710000	-1.2850460000	0.3690000000
C7	2.9602960000	-1.6657500000	1.1324620000
C8	3.1608720000	-2.2145480000	2.4062610000
C9	4.4558070000	-2.3795290000	2.9063310000
H10	6.5652690000	-2.1431520000	2.5297450000
H11	6.2240450000	-1.1780880000	0.2609770000
H12	3.9452880000	-0.8671690000	-0.6263490000

H13	2.3127620000	-2.5237560000	3.0091890000
H14	4.5976890000	-2.8105670000	3.8938330000
C15	-1.5521510000	-3.6335920000	3.3361490000
C16	-1.1958920000	-2.3019120000	3.5634290000
C17	-0.3584320000	-1.6391110000	2.6648610000
C18	0.1454520000	-2.3040230000	1.5340700000
C19	-0.2192420000	-3.6399010000	1.3116270000
C20	-1.0648690000	-4.2968040000	2.2079020000
H21	-2.2081990000	-4.1493680000	4.0316160000
H22	-1.5740320000	-1.7762150000	4.4360520000
H23	-0.0978590000	-0.5975420000	2.8417740000
H24	0.1499070000	-4.1689030000	0.4383740000
H25	-1.3409790000	-5.3314930000	2.0228990000
C26	1.4559960000	-3.6753560000	-3.6105720000
C27	2.1816590000	-4.1476510000	-2.5145680000
C28	2.1339110000	-3.4692490000	-1.2976560000
C29	1.3524640000	-2.3084030000	-1.1636880000
C30	0.6288230000	-1.8409810000	-2.2699340000
C31	0.6794200000	-2.5233030000	-3.4861090000
H32	1.5016720000	-4.2020090000	-4.5600200000
H33	2.7922110000	-5.0416440000	-2.6087320000
H34	2.7175530000	-3.8351600000	-0.4579450000
H35	0.0220810000	-0.9455520000	-2.1821650000
H36	0.1156420000	-2.1499380000	-4.3367380000
C37	-3.6720700000	-1.8241210000	-2.2671850000
C38	-3.3322230000	-0.7156080000	-3.0420420000
C39	-2.5970880000	0.3341750000	-2.4864610000
C40	-2.1961230000	0.2775840000	-1.1431000000
C41	-2.5449610000	-0.8410890000	-0.3666160000
C42	-3.2785370000	-1.8833930000	-0.9276170000
H43	-4.2439590000	-2.6385130000	-2.7034610000
H44	-3.6433740000	-0.6591210000	-4.0818080000
H45	-2.3483840000	1.1940070000	-3.0996440000
H46	-2.2486150000	-0.8984090000	0.6765370000
H47	-3.5409660000	-2.7431230000	-0.3175230000
C48	-1.1259160000	5.0006940000	-3.5287380000
C49	-0.2684360000	3.9004920000	-3.6163110000
C50	-0.3111760000	2.9042730000	-2.6430210000
C51	-1.2253900000	2.9879880000	-1.5770680000
C52	-2.0788130000	4.0963160000	-1.4938700000
C53	-2.0242490000	5.0974960000	-2.4667880000
H54	-1.0872100000	5.7819860000	-4.2827680000
H55	0.4401040000	3.8227330000	-4.4364320000
H56	0.3754660000	2.0625920000	-2.7068490000
H57	-2.7826950000	4.1879190000	-0.6730130000
H58	-2.6869900000	5.9550820000	-2.3897750000
C59	-3.9725380000	2.9323100000	3.1622800000
C60	-4.5269570000	2.6180090000	1.9189870000
C61	-3.7057570000	2.2168870000	0.8671270000
C62	-2.3128630000	2.1377430000	1.0469980000
C63	-1.7663980000	2.4420140000	2.3021870000
C64	-2.5939110000	2.8390340000	3.3536770000
H65	-4.6163130000	3.2411210000	3.9812210000
H66	-5.6013170000	2.6790920000	1.7689000000
H67	-4.1497120000	1.9577910000	-0.0900040000
H68	-0.6957700000	2.3558310000	2.4629750000
H69	-2.1592540000	3.0710330000	4.3220400000
C70	1.3114530000	3.1178660000	0.4983520000
H71	0.6836730000	3.6194510000	1.2331790000
C72	2.7170080000	2.7887080000	0.9486150000

H74	2.8073630000	1.6443390000	0.9631860000
H75	1.2200420000	3.5566590000	-0.4931120000
C86	3.4719640000	3.9138530000	5.0704490000
C87	3.5390140000	2.5736770000	4.6921320000
C88	3.2963580000	2.2060260000	3.3661210000
C89	2.9813710000	3.1739970000	2.4069320000
C90	2.9221210000	4.5197420000	2.7935780000
C91	3.1644740000	4.8866370000	4.1160340000
H92	3.6622950000	4.2014330000	6.1008930000
H93	3.7841590000	1.8106880000	5.4263460000
H94	3.3607650000	1.1576810000	3.0790240000
H95	2.6990870000	5.2853250000	2.0538280000
H96	3.1160670000	5.9341810000	4.4017630000
C92	5.9728080000	4.1178210000	-1.5914470000
C93	4.8125240000	4.8847920000	-1.4913100000
C94	3.7489570000	4.4523270000	-0.6970520000
C95	3.8326930000	3.2454480000	0.0092080000
C96	5.0054990000	2.4852130000	-0.0926400000
C97	6.0662570000	2.9153020000	-0.8878770000
H97	6.8003790000	4.4561600000	-2.2089620000
H98	4.7331590000	5.8261980000	-2.0287150000
H99	2.8576930000	5.0700330000	-0.6224740000
H100	5.0919020000	1.5541630000	0.4632910000
H101	6.9690990000	2.3137100000	-0.9555050000

β-elimination TS leading to α-phenyl styrene

Gas phase energy (Lacvp*): -2740.465278 au
Gas phase energy (Lacv3p**+): -2741.03636662272au
Solvation energy: -0.050122187 au
Total Gibbs free energy: -2740.540286au
Dispersion energy: -0.14366828 au
ZPE: 2039.05 kJ/mol
Neg. Freq: -603.54 cm^{-1}

Pd1	0.9863980000	1.1983970000	0.3897130000
P2	1.4519520000	-1.1555500000	0.4394980000
P3	-1.3319610000	1.5508760000	-0.3086540000
C4	5.5886030000	-2.2158960000	2.2833680000
C5	5.4742830000	-1.2144860000	1.3146850000
C6	4.2252110000	-0.8919580000	0.7866720000
C7	3.0743370000	-1.5776170000	1.2109330000
C8	3.1978670000	-2.5845060000	2.1772320000
C9	4.4503690000	-2.8954600000	2.7137470000
H10	6.5615880000	-2.4634200000	2.6990020000
H11	6.3571830000	-0.6820110000	0.9712180000
H12	4.1503010000	-0.1080230000	0.0363580000
H13	2.3232380000	-3.1306740000	2.5150560000
H14	4.5317390000	-3.6746000000	3.4669210000
C15	-1.5538900000	-3.6402910000	2.9468220000
C16	-1.1468810000	-2.3717730000	3.3695250000
C17	-0.2592610000	-1.6290960000	2.5915030000
C18	0.2376580000	-2.1532980000	1.3868470000
C19	-0.1749310000	-3.4260070000	0.9679150000
C20	-1.0692100000	-4.1633370000	1.7468930000
H21	-2.2481740000	-4.2177130000	3.5512450000
H22	-1.5235980000	-1.9599430000	4.3018610000
H23	0.0484440000	-0.6385970000	2.9194930000
H24	0.1976250000	-3.8419090000	0.0366570000
H25	-1.3847090000	-5.1488480000	1.4149080000
C26	1.6211670000	-3.0668510000	-3.7929440000
C27	2.5968060000	-3.3948330000	-2.8515140000

C28	2.5639800000	-2.8289020000	-1.5757110000
C29	1.5491620000	-1.9224040000	-1.2314020000
C30	0.5720510000	-1.5960280000	-2.1860280000
C31	0.6062260000	-2.1689990000	-3.4561250000
H32	1.6506820000	-3.5097360000	-4.7848490000
H33	3.3875000000	-4.0951480000	-3.1069290000
H34	3.3291380000	-3.0952070000	-0.8539060000
H35	-0.2287920000	-0.9093150000	-1.9333320000
H36	-0.1619160000	-1.9135290000	-4.1812310000
C37	-4.0806130000	-1.8444600000	-1.9063390000
C38	-3.7316220000	-0.7951800000	-2.7556070000
C39	-2.9010270000	0.2325310000	-2.3023400000
C40	-2.4102840000	0.2151070000	-0.9882680000
C41	-2.7672350000	-0.8452970000	-0.1379410000
C42	-3.5972370000	-1.8660760000	-0.5959490000
H43	-4.7294990000	-2.6403660000	-2.2617050000
H44	-4.1117550000	-0.7664920000	-3.7734360000
H45	-2.6492690000	1.0479670000	-2.9724010000
H46	-2.4058130000	-0.8724810000	0.8857820000
H47	-3.8656380000	-2.6785730000	0.0734860000
C48	-1.1303730000	4.6943270000	-3.7252560000
C49	-0.3842390000	3.5139140000	-3.7797650000
C50	-0.4637740000	2.5897570000	-2.7395050000
C51	-1.3064450000	2.8242130000	-1.6370000000
C52	-2.0479000000	4.0120100000	-1.5893920000
C53	-1.9553960000	4.9415530000	-2.6288130000
H54	-1.0634930000	5.4186080000	-4.5323460000
H55	0.2634080000	3.3158160000	-4.6297580000
H56	0.1298410000	1.6785940000	-2.7862720000
H57	-2.6959900000	4.2202550000	-0.7441280000
H58	-2.5326850000	5.8608070000	-2.5780060000
C59	-3.9193900000	3.2305310000	3.1609520000
C60	-4.5118020000	2.9295310000	1.9316940000
C61	-3.7409280000	2.4197940000	0.8887610000
C62	-2.3597790000	2.2167050000	1.0591410000
C63	-1.7782290000	2.5072130000	2.3021310000
C64	-2.5544120000	3.0132260000	3.3465750000
H65	-4.5238860000	3.6248310000	3.9731990000
H66	-5.5772390000	3.0864330000	1.7868440000
H67	-4.2155540000	2.1716530000	-0.0566260000
H68	-0.7189370000	2.3230120000	2.4612940000
H69	-2.0914410000	3.2317590000	4.3050840000
C70	1.3264780000	3.3697880000	0.4703280000
H71	0.5801520000	3.7423090000	1.1649630000
C72	2.6098100000	3.0162570000	0.9774680000
H74	2.5107100000	1.3613100000	0.9121160000
H75	1.2400890000	3.7276050000	-0.5512000000
C86	3.3440120000	3.4382240000	5.2078080000
C87	3.8383110000	2.3242080000	4.5234320000
C88	3.6002000000	2.1773090000	3.1594150000
C89	2.8507900000	3.1354770000	2.4584480000
C90	2.3640130000	4.2532270000	3.1520770000
C91	2.6116690000	4.4033160000	4.5180560000
H92	3.5340900000	3.5536570000	6.2713980000
H93	4.4109630000	1.5679470000	5.0534150000
H94	3.9883740000	1.3075310000	2.6352910000
H95	1.8137660000	5.0240080000	2.6195090000
H96	2.2353330000	5.2797570000	5.0385070000
C92	5.9981380000	3.3611870000	-1.6773200000
C93	4.7964320000	2.8176510000	-2.1419930000

C94	3.7114500000	2.6835790000	-1.2813980000
C95	3.8041370000	3.0917130000	0.0600740000
C96	5.0152640000	3.6270070000	0.5192120000
C97	6.1015670000	3.7645190000	-0.3478330000
H97	6.8471200000	3.4619560000	-2.3479380000
H98	4.7093700000	2.4895990000	-3.1744760000
H99	2.7881170000	2.2379180000	-1.6449240000
H100	5.1098100000	3.9501440000	1.5504100000
H101	7.0307150000	4.1880670000	0.0234970000

Cationic Square planar complex (leading to α-phenyl styrene)

Gas phase energy (Lacvp*): -2740.468438 au
Gas phase energy (Lacv3p**+): -2741.03851933939au
Solvation energy: -0.050081515 au
Total Gibbs free energy: -2740.553122au
Dispersion energy: -0.14423637 au
ZPE: 2050.97 kJ/mol

Pd1	1.1326648852	1.0845676044	0.3480551785
P2	1.5250273927	-1.2201255505	0.2518151810
P3	-1.2707277899	1.4591320061	-0.2906199085
C4	5.7438309529	-2.6656092192	1.5790569256
C5	5.5973257202	-1.4389710595	0.9280116960
C6	4.3310136978	-0.9926219729	0.5507576551
C7	3.1941640588	-1.7748524696	0.8088198861
C8	3.3519006529	-3.0115095212	1.4541083968
C9	4.6195257672	-3.4483694326	1.8411101531
H10	6.7291877838	-3.0073029409	1.8839977682
H11	6.4674350199	-0.8224807509	0.7192696150
H12	4.2330662276	-0.0301504371	0.0557088281
H13	2.4890010629	-3.6341605793	1.6667835156
H14	4.7246365687	-4.4018204054	2.3517425917
C15	-1.2742102601	-3.5680402167	3.1042918835
C16	-0.7391488171	-2.3320906932	3.4777186098
C17	0.0744578766	-1.6271847439	2.5918510959
C18	0.3671300394	-2.1561701700	1.3240375332
C19	-0.1705716755	-3.3981376218	0.9558730935
C20	-0.9902751254	-4.0969632449	1.8447198612
H21	-1.9099979322	-4.1163420477	3.7942507293
H22	-0.9572993155	-1.9165194344	4.4577904133
H23	0.4859867066	-0.6636592596	2.8841186011
H24	0.0461343301	-3.8223009822	-0.0194679612
H25	-1.4029750293	-5.0583565590	1.5509743554
C26	1.0548502691	-2.9085345617	-4.0571571774
C27	2.3148998206	-2.8671846037	-3.4593270143
C28	2.4669763986	-2.3751691677	-2.1610421165
C29	1.3519814358	-1.9134064995	-1.4452398797
C30	0.0851537285	-1.9523666507	-2.0544363930
C31	-0.0597165578	-2.4515466702	-3.3486814841
H32	0.9407245041	-3.2979140460	-5.0649844391
H33	3.1869274974	-3.2262411864	-3.9993039267
H34	3.4534281737	-2.3615568590	-1.7091884369
H35	-0.7934237110	-1.6121828639	-1.5163387508
H36	-1.0479126583	-2.4846733011	-3.7995977725
C37	-4.4577779138	-1.8131642862	-1.1827542753
C38	-4.1085301716	-0.9126266907	-2.1889306244
C39	-3.1426364820	0.0689145586	-1.9535803561
C40	-2.5133682687	0.1553582080	-0.7031128883
C41	-2.8700378802	-0.7560167291	0.3055124855
C42	-3.8362473238	-1.7315159368	0.0656565712
H43	-5.2118530662	-2.5732668438	-1.3686183489

H44	-4.5931432234	-0.9648576472	-3.1605278371
H45	-2.8877175586	0.7662805821	-2.7450270458
H46	-2.3988487459	-0.7035846701	1.2834212483
H47	-4.1022487139	-2.4279769313	0.8560480446
C48	-0.8325651359	3.9552805244	-4.1847416682
C49	-0.2934016759	2.6708372055	-4.0742781197
C50	-0.4523400561	1.9455748067	-2.8948329760
C51	-1.1708100423	2.4882244921	-1.8126399097
C52	-1.7034213396	3.7790902352	-1.9305528344
C53	-1.5317430320	4.5065370752	-3.1114468151
H54	-0.7036371941	4.5235182951	-5.1018840885
H55	0.2548290150	2.2345947617	-4.9052682713
H56	-0.0214566205	0.9493127506	-2.8186500688
H57	-2.2494150460	4.2251550624	-1.1055439398
H58	-1.9480637504	5.5073136749	-3.1894253036
C59	-3.6308061338	3.7909670702	2.9612102858
C60	-4.2201300545	3.5450613273	1.7177589050
C61	-3.5159391052	2.8554719137	0.7332617389
C62	-2.2011434371	2.4176674355	0.9731155712
C63	-1.6263794670	2.6533676144	2.2305349996
C64	-2.3375831189	3.3380444945	3.2187369225
H65	-4.1846633752	4.3250926017	3.7284417576
H66	-5.2334180949	3.8830431647	1.5182545762
H67	-3.9944963817	2.6456716080	-0.2194779242
H68	-0.6239465674	2.2919151321	2.4458799921
H69	-1.8778396302	3.5124053210	4.1878027819
C70	1.3758623182	3.4473708978	0.3952652784
H71	0.4515299451	3.6530885353	0.9241637539
C72	2.5594028516	3.3895585698	1.1101363113
H74	2.6309223648	0.9829742506	0.7602173154
H75	1.3817163439	3.6694076525	-0.6671630401
C86	2.4524374288	3.4725901333	5.4065221281
C87	3.3005338637	2.5794423579	4.7449576269
C88	3.3482955551	2.5579588002	3.3535188701
C89	2.5254064866	3.4143656439	2.5986272560
C90	1.6774253179	4.3078388951	3.2739598556
C91	1.6474580316	4.3407337001	4.6685851473
H92	2.4272058032	3.4963323945	6.4926410336
H93	3.9300083775	1.9023580326	5.3159247285
H94	4.0073827036	1.8610558108	2.8434141375
H95	1.0659076752	5.0030311419	2.7055239423
H96	1.0027055531	5.0528461846	5.1766505370
C92	6.3642216272	3.7563251770	-0.8582255649
C93	5.2864919960	3.1666948641	-1.5284506882
C94	4.0607622466	3.0212665368	-0.8896455356
C95	3.8827057665	3.4580275103	0.4376285900
C96	4.9754093540	4.0447316023	1.1012740560
C97	6.2024702648	4.1960118426	0.4541636160
H97	7.3226641093	3.8672678135	-1.3580172613
H98	5.4075235742	2.8134422638	-2.5490068044
H99	3.2392243116	2.5376164254	-1.4109841251
H100	4.8606216451	4.4075398437	2.1167946928
H101	7.0314214782	4.6605950152	0.9809041843

α-Phenyl styrene

Gas phase energy (Lacvp*): -540.6908803 au
Gas phase energy (Lacv3p**+): -540.83859884033au
Solvation energy: -0.006339727 au
Total Gibbs free energy: -540.6877694au
Dispersion energy: -0.02082306 au

ZPE: 566.24 kJ/mol

C1	0.4887620000	2.2847880000	-0.2430390000
C2	-0.8577460000	2.3025120000	-0.2455920000
H4	-1.4391630000	1.3921050000	-0.1357220000
H5	-1.4147300000	3.2273670000	-0.3607830000
C6	2.5981510000	-1.4626240000	0.0497700000
C7	3.0676350000	-0.3363890000	0.7278340000
C8	2.3964480000	0.8801910000	0.6179470000
C9	1.2334020000	0.9955020000	-0.1627880000
C10	0.7784990000	-0.1447090000	-0.8460760000
C11	1.4512600000	-1.3610420000	-0.7392890000
H12	3.1261180000	-2.4093700000	0.1296850000
H13	3.9601100000	-0.4041660000	1.3448930000
H14	2.7683910000	1.7497970000	1.1515980000
H15	-0.0979100000	-0.0659540000	-1.4833830000
H16	1.0855430000	-2.2282270000	-1.2834620000
C16	2.6920620000	5.9783950000	-0.5336070000
C17	3.1399940000	4.8379440000	-1.2026980000
C18	2.4392670000	3.6380240000	-1.0931630000
C19	1.2675430000	3.5537440000	-0.3213000000
C20	0.8348730000	4.7076900000	0.3531620000
C21	1.5368560000	5.9073760000	0.2466090000
H22	3.2425980000	6.9121800000	-0.6136670000
H23	4.0385940000	4.8818390000	-1.8129600000
H24	2.7946340000	2.7579110000	-1.6208160000
H25	-0.0483200000	4.6530310000	0.9831570000
H26	1.1868680000	6.7853690000	0.7838200000

Anionic Pd° complex ($ClPdPPh_3$)

Gas phase energy (Lacvp*): -1623.365784 au
Gas phase energy (Lacv3p**+): -1623.62844080727au
Solvation energy: -0.083776104 au
Total Gibbs free energy: -1623.531509au
Dispersion energy: -0.04172953 au
ZPE: 724.19 kJ/mol

Pd1	-0.1456650000	0.3616480000	0.0064820000
P3	-0.0204230000	1.9319080000	1.5232390000
Cl7	-0.2648610000	-1.3618230000	-1.6886740000
C34	4.2931240000	2.8379450000	3.1196670000
C35	3.2176720000	2.9518590000	4.0010900000
C36	1.9163720000	2.6908850000	3.5620840000
C37	1.6684640000	2.3048800000	2.2356050000
C38	2.7632660000	2.1745030000	1.3650350000
C39	4.0602710000	2.4485060000	1.7980000000
H40	5.3059980000	3.0414270000	3.4617330000
H41	3.3889200000	3.2453020000	5.0353500000
H42	1.0902790000	2.7864990000	4.2612060000
H43	2.5795200000	1.8340180000	0.3480910000
H44	4.8927860000	2.3450190000	1.1051320000
C44	-2.4660590000	1.1738360000	5.4541660000
C45	-2.3477540000	2.4818650000	4.9824550000
C46	-1.6237900000	2.7485830000	3.8164190000
C47	-1.0101590000	1.7114330000	3.0964230000
C48	-1.1552760000	0.3974230000	3.5716970000
C49	-1.8649090000	0.1317320000	4.7428140000
H50	-3.0300620000	0.9665160000	6.3612460000
H51	-2.8205930000	3.3009190000	5.5216110000
H52	-1.5418000000	3.7732350000	3.4645670000
H53	-0.7188400000	-0.4144340000	2.9935790000
H54	-1.9602810000	-0.8938990000	5.0932210000

C54	-1.4807260000	6.1638340000	0.1303120000
C55	-2.0592440000	4.9870700000	-0.3520510000
C56	-1.5920650000	3.7462360000	0.0808940000
C57	-0.5518690000	3.6536700000	1.0201980000
C58	0.0239730000	4.8434930000	1.4933660000
C59	-0.4343350000	6.0873410000	1.0500860000
H60	-1.8358720000	7.1323710000	-0.2162710000
H61	-2.8673420000	5.0348130000	-1.0790210000
H62	-2.0108910000	2.8260030000	-0.3210760000
H63	0.8410270000	4.8023300000	2.2081870000
H64	0.0304750000	6.9978950000	1.4242500000

Anionic square planar complex (most stable complex, Chlorides trans to Ph and Phosphine)

Gas phase energy(Lacvp*): -2315.228712 au
Gas phase energy (Lacv3p**+): -2315.59068666723 au
Solvation energy: -0.091837772 au
Total Gibbs free energy: -2315.442674au
Dispersion energy: -0.06830818 au
ZPE: 965.72 kJ/mol

Pd1	-0.2359010000	0.1793300000	0.0019110000
P3	0.0388310000	1.9219210000	1.5381890000
Cl7	-2.7010050000	0.3009800000	0.4706030000
C8	4.4333660000	0.1564990000	-1.3033600000
C9	3.4815110000	0.8718490000	-2.0350260000
C10	2.1381620000	0.8694510000	-1.6427950000
C11	1.7174790000	0.1609200000	-0.5050860000
C12	2.6807950000	-0.5600300000	0.2142950000
C13	4.0230860000	-0.5647180000	-0.1800780000
H14	5.4779770000	0.1547300000	-1.6095360000
H15	3.7823940000	1.4283800000	-2.9222020000
H16	1.4092520000	1.4123330000	-2.2397540000
H17	2.3853800000	-1.1304220000	1.0918320000
H18	4.7509590000	-1.1346880000	0.3963730000
Cl15	-0.4652010000	-1.6301260000	-1.5649210000
C34	4.3320230000	2.7884150000	3.1806690000
C35	3.3255630000	2.3838710000	4.0566900000
C36	2.0346270000	2.1341340000	3.5831640000
C37	1.7274840000	2.2827500000	2.2223600000
C38	2.7547830000	2.6759790000	1.3464910000
C39	4.0398200000	2.9312380000	1.8222050000
H40	5.3366270000	2.9825680000	3.5497970000
H41	3.5390920000	2.2623980000	5.1166170000
H42	1.2649330000	1.8245940000	4.2821700000
H43	2.5562420000	2.7649460000	0.2837890000
H44	4.8171630000	3.2273640000	1.1222390000
C44	-2.3838920000	1.4285420000	5.4804540000
C45	-2.0654940000	2.7097820000	5.0274320000
C46	-1.3563700000	2.8743750000	3.8365480000
C47	-0.9632230000	1.7592420000	3.0834940000
C48	-1.3018220000	0.4764920000	3.5359030000
C49	-1.9995020000	0.3139720000	4.7331200000
H50	-2.9389570000	1.2998990000	6.4073210000
H51	-2.3716020000	3.5838430000	5.5983640000
H52	-1.1159850000	3.8756490000	3.4904150000
H53	-1.0443820000	-0.3865510000	2.9304780000
H54	-2.2614530000	-0.6863440000	5.0689430000
C54	-1.3460400000	6.0100480000	-0.2288420000
C55	-2.0051150000	4.8212000000	-0.5479920000
C56	-1.5752630000	3.6063470000	-0.0134440000

C57	-0.4738510000	3.5699330000	0.8581930000
C58	0.1808880000	4.7693920000	1.1793070000
C59	-0.2527350000	5.9813010000	0.6371550000
H60	-1.6811110000	6.9537300000	-0.6544310000
H61	-2.8587680000	4.8333840000	-1.2215920000
H62	-2.0955810000	2.6808340000	-0.2521870000
H63	1.0370630000	4.7610870000	1.8466080000
H64	0.2685520000	6.9017200000	0.8921770000

Complex **1**

Gas phase energy (Lacvp*): -1854.921645 au
Gas phase energy (Lacv3p**+): -1855.238066au
Solvation energy: -0.026145118 au
Total Gibbs free energy: -1855.01774au
Dispersion energy: -0.06046502 au
ZPE: 965.22 kJ/mol

Pd1	1.4229430306	0.8962746655	0.9974274703
Cl2	0.8626801619	3.1401538088	1.3507588538
P3	1.5673524940	-1.4190056254	0.7753535429
C4	4.9347816350	-3.7308408804	2.9885111199
C5	5.2455224469	-2.7742550499	2.0194372419
C6	4.2299221983	-2.0840644437	1.3595826172
C7	2.8826927679	-2.3534289058	1.6585795068
C8	2.5777821145	-3.3154463676	2.6332882188
C9	3.6006965200	-3.9979855544	3.2942231247
H10	5.7297453960	-4.2636802761	3.5038638548
H11	6.2828745709	-2.5581990357	1.7782281042
H12	4.4870481917	-1.3380154492	0.6144517126
H13	1.5440145804	-3.5360354316	2.8787972970
H14	3.3502500896	-4.7406769556	4.0474070110
C15	-2.4453489697	-2.8949556126	2.5850002956
C16	-1.7178281097	-1.8698083766	3.1919659504
C17	-0.5127704039	-1.4443647305	2.6334727686
C18	-0.0186600805	-2.0469303534	1.4631790031
C19	-0.7574620799	-3.0750334939	0.8584960175
C20	-1.9638517709	-3.4948646010	1.4197019818
H21	-3.3875562187	-3.2224815657	3.0163218153
H22	-2.0893267243	-1.3946987804	4.0957076317
H23	0.0472999398	-0.6422967973	3.1102074297
H24	-0.3937429965	-3.5455875912	-0.0497792656
H25	-2.5295547986	-4.2913296747	0.9434029743
C26	1.5914328637	-2.9305374415	-3.6143786070
C27	2.2308249607	-3.6859578130	-2.6299036053
C28	2.2468965602	-3.2469303483	-1.3044923710
C29	1.6211069734	-2.0418211520	-0.9523931533
C30	0.9857962794	-1.2832374394	-1.9494323674
C31	0.9680635572	-1.7282791376	-3.2710981513
H32	1.5837383697	-3.2735886241	-4.6454493138
H33	2.7209154193	-4.6201174000	-2.8917368120
H34	2.7502318083	-3.8405572834	-0.5473150120
H35	0.5122327802	-0.3394468302	-1.6874116042
H36	0.4744855838	-1.1309645170	-4.0329540509
C37	5.9906339602	1.6026962628	-0.2103782387
C38	5.0634827266	1.2582279867	-1.1952949729
C39	3.7202480844	1.0365909124	-0.8622663515
C40	3.3196743204	1.1624522577	0.4687213118
C41	4.2325134395	1.5217748326	1.4621974500
C42	5.5706028024	1.7378154326	1.1147812876
H43	7.0313576216	1.7719960557	-0.4740775783
H44	5.3777052987	1.1580280677	-2.2316885221

H45	3.0113579010	0.7632932816	-1.6369510129
H46	3.9126895411	1.6439770953	2.4917352296
H47	6.2814544382	2.0183075286	1.8886395453

Complex **2**

Gas phase energy (Lacvp*): -1854.91815 au
Gas phase energy (Lacv3p**+): -1855.234675au
Solvation energy: -0.023700344au
Total Gibbs free energy: -1855.013021au
Dispersion energy: -0.06229580 au
ZPE: 965.63 kJ/mol

Pd1	1.3749940000	0.8256130000	0.5404620000
Cl2	-0.9055980000	1.4367270000	0.1503890000
P3	1.4390470000	-1.4330180000	0.6919480000
C4	4.9366980000	-3.5623310000	2.8919050000
C5	5.1698030000	-2.8756400000	1.6977330000
C6	4.1226200000	-2.2346040000	1.0398190000
C7	2.8179590000	-2.2851140000	1.5616430000
C8	2.5931510000	-2.9732130000	2.7634010000
C9	3.6489950000	-3.6048680000	3.4237490000
H10	5.7567660000	-4.0575750000	3.4055210000
H11	6.1719410000	-2.8303930000	1.2798520000
H12	4.3245490000	-1.6855350000	0.1260770000
H13	1.5961010000	-3.0218560000	3.1873910000
H14	3.4582000000	-4.1338520000	4.3538570000
C15	-2.3156550000	-3.0562520000	2.8792870000
C16	-1.8480520000	-1.7703130000	3.1530790000
C17	-0.7357640000	-1.2671910000	2.4762450000
C18	-0.0751590000	-2.0568440000	1.5256680000
C19	-0.5522800000	-3.3484550000	1.2484560000
C20	-1.6681780000	-3.8424780000	1.9229900000
H21	-3.1875480000	-3.4418650000	3.4009880000
H22	-2.3570080000	-1.1467480000	3.8827310000
H23	-0.3986510000	-0.2530910000	2.6653790000
H24	-0.0587380000	-3.9663500000	0.5038530000
H25	-2.0339560000	-4.8407460000	1.6973500000
C26	1.1815530000	-3.1768900000	-3.6016280000
C27	1.9885980000	-3.8136240000	-2.6582320000
C28	2.0924610000	-3.3041390000	-1.3621210000
C29	1.3875610000	-2.1452310000	-1.0030260000
C30	0.5727900000	-1.5080190000	-1.9548480000
C31	0.4721700000	-2.0271290000	-3.2449440000
H32	1.1069210000	-3.5729930000	-4.6109150000
H33	2.5426170000	-4.7091350000	-2.9278380000
H34	2.7249390000	-3.8083810000	-0.6386350000
H35	0.0176230000	-0.6129500000	-1.6816040000
H36	-0.1599180000	-1.5265350000	-3.9733670000
C37	6.0717700000	1.6497060000	0.7585830000
C38	5.4368680000	1.4589440000	-0.4704380000
C39	4.0876520000	1.0883580000	-0.5164850000
C40	3.3645780000	0.9276890000	0.6745170000
C41	4.0097850000	1.0965600000	1.9059870000
C42	5.3564860000	1.4709240000	1.9448160000
H43	7.1216000000	1.9302310000	0.7923310000
H44	5.9906340000	1.5922400000	-1.3971390000
H45	3.6062150000	0.9347010000	-1.4798300000
H46	3.4702990000	0.9414930000	2.8371990000
H47	5.8472100000	1.6148950000	2.9049370000

Complex **3**

Gas phase energy (Lacvp*): -1854.899812au
Gas phase energy (Lacv3p**+): -1855.216904au
Solvation energy: -0.01830786 au
Total Gibbs free energy: -1854.986561au
Dispersion energy: -0.05511741 au
ZPE: 962.93 kJ/mol

Pd1	1.1736800000	1.4410900000	0.3507430000
Cl2	1.5917270000	3.5855880000	1.2101650000
P3	-1.1587300000	1.6639550000	-0.4698510000
C4	-2.1475650000	-2.4169200000	-2.4680160000
C5	-2.3977280000	-1.2424540000	-3.1778210000
C6	-2.1386320000	0.0021290000	-2.5984690000
C7	-1.6226680000	0.0834210000	-1.2978240000
C8	-1.3665910000	-1.1072440000	-0.5930700000
C9	-1.6326910000	-2.3468470000	-1.1711000000
H10	-2.3482290000	-3.3832170000	-2.9232080000
H11	-2.7953020000	-1.2913620000	-4.1883780000
H12	-2.3365050000	0.9088030000	-3.1619130000
H13	-0.9632520000	-1.0626260000	0.4172370000
H14	-1.4327530000	-3.2569740000	-0.6115860000
C15	-1.8220490000	4.9874200000	-3.6376380000
C16	-0.5373130000	4.5455550000	-3.3207540000
C17	-0.3574070000	3.5501550000	-2.3593020000
C18	-1.4640610000	2.9809130000	-1.7124890000
C19	-2.7529800000	3.4412370000	-2.0266320000
C20	-2.9289550000	4.4367370000	-2.9869630000
H21	-1.9615710000	5.7674510000	-4.3817240000
H22	0.3283190000	4.9829540000	-3.8109340000
H23	0.6454970000	3.2284530000	-2.0914330000
H24	-3.6177220000	3.0291260000	-1.5139000000
H25	-3.9303530000	4.7876850000	-3.2228960000
C26	-4.3769770000	2.4100260000	2.7879170000
C27	-4.6618280000	1.5242610000	1.7474070000
C28	-3.7090090000	1.2756070000	0.7583310000
C29	-2.4607860000	1.9144400000	0.8050970000
C30	-2.1745240000	2.7960640000	1.8604780000
C31	-3.1339140000	3.0439260000	2.8422100000
H32	-5.1202140000	2.6012100000	3.5578550000
H33	-5.6259630000	1.0235900000	1.7048320000
H34	-3.9353620000	0.5796270000	-0.0446170000
H35	-1.2018810000	3.2802430000	1.9124070000
H36	-2.9055440000	3.7284890000	3.6549360000
C37	5.3217710000	-0.4984670000	1.4923660000
C38	4.8901190000	-0.4015450000	0.1682760000
C39	3.7346240000	0.3279920000	-0.1416820000
C40	2.9986290000	0.9146240000	0.8935510000
C41	3.4480600000	0.8641840000	2.2148290000
C42	4.6042330000	0.1358840000	2.5109230000
H43	6.2266610000	-1.0521040000	1.7291640000
H44	5.4585690000	-0.8733910000	-0.6296940000
H45	3.4214480000	0.4278930000	-1.1800610000
H46	2.9039230000	1.3797770000	2.9997950000
H47	4.9484810000	0.0721880000	3.5407200000

Neutral square planar pre-insertion complex (Chloride trans to Phenyl)

Gas phase energy (Lacvp*): -2164.580237 au
Gas phase energy (Lacv3p**+): -2164.981573au
Solvation energy: -0.0205175 au

Total Gibbs free energy: -2164.652757au
Dispersion energy: -0.08953452 au
ZPE: 1322.86 kJ/mol

Pd1	0.0956585877	0.5519667780	0.9794067375
Cl2	1.5381870162	2.5126168101	1.4372101353
P3	0.4722133891	0.7382585922	-1.3453217983
C4	0.3896500209	5.1452617533	-2.7947542082
C5	-0.3898176603	4.7437240732	-1.7091082655
C6	-0.3384684669	3.4246967779	-1.2601418712
C7	0.4829840109	2.4904971625	-1.9055217339
C8	1.2642974094	2.8994706806	-2.9954505115
C9	1.2184470215	4.2226293728	-3.4343910171
H10	0.3583223826	6.1770592990	-3.1356038808
H11	-1.0247134745	5.4614471388	-1.1965604276
H12	-0.9153742793	3.1247395407	-0.3910198573
H13	1.9159724648	2.1908629189	-3.4977552877
H14	1.8346272948	4.5321521142	-4.2746997569
C15	4.6980478636	-0.8309847061	-2.4738642627
C16	4.4712630457	-0.1904565115	-1.2543818759
C17	3.1946733369	0.2607404067	-0.9208175710
C18	2.1271235292	0.0758253008	-1.8147189367
C19	2.3624048280	-0.5614035903	-3.0432666121
C20	3.6424620355	-1.0133105203	-3.3673646970
H21	5.6939369048	-1.1854226387	-2.7279979569
H22	5.2907286812	-0.0392891048	-0.5564733969
H23	3.0250383976	0.7756802739	0.0214167071
H24	1.5503768220	-0.7099258919	-3.7475735611
H25	3.8116387375	-1.5077128839	-4.3207640822
C26	-2.5235421272	-1.3333892190	-4.2525977873
C27	-1.6546635735	-2.0965663542	-3.4691791877
C28	-0.7565769555	-1.4751603991	-2.6038850074
C29	-0.7029962953	-0.0734236791	-2.5146082676
C30	-1.5807895510	0.6850216017	-3.3033171977
C31	-2.4853690875	0.0573091319	-4.1627735596
H32	-3.2255212332	-1.8202957550	-4.9245489887
H33	-1.6796606948	-3.1817555866	-3.5231596237
H34	-0.1044341011	-2.0863700275	-1.9890299253
H35	-1.5597594482	1.7685773358	-3.2542954774
H36	-3.1564222405	0.6629782885	-4.7666556850
C37	0.3111583062	0.2663845934	3.4832251719
C38	-0.9324050708	0.6965018323	3.1031549495
H39	-1.7967390700	0.0407201119	3.0894671516
H40	-1.1169551473	1.7615026468	2.9956474961
H41	1.0915984997	1.0214748575	3.5397281055
C42	-2.4388237755	-3.5307733291	0.4024219650
C43	-3.0850767631	-2.2968218680	0.2955351141
C44	-2.3622375365	-1.1059136327	0.4239563047
C45	-0.9833572428	-1.1321879741	0.6768018288
C46	-0.3410709460	-2.3739812764	0.7875012266
C47	-1.0649972871	-3.5650839100	0.6479322128
H48	-3.0006382445	-4.4554643960	0.2952267537
H49	-4.1554677722	-2.2575958879	0.1036980510
H50	-2.8830502260	-0.1566545268	0.3196214185
H51	0.7269928876	-2.4243068302	0.9863695755
H52	-0.5493346022	-4.5194509467	0.7352894321
C53	1.6108000668	-3.5929989817	4.8018761000
C54	0.2511154621	-3.3747363692	4.5636297256
C55	-0.1953095012	-2.1317199135	4.1250878965
C56	0.7125049194	-1.0779552482	3.9180075968
C57	2.0773132813	-1.3105343336	4.1687775037

C58	2.5241742322	-2.5563472561	4.6023295220
H59	1.9551758881	-4.5659447817	5.1434782730
H60	-0.4640267453	-4.1783381904	4.7188993683
H61	-1.2541406759	-1.9793497669	3.9424624883
H62	2.7869667111	-0.5009605528	4.0143448498
H63	3.5831409876	-2.7172767812	4.7869695347

Neutral TS leading to Stilbene (Chloride trans to Phenyl)

Gas phase energy (Lacvp*): -2164.548161 au
Gas phase energy (Lacv3p**+): -2164.947577au
Solvation energy: -0.0214471 au
Total Gibbs free energy: -2164.620056au
Dispersion energy: -0.08752605 au
ZPE: 1318.40 kJ/mol
Neg. Freq: -362.04 cm^{-1}

Pd1	0.1130350000	0.3071820000	1.1075010000
Cl2	1.9552210000	1.8944520000	1.5837120000
P3	0.5209230000	0.6165880000	-1.3461340000
C4	0.5680040000	5.1525320000	-2.5536240000
C5	-0.0575410000	4.7348910000	-1.3739430000
C6	-0.0488810000	3.3815730000	-1.0155600000
C7	0.5773690000	2.4376110000	-1.8426580000
C8	1.2091980000	2.8600500000	-3.0226450000
C9	1.2043370000	4.2141660000	-3.3753360000
H10	0.5691640000	6.2032110000	-2.8265210000
H11	-0.5362310000	5.4598710000	-0.7235480000
H12	-0.4961020000	3.0622200000	-0.0809650000
H13	1.7141040000	2.1416300000	-3.6592210000
H14	1.7010580000	4.5347650000	-4.2857850000
C15	4.6595160000	-1.0846800000	-2.7953560000
C16	4.4881670000	-0.6333450000	-1.4819370000
C17	3.2491910000	-0.1372590000	-1.0584120000
C18	2.1684900000	-0.0903820000	-1.9553970000
C19	2.3442480000	-0.5396320000	-3.2756580000
C20	3.5859560000	-1.0355540000	-3.6915960000
H21	5.6212190000	-1.4708650000	-3.1187320000
H22	5.3168350000	-0.6637070000	-0.7817270000
H23	3.1262180000	0.2302120000	-0.0452860000
H24	1.5178520000	-0.5167430000	-3.9771650000
H25	3.7107120000	-1.3817290000	-4.7130810000
C26	-2.6240530000	-1.2246600000	-4.3201020000
C27	-1.7008660000	-2.0466830000	-3.6623200000
C28	-0.7612010000	-1.4914900000	-2.7879910000
C29	-0.7255390000	-0.1030600000	-2.5722470000
C30	-1.6568520000	0.7161700000	-3.2294510000
C31	-2.6026490000	0.1561600000	-4.0976660000
H32	-3.3522930000	-1.6569540000	-4.9992290000
H33	-1.7131350000	-3.1197280000	-3.8257570000
H34	-0.0574480000	-2.1398940000	-2.2774140000
H35	-1.6406780000	1.7890580000	-3.0747460000
H36	-3.3141490000	0.8014690000	-4.6036800000
C37	-0.2160080000	0.1062670000	3.2729330000
C38	-1.5275730000	-0.2541160000	2.8349270000
H39	-1.9767960000	-1.1687870000	3.2042190000
H40	-2.2432220000	0.5531740000	2.7140540000
H41	-0.0225920000	1.1596410000	3.4608990000
C42	-3.1512180000	-2.9399610000	-0.3670350000
C43	-3.5512610000	-1.5977780000	-0.3199180000
C44	-2.7638780000	-0.6519080000	0.3438000000
C45	-1.5589400000	-1.0331460000	0.9705330000

C46	-1.1642310000	-2.3891470000	0.9160810000
C47	-1.9515560000	-3.3305300000	0.2427770000
H48	-3.7685370000	-3.6739760000	-0.8750860000
H49	-4.4739070000	-1.2877320000	-0.8005640000
H50	-3.0913480000	0.3825880000	0.3881780000
H51	-0.2516140000	-2.7060370000	1.4107800000
H52	-1.6341530000	-4.3686350000	0.2050230000
C53	2.5545540000	-2.5359760000	5.2396090000
C54	1.3185990000	-3.0311050000	4.8067430000
C55	0.4088220000	-2.1901030000	4.1606020000
C56	0.7168840000	-0.8307230000	3.9291790000
C57	1.9678870000	-0.3464500000	4.3749350000
C58	2.8728520000	-1.1890840000	5.0210250000
H59	3.2587800000	-3.1903640000	5.7435550000
H60	1.0592680000	-4.0713630000	4.9786500000
H61	-0.5479020000	-2.5960070000	3.8488690000
H62	2.2291420000	0.6864500000	4.1734430000
H63	3.8296910000	-0.7961580000	5.3498890000

Neutral complex after TS leading to Stilbene (Chloride trans to Phenyl)

Gas phase energy (Lacvp*): -2164.587665 au
Gas phase energy (Lacv3p**+): -2164.984281au
Solvation energy: -0.0209573 au
Total Gibbs free energy: -2164.654881au
Dispersion energy: -0.08869816 au
ZPE: 1328.86 kJ/mol

Pd1	0.2855723541	0.2536569912	1.1557363455
Cl2	1.9049530885	1.9687296398	1.7188074648
P3	0.7485154622	0.4301330208	-1.3135371106
C4	-0.5730755245	4.5828629617	-2.9385771975
C5	-1.2023342814	4.0034319315	-1.8354137718
C6	-0.7749747239	2.7653533824	-1.3544150874
C7	0.2786753871	2.0825281406	-1.9812936810
C8	0.9106695538	2.6745643741	-3.0844749075
C9	0.4869032664	3.9172887431	-3.5575872497
H10	-0.8997990283	5.5516810953	-3.3078256126
H11	-2.0195681704	4.5203906864	-1.3385984581
H12	-1.2550076885	2.3299358314	-0.4818796957
H13	1.7394644322	2.1699425760	-3.5719337222
H14	0.9890599211	4.3671948495	-4.4105361735
C15	5.1402384317	-0.2604533987	-2.7178547892
C16	4.8676721661	0.2306009647	-1.4404406435
C17	3.5503405400	0.4327916077	-1.0239849475
C18	2.4845170680	0.1469539059	-1.8907835623
C19	2.7660942105	-0.3481740697	-3.1758836127
C20	4.0845905892	-0.5485469091	-3.5852159348
H21	6.1673425471	-0.4205050086	-3.0363270228
H22	5.6825638423	0.4571249370	-0.7574632125
H23	3.3463586997	0.8224018452	-0.0308834375
H24	1.9560177992	-0.5869932679	-3.8585077760
H25	4.2849056289	-0.9336341903	-4.5822917151
C26	-1.5888816626	-2.6702214014	-3.8931373988
C27	-0.6485057379	-3.0783166684	-2.9421596948
C28	0.0441626875	-2.1301156661	-2.1920252326
C29	-0.1809763661	-0.7558876378	-2.3859588729
C30	-1.1232556417	-0.3572098715	-3.3427597843
C31	-1.8236423301	-1.3098246614	-4.0888652950
H32	-2.1319505637	-3.4093568108	-4.4767203406
H33	-0.4558467045	-4.1367465231	-2.7844503109
H34	0.7711796449	-2.4601113460	-1.4529619076

H35	-1.3122117929	0.6985324720	-3.5105185547
H36	-2.5505743469	-0.9833448533	-4.8288605988
C37	0.0250402958	-0.0272568202	3.2263710409
C38	-1.4856530442	0.0710503685	3.4383703239
H39	-1.8629290569	-0.7105910018	4.1143155487
H40	-1.7165082831	1.0274647969	3.9183793966
H41	0.5686694271	0.8157373845	3.6448408941
C42	-3.6504142137	-0.1367074195	-0.3236445751
C43	-3.9025749485	0.8974390368	0.5877039918
C44	-3.1865052317	0.9791401913	1.7777439534
C45	-2.2163404580	0.0145323360	2.1036753313
C46	-1.9551321830	-1.0177497871	1.1710921641
C47	-2.6797640691	-1.0866327473	-0.0328313761
H48	-4.2114684385	-0.1968089201	-1.2521248114
H49	-4.6654319715	1.6402545210	0.3665899575
H50	-3.3876989687	1.7851705111	2.4792130461
H51	-1.2941467102	-1.8394117749	1.4336880434
H52	-2.4768687295	-1.8921818963	-0.7316856013
C53	2.1639013246	-3.7085182366	3.8806832485
C54	0.7701068720	-3.7289400402	3.8127154962
C55	0.0580471446	-2.5503743774	3.5974762376
C56	0.7212133524	-1.3140572807	3.4474251968
C57	2.1335202091	-1.3156768989	3.5216245360
C58	2.8407131679	-2.4932331238	3.7354328396
H59	2.7176867314	-4.6288970961	4.0477351510
H60	0.2322822847	-4.6664215587	3.9333908723
H61	-1.0265386806	-2.5955866575	3.5637693284
H62	2.6582812946	-0.3723423660	3.3967644210
H63	3.9261286824	-2.4652585763	3.7905549879

Neutral TS leading to α-phenyl styrene (Chloride trans to Phenyl)

Gas phase energy (Lacvp*): -2164.543176 au
Gas phase energy (Lacv3p**+): -2164.942135au
Solvation energy: -0.0233126 au
Total Gibbs free energy: -2164.617698au
Dispersion energy: -0.08753908 au
ZPE: 1316.64 kJ/mol
Neg. Freq: -359.10 cm^{-1-}

Pd1	-1.3469960000	-1.3339070000	-0.1453570000
P2	-1.7976980000	1.0486720000	0.6118740000
Cl3	-3.6975130000	-1.9267170000	0.2468280000
C4	1.5729950000	4.2698960000	-0.0381120000
C5	1.6516930000	3.3678870000	1.0298310000
C6	0.6433750000	2.4185910000	1.2263930000
C7	-0.4663320000	2.3714690000	0.3655230000
C8	-0.5359850000	3.2728520000	-0.7088580000
C9	0.4803190000	4.2151740000	-0.9101270000
H10	2.3554550000	5.0071640000	-0.1886390000
H11	2.4983410000	3.3993830000	1.7086370000
H12	0.7226430000	1.7178720000	2.0504840000
H13	-1.3855360000	3.2499240000	-1.3821430000
H14	0.4107700000	4.9093660000	-1.7419790000
C15	-2.8948410000	1.3326230000	5.1795380000
C16	-2.2885600000	2.4271610000	4.5529140000
C17	-1.9447500000	2.3602090000	3.1971710000
C18	-2.2032580000	1.1930460000	2.4580900000
C19	-2.8164100000	0.0971480000	3.0889300000
C20	-3.1590680000	0.1714680000	4.4446190000

H21	-3.1602330000	1.3855950000	6.2309110000
H22	-2.0825700000	3.3330900000	5.1149050000
H23	-1.4662760000	3.2115720000	2.7262860000
H24	-3.0437040000	-0.7965630000	2.5174270000
H25	-3.6352010000	-0.6796580000	4.9209970000
C26	-5.4769940000	2.9939040000	-1.5690490000
C27	-4.8659100000	1.8483560000	-2.0892660000
C28	-3.7793760000	1.2667090000	-1.4236510000
C29	-3.2940560000	1.8351170000	-0.2370290000
C30	-3.9144720000	2.9807450000	0.2863190000
C31	-5.0018210000	3.5575420000	-0.3782150000
H32	-6.3237680000	3.4398050000	-2.0814950000
H33	-5.2409050000	1.3961120000	-3.0017970000
H34	-3.3315970000	0.3560060000	-1.8040100000
H35	-3.5612380000	3.4171190000	1.2143000000
H36	-5.4794210000	4.4401120000	0.0358870000
C37	-1.0281940000	-3.3161300000	-0.7591320000
C38	0.2041860000	-2.9424710000	-1.4023250000
H39	-0.9694320000	-3.9016140000	0.1565840000
H40	1.1083220000	-3.3928720000	-1.0035190000
H41	-1.9008440000	-3.5323090000	-1.3672460000
C42	3.1978920000	0.1789600000	-0.0044850000
C43	2.4819720000	0.4323290000	-1.1814650000
C44	1.2879650000	-0.2504270000	-1.4393330000
C45	0.7901450000	-1.1868460000	-0.5144650000
C46	1.5229120000	-1.4413370000	0.6661360000
C47	2.7121920000	-0.7514360000	0.9251460000
H48	4.1311830000	0.6996340000	0.1855470000
H49	2.8516790000	1.1593860000	-1.8974290000
H50	0.7539650000	-0.0709520000	-2.3662400000
H51	1.1712540000	-2.1906620000	1.3701480000
H52	3.2663210000	-0.9522250000	1.8373150000
C53	0.4385920000	-2.4525410000	-5.6764940000
C54	1.5364350000	-2.9285420000	-4.9506710000
C55	1.4515590000	-3.0628290000	-3.5618890000
C56	0.2671260000	-2.7340710000	-2.8766790000
C57	-0.8285320000	-2.2488130000	-3.6161420000
C58	-0.7425210000	-2.1118260000	-5.0039870000
H59	0.5022810000	-2.3451090000	-6.7545490000
H60	2.4554330000	-3.1941340000	-5.4633220000
H61	2.3072100000	-3.4293370000	-3.0015430000
H62	-1.7438370000	-1.9728950000	-3.1016790000
H63	-1.5961680000	-1.7385220000	-5.5606120000

Neutral complex after TS leading to α-phenyl styrene (Chloride trans to Phenyl)

Gas phase energy (Lacvp*): -2164.577511 au
Gas phase energy (Lacv3p**+): -2164.974694au
Solvation energy: -0.0202109 au
Total Gibbs free energy: -2164.644152au
Dispersion energy: -0.08831349 au
ZPE: 1320.75kJ/mol

Pd1	-1.0713177172	-1.1835062321	-0.0180999096
P2	-1.6659607901	1.1852375807	0.7776011439
Cl3	-3.3780737956	-1.7734417601	0.0408815950
C4	1.5435783464	4.5815921954	0.9194579215
C5	1.4928075829	3.6036601534	1.9167342850
C6	0.5206086318	2.6050676473	1.8722386728
C7	-0.4321617026	2.5699246300	0.8389757794
C8	-0.3710164397	3.5555092221	-0.1564271655

C9	0.6093499953	4.5506815121	-0.1163555310
H10	2.2987409414	5.3625311993	0.9549638044
H11	2.2100483092	3.6197633065	2.7339904127
H12	0.4918516067	1.8568872422	2.6599283419
H13	-1.0972713793	3.5562212537	-0.9634658195
H14	0.6333419337	5.3095319151	-0.8946537191
C15	-3.2877435368	1.0902942516	5.1465675457
C16	-2.8507032539	2.3001736973	4.6038113399
C17	-2.3660622395	2.3474846053	3.2968722684
C18	-2.3125796721	1.1834513088	2.5098632388
C19	-2.7588325681	-0.0264652351	3.0644783791
C20	-3.2419459093	-0.0693619517	4.3735178116
H21	-3.6601493576	1.0531541104	6.1673178220
H22	-2.8825789906	3.2094071410	5.1991256814
H23	-2.0140017661	3.2930194589	2.8956083334
H24	-2.7478846478	-0.9299189475	2.4637683586
H25	-3.5832514213	-1.0155558467	4.7855920417
C26	-5.0019112548	2.9469382243	-1.9484849100
C27	-4.0371176355	2.0762856776	-2.4572199685
C28	-3.0598159380	1.5445360243	-1.6149954445
C29	-3.0230538121	1.8920894746	-0.2564321261
C30	-4.0005640105	2.7614816462	0.2478464522
C31	-4.9836213809	3.2830305498	-0.5934237669
H32	-5.7708030986	3.3523211566	-2.6010866726
H33	-4.0530053649	1.7960802267	-3.5073822079
H34	-2.3309410568	0.8411786165	-2.0087517208
H35	-4.0050585863	3.0239838537	1.3012560579
H36	-5.7398898742	3.9498408921	-0.1866407014
C37	-0.6859194243	-3.1329068682	-0.5512267354
C38	0.4744131828	-2.9601147510	-1.5369472773
H39	-0.3991710768	-3.6166518222	0.3876490954
H40	1.2775126070	-3.6810587442	-1.3213172979
H41	-1.5837219252	-3.5914276282	-0.9570213545
C42	2.3222955387	0.8759278200	-0.5607263062
C43	1.8975250065	0.6272094553	-1.8737554612
C44	1.2555318507	-0.5602950243	-2.2000136942
C45	1.0334678039	-1.5512336669	-1.2183645179
C46	1.4343236082	-1.2755363640	0.1149084075
C47	2.0873547308	-0.0688522166	0.4270776621
H48	2.8196541197	1.8096255392	-0.3160005535
H49	2.0776252213	1.3688650123	-2.6480979563
H50	0.9487096775	-0.7505612005	-3.2224924896
H51	1.3834678729	-2.0591415365	0.8664050826
H52	2.4145724232	0.1111123514	1.4472569562
C53	-0.5099383245	-3.4208731064	-5.7335933374
C54	0.7343231106	-3.8219104477	-5.2461967943
C55	1.0308996054	-3.6796549066	-3.8902046042
C56	0.0965125916	-3.1366206925	-2.9982723466
C57	-1.1525751542	-2.7402853189	-3.4985872930
C58	-1.4511314949	-2.8821913229	-4.8547251334
H59	-0.7462504394	-3.5319102295	-6.7889675883
H60	1.4741483210	-4.2483213676	-5.9193653562
H61	2.0039534957	-3.9945968957	-3.5171742641
H62	-1.8977317332	-2.3225259257	-2.8260829560
H63	-2.4263820472	-2.5737198716	-5.2233432042

Anionic square planar complex (less stable complex, Chloride trans to Chloride)

Gas phase energy (Lacvp*): -2315.229763 au

Gas phase energy (Lacv3p**+): -2315.591418au

Solvation energy: -0.080996778 au
Total Gibbs free energy: -2315.429386au
Dispersion energy: -0.06282397 au
ZPE: 964.39kJ/mol

Pd1	1.4363309108	-0.1332507779	-0.0886262253
P2	-1.1024191218	-0.0200274332	0.0131162453
Cl3	1.4885070572	2.1996626998	0.5870860380
C4	6.2643722362	-0.0915928611	-0.2075946844
C5	5.5249601609	0.6295369674	-1.1478391225
C6	4.1260992688	0.6215456815	-1.1070000149
C7	3.4456328894	-0.1187760104	-0.1324187211
C8	4.1908024191	-0.8452651283	0.8046932359
C9	5.5897072349	-0.8256388146	0.7708513883
H10	7.3526904981	-0.0828227000	-0.2377994396
H11	6.0376032003	1.2082467505	-1.9158037291
H12	3.5669276821	1.2070800898	-1.8316837553
H13	3.6815787176	-1.4453543815	1.5535956350
H14	6.1535408173	-1.3966446473	1.5081225336
Cl15	1.5477055045	-2.4538121622	-0.7332260041
C16	-3.6093555799	-3.4697895044	-1.8785675241
C17	-3.9474974107	-2.1487423777	-2.1727442773
C18	-3.2176584612	-1.0952153424	-1.6168318840
C19	-2.1365146906	-1.3488042374	-0.7589943805
C20	-1.7941380115	-2.6837108501	-0.4814837481
C21	-2.5305162766	-3.7321029438	-1.0322251762
H22	-4.1765167179	-4.2901730230	-2.3136830355
H23	-4.7816827748	-1.9326896557	-2.8373004550
H24	-3.4953527834	-0.0727871329	-1.8530007027
H25	-0.9251846244	-2.8987478601	0.1311880703
H26	-2.2449980017	-4.7580090842	-0.8114694837
C27	-2.7534262808	3.7879671855	-2.1035205540
C28	-3.4100363481	3.3085416433	-0.9686756204
C29	-2.9302656375	2.1774215711	-0.3044175241
C30	-1.7853368592	1.5128492054	-0.7655845981
C31	-1.1210800897	2.0136664228	-1.8953933543
C32	-1.6070193387	3.1371558594	-2.5638931955
H33	-3.1266670954	4.6699168442	-2.6194631550
H34	-4.2971821434	3.8165162768	-0.5961246456
H35	-3.4468081675	1.8126820591	0.5792574766
H36	-0.2085045979	1.5304186210	-2.2326743138
H37	-1.0779631456	3.5133762748	-3.4363199810
C38	-2.6591945719	0.1641755496	4.4126932693
C39	-1.4916137741	0.8260669708	4.0253949948
C40	-1.0449007318	0.7626205378	2.7048121913
C41	-1.7723756480	0.0381834793	1.7441130362
C42	-2.9444587223	-0.6241531300	2.1406937321
C43	-3.3829641322	-0.5619308810	3.4657979139
H44	-2.9991572988	0.2092690639	5.4451876596
H45	-0.9160847902	1.3908476519	4.7553582326
H46	-0.1330419975	1.2761576284	2.4074497046
H47	-3.5137966245	-1.1980096219	1.4156551823
H48	-4.2915123068	-1.0859078027	3.7560120127

Neutral square planar pre-insertion complex (Chloride trans to alkene)

Gas phase energy (Lacvp*): -2164.568153 au
Gas phase energy (Lacv3p**+): -2164.969162au
Solvation energy: -0.0221388 au
Total Gibbs free energy: -2164.645212au
Dispersion energy: -0.08720452 au

ZPE: 1322.45 kJ/mol

Pd1	-1.5832167197	-0.6564563563	-0.6526667984
P2	0.9851503094	-0.4611837280	-0.4659111658
Cl3	-1.2299014323	-3.0200453592	-0.6556457353
C4	2.9372394486	3.7526872815	-0.9258794174
C5	3.1974723939	2.7679955114	-1.8788434738
C6	2.6410532524	1.4928200183	-1.7483440990
C7	1.8173234453	1.1822421827	-0.6571564330
C8	1.5670997823	2.1815961733	0.3011312882
C9	2.1213273923	3.4542767231	0.1685018634
H10	3.3692339077	4.7444148038	-1.0309265658
H11	3.8390390753	2.9880698268	-2.7286214276
H12	2.8523276242	0.7377681924	-2.4984897059
H13	0.9523159454	1.9569029107	1.1698374115
H14	1.9186140400	4.2115411828	0.9215309499
C15	3.0415592316	-3.0394020110	-3.7345813396
C16	3.6371133545	-2.9367906639	-2.4767931417
C17	3.0345342931	-2.1755391939	-1.4747104060
C18	1.8258383859	-1.5110030898	-1.7229878585
C19	1.2255429363	-1.6305400888	-2.9854193907
C20	1.8355709114	-2.3839885640	-3.9875870791
H21	3.5109925567	-3.6363044380	-4.5125515004
H22	4.5710999376	-3.4538502241	-2.2713463621
H23	3.5027227033	-2.1085769653	-0.4973947554
H24	0.2723630817	-1.1461596339	-3.1785453092
H25	1.3593573247	-2.4714583296	-4.9606984179
C26	2.5996656971	-1.8797260728	3.6733408946
C27	1.3735886278	-2.3388976843	3.1909899204
C28	0.8950162326	-1.9120602049	1.9506331217
C29	1.6437604962	-1.0140809297	1.1733950090
C30	2.8793658579	-0.5584388655	1.6656742682
C31	3.3524501499	-0.9893704165	2.9052872336
H32	2.9670170704	-2.2118029454	4.6409201248
H33	0.7813871653	-3.0353826626	3.7787778118
H34	-0.0490742365	-2.2927502334	1.5740714357
H35	3.4729166002	0.1415415120	1.0855842935
H36	4.3097689975	-0.6254784735	3.2702188444
C37	-1.9412050710	1.5562763538	-0.3708212260
C38	-2.4519743858	1.3057498239	-1.6304892655
H39	-2.6156527015	1.5686275015	0.4800999513
H40	-3.4993660767	1.0286760961	-1.6914043919
H41	-0.9782747145	2.0342312929	-0.2323009116
C42	-6.2903271696	-1.7446486422	-0.3453078867
C43	-5.5805171228	-2.0496749815	-1.5095249034
C44	-4.2194766664	-1.7453935724	-1.6099094448
C45	-3.5617157582	-1.1211882028	-0.5444807568
C46	-4.2683118827	-0.8164910804	0.6221273364
C47	-5.6303454435	-1.1329462999	0.7200482669
H48	-7.3465244144	-1.9898073785	-0.2676725489
H49	-6.0827288273	-2.5399507453	-2.3410815825
H50	-3.6706190166	-2.0227513391	-2.5054599204
H51	-3.7702339292	-0.3514486489	1.4698708987
H52	-6.1694584067	-0.9014158027	1.6363487168
C53	-0.7840532910	2.0657484616	-5.5017087523
C54	-1.9663780172	1.3364804227	-5.3585176787
C55	-2.4843021727	1.0957297918	-4.0890910696
C56	-1.8268782141	1.5688471133	-2.9380501716
C57	-0.6420695063	2.3074874826	-3.0968295753
C58	-0.1275359070	2.5508069527	-4.3679305367
H59	-0.3795992172	2.2604785868	-6.4917382504

H60	-2.4865703427	0.9595441957	-6.2352742438
H61	-3.4052096398	0.5283923960	-3.9753762690
H62	-0.1270168127	2.7042628629	-2.2287218550
H63	0.7883104523	3.1262642800	-4.4726857701

Neutral TS leading to stilbene (Chloride trans to alkene)

Gas phase energy (Lacvp*): -2164.545598 au
Gas phase energy (Lacv3p**+): -2164.944853au
Solvation energy: -0.0254148 au
Total Gibbs free energy: -2164.621533au
Dispersion energy: -0.08779032 au
ZPE: 1318.43 kJ/mol
Neg. Freq: -299.24 cm^{-1}

Pd1	-0.4527920000	0.1166860000	-0.5960140000
P2	1.6880600000	-0.4658030000	0.5265020000
Cl3	-0.5393670000	2.1290980000	0.8422010000
C4	3.8400770000	-4.3369510000	-1.0618750000
C5	2.5686020000	-4.4080660000	-0.4758390000
C6	1.9513120000	-3.2473060000	0.0014060000
C7	2.5990540000	-2.0019890000	-0.0987180000
C8	3.8713530000	-1.9371470000	-0.6840410000
C9	4.4883760000	-3.1016520000	-1.1627770000
H10	4.3200300000	-5.2374040000	-1.4316570000
H11	2.0618600000	-5.3639370000	-0.3873170000
H12	0.9723440000	-3.3122800000	0.4677520000
H13	4.3822170000	-0.9849660000	-0.7671210000
H14	5.4751460000	-3.0393760000	-1.6108410000
C15	1.3005130000	-1.4178830000	5.1176320000
C16	2.3132840000	-2.0225730000	4.3643610000
C17	2.4311780000	-1.7480350000	2.9967660000
C18	1.5338490000	-0.8627470000	2.3726800000
C19	0.5217400000	-0.2526710000	3.1316000000
C20	0.4094700000	-0.5341650000	4.4990900000
H21	1.2082910000	-1.6335290000	6.1776340000
H22	3.0106960000	-2.7078060000	4.8363600000
H23	3.2141450000	-2.2300170000	2.4222000000
H24	-0.1550260000	0.4515000000	2.6602000000
H25	-0.3755390000	-0.0567870000	5.0768180000
C26	4.8997600000	2.9237740000	0.1292290000
C27	3.9321860000	2.7324750000	-0.8638960000
C28	2.9718420000	1.7245390000	-0.7242420000
C29	2.9833450000	0.8951910000	0.4081950000
C30	3.9506480000	1.0909020000	1.4050140000
C31	4.9060490000	2.1042940000	1.2638470000
H32	5.6380930000	3.7125410000	0.0244500000
H33	3.9136180000	3.3740810000	-1.7388520000
H34	2.2061300000	1.5958060000	-1.4817360000
H35	3.9532480000	0.4690700000	2.2934670000
H36	5.6469280000	2.2564690000	2.0424550000
C37	-0.3259540000	-1.3776080000	-2.1965830000
H38	-0.0230100000	-2.2758580000	-1.6642240000
C39	-1.7228880000	-1.0932660000	-2.2429680000
H40	-2.1340260000	-0.6556340000	-3.1449660000
H41	-2.3913720000	-1.7802630000	-1.7374650000
C42	-4.8421380000	2.0521760000	-0.9575280000
C43	-4.6526320000	0.8979950000	-0.1886490000
C44	-3.4719770000	0.1559220000	-0.3127080000
C45	-2.4622920000	0.5789010000	-1.1932350000
C46	-2.6613030000	1.7293810000	-1.9747920000
C47	-3.8438880000	2.4658130000	-1.8490690000

H48	-5.7591160000	2.6251370000	-0.8631910000
H49	-5.4206370000	0.5731140000	0.5069620000
H50	-3.3345530000	-0.7399650000	0.2854790000
H51	-1.8877470000	2.0744160000	-2.6527600000
H52	-3.9808270000	3.3659000000	-2.4408520000
C53	2.4007020000	-0.1934770000	-5.3185860000
C54	1.2600880000	0.5784860000	-5.0610460000
C55	0.3740880000	0.2115690000	-4.0461470000
C56	0.6087100000	-0.9370620000	-3.2581550000
C57	1.7606780000	-1.7043860000	-3.5314400000
C58	2.6443270000	-1.3372850000	-4.5499290000
H59	3.0876090000	0.0927760000	-6.1085130000
H60	1.0608930000	1.4673780000	-5.6515930000
H61	-0.5008470000	0.8248040000	-3.8603710000
H62	1.9555510000	-2.5965320000	-2.9464880000
H63	3.5220600000	-1.9463120000	-4.7420920000

Neutral structure after TS leading to stilbene (Chloride trans to alkene)

Gas phase energy (Lacvp*): -2164.593767 au
Gas phase energy (Lacv3p**+): -2164.990714au
Solvation energy: -0.0240685 au
Total Gibbs free energy: -2164.666939au
Dispersion energy: -0.09223477 au
ZPE: 1329.24kJ/mol

Pd1	-0.2788275445	0.2309283550	-0.6667088894
P2	1.6344189310	-0.4229629492	0.4680517988
Cl3	-0.4716825103	2.3625930823	0.5266007007
C4	3.6631572456	-4.3584126069	-0.9606586056
C5	2.3775690490	-4.3736854235	-0.4119174482
C6	1.7881904895	-3.1868138955	0.0189524545
C7	2.4776877579	-1.9657582117	-0.0842329026
C8	3.7647250178	-1.9604883405	-0.6379751699
C9	4.3523484723	-3.1514890644	-1.0716499936
H10	4.1225067235	-5.2835306249	-1.2992905588
H11	1.8337029718	-5.3103803776	-0.3200856186
H12	0.7904079251	-3.2092005200	0.4508840756
H13	4.3121197508	-1.0282756925	-0.7307503275
H14	5.3525816025	-3.1315309545	-1.4969735327
C15	0.9169692583	-1.1757245387	5.0109566243
C16	1.8755935556	-1.9238777411	4.3261783037
C17	2.0888780090	-1.7139333974	2.9631566592
C18	1.3416027582	-0.7494564206	2.2641444897
C19	0.3819951508	0.0027670899	2.9599393381
C20	0.1768255509	-0.2125632682	4.3237296788
H21	0.7500927743	-1.3420761978	6.0721466273
H22	2.4615966794	-2.6749224696	4.8502843642
H23	2.8379408593	-2.3065631800	2.4479748609
H24	-0.1870737290	0.7655526061	2.4350281392
H25	-0.5681517183	0.3801530227	4.8483789225
C26	4.9735616149	2.7859716777	0.2261211577
C27	4.0058337630	2.6910375870	-0.7744431411
C28	2.9934558673	1.7360137661	-0.6822657188
C29	2.9506002900	0.8572052622	0.4089727711
C30	3.9230329064	0.9604701183	1.4149830582
C31	4.9286246419	1.9220888653	1.3219661259
H32	5.7558751958	3.5378091360	0.1579223783
H33	4.0273681719	3.3704044678	-1.6223646355
H34	2.2248843019	1.6818120066	-1.4474058834
H35	3.8915728839	0.2988254159	2.2756186939
H36	5.6741414867	1.9993507787	2.1093827443

C37	-0.3106675680	-1.2846637419	-2.1140498466
H38	0.0115547630	-2.2374132792	-1.6944905061
C39	-1.8208921291	-1.2782166371	-2.4393912937
H40	-1.9832245103	-1.1461641272	-3.5154281438
H41	-2.2524609241	-2.2495515090	-2.1697216992
C42	-4.1134427975	1.7298959985	-0.2881806902
C43	-3.7653851738	0.5316393741	0.3334681267
C44	-3.0018145839	-0.4160532820	-0.3496603844
C45	-2.5782662999	-0.1849157404	-1.6766460850
C46	-2.9491016261	1.0288428462	-2.2884640075
C47	-3.7044543163	1.9755644001	-1.6006529633
H48	-4.6997189986	2.4714170872	0.2470830694
H49	-4.0816539590	0.3338304891	1.3540028086
H50	-2.7643125683	-1.3650397236	0.1254742799
H51	-2.6640870533	1.2151946787	-3.3210077786
H52	-3.9739884160	2.9080190280	-2.0891384294
C53	2.3449609881	-0.0534104246	-5.2921390475
C54	1.2101801049	0.7045629435	-4.9950312699
C55	0.3500924406	0.3130238905	-3.9720054530
C56	0.6014939719	-0.8453002799	-3.2058331669
C57	1.7503232001	-1.5958868744	-3.5233295717
C58	2.6074600510	-1.2067603948	-4.5511216129
H59	3.0133203043	0.2496743099	-6.0940693366
H60	0.9921494341	1.6055029882	-5.5637386597
H61	-0.5207236992	0.9233563778	-3.7530415681
H62	1.9610481352	-2.5032393724	-2.9654265428
H63	3.4814027845	-1.8128908531	-4.7781246659

Neutral TS leading to α-phenyl styrene (Chloride trans to alkene)

Gas phase energy (Lacvp*): -2164.545655 au
Gas phase energy (Lacv3p**+): -2164.94525au
Solvation energy: -0.0262941 au
Total Gibbs free energy: -2164.620919au
Dispersion energy: -0.08468807 au
ZPE: 1316.6 kJ/mol
Neg. Freq: -296.25 cm^{-1}

Pd1	-1.2139650000	-0.4869210000	-0.8386050000
P2	1.1838170000	-0.5797390000	-0.2799580000
Cl3	-1.3692910000	-2.9716530000	-0.8063420000
C4	3.0597170000	3.7315520000	-0.3530990000
C5	3.3063300000	2.8491630000	-1.4097530000
C6	2.7864860000	1.5481060000	-1.3803210000
C7	2.0140760000	1.1173770000	-0.2899640000
C8	1.7576440000	2.0146030000	0.7631040000
C9	2.2829550000	3.3107440000	0.7336850000
H10	3.4656010000	4.7377880000	-0.3759180000
H11	3.9053460000	3.1674130000	-2.2572240000
H12	2.9920720000	0.8711510000	-2.2018990000
H13	1.1563670000	1.6999020000	1.6103920000
H14	2.0848840000	3.9895310000	1.5573080000
C15	3.8151730000	-3.1332890000	-3.2071600000
C16	4.4171780000	-2.4847290000	-2.1206960000
C17	3.6406390000	-1.7237090000	-1.2414400000
C18	2.2560010000	-1.6031850000	-1.4482620000
C19	1.6527850000	-2.2619590000	-2.5292580000
C20	2.4355790000	-3.0236120000	-3.4073460000
H21	4.4186430000	-3.7274280000	-3.8863300000
H22	5.4861650000	-2.5755160000	-1.9551150000
H23	4.1135940000	-1.2318160000	-0.3979980000

H24	0.5768270000	-2.2169870000	-2.6516730000
H25	1.9608890000	-3.5397200000	-4.2355310000
C26	2.1447210000	-2.3581730000	3.9601660000
C27	1.0215230000	-2.7823680000	3.2416810000
C28	0.7342070000	-2.2342220000	1.9853120000
C29	1.5795990000	-1.2525410000	1.4425440000
C30	2.7096550000	-0.8292810000	2.1630040000
C31	2.9884590000	-1.3812270000	3.4187710000
H32	2.3624030000	-2.7848840000	4.9343800000
H33	0.3649260000	-3.5423270000	3.6529370000
H34	-0.1277040000	-2.5769180000	1.4212920000
H35	3.3647000000	-0.0644110000	1.7601430000
H36	3.8621290000	-1.0474590000	3.9702170000
C37	-1.2228480000	1.6193560000	-1.0591460000
C38	-2.5035260000	1.5286500000	-1.6935740000
H39	-1.1840710000	2.0506580000	-0.0604270000
H40	-3.3464340000	1.9420590000	-1.1508570000
H41	-0.3572600000	1.8505930000	-1.6741040000
C42	-5.8411850000	-1.5894730000	-0.7247710000
C43	-5.1912280000	-1.6833820000	-1.9622860000
C44	-3.9485410000	-1.0691250000	-2.1546480000
C45	-3.3447090000	-0.3746440000	-1.0972610000
C46	-4.0113040000	-0.2506430000	0.1353260000
C47	-5.2507270000	-0.8738170000	0.3246490000
H48	-6.8056280000	-2.0665440000	-0.5808440000
H49	-5.6459080000	-2.2412250000	-2.7751980000
H50	-3.4478370000	-1.1477790000	-3.1129710000
H51	-3.5637740000	0.3169500000	0.9467350000
H52	-5.7535960000	-0.7958050000	1.2840160000
C53	-2.9923470000	1.8288610000	-5.9573280000
C54	-3.9738250000	2.3198830000	-5.0888660000
C55	-3.8116290000	2.1930780000	-3.7065080000
C56	-2.6612010000	1.5856190000	-3.1686330000
C57	-1.6856350000	1.0850590000	-4.0527170000
C58	-1.8499430000	1.2082730000	-5.4341260000
H59	-3.1189400000	1.9205330000	-7.0312440000
H60	-4.8644930000	2.7960590000	-5.4859910000
H61	-4.5788050000	2.5689070000	-3.0354910000
H62	-0.8108220000	0.5801450000	-3.6548300000
H63	-1.0918710000	0.8136310000	-6.1030320000

Neutral structure after TS leading to α-phenyl styrene (Chloride trans to alkene)

Gas phase energy (Lacvp*): -2164.590154 au
Gas phase energy (Lacv3p**+): -2164.988047au
Solvation energy: -0.0243279 au
Total Gibbs free energy: -2164.660793au
Dispersion energy: -0.08805159 au
ZPE: 1328.33 kJ/mol

Pd1	-1.2455117279	-0.6655553540	-0.6189253712
P2	1.0148798687	-0.5777012774	-0.2133325878
Cl3	-1.3793942242	-3.1139382939	-0.4576725175
C4	2.7942109592	3.6951946791	-0.7067442806
C5	3.0740855973	2.7148330355	-1.6584106701
C6	2.5742892312	1.4190992793	-1.5064639563
C7	1.7834415237	1.0869310077	-0.3973101828
C8	1.4979658085	2.0846377855	0.5512599280
C9	2.0044480122	3.3743238997	0.4002992680
H10	3.1846001237	4.7022358472	-0.8267294736
H11	3.6863131269	2.9537845381	-2.5243130106
H12	2.8056293706	0.6667302618	-2.2539502088

H13	0.8823596182	1.8501689424	1.4157384291
H14	1.7782270490	4.1308272801	1.1473511875
C15	3.4109401407	-3.2419491123	-3.1607573783
C16	4.0216126011	-2.7795707781	-1.9926800365
C17	3.3065198005	-1.9885055345	-1.0954060462
C18	1.9698565295	-1.6510707068	-1.3601548443
C19	1.3585978528	-2.1311040779	-2.5260246331
C20	2.0803682243	-2.9182891246	-3.4245613106
H21	3.9691107100	-3.8627901491	-3.8571169174
H22	5.0547305725	-3.0397290640	-1.7768934352
H23	3.7876820654	-1.6439993425	-0.1847837601
H24	0.3103796141	-1.9159236473	-2.7084682657
H25	1.5936603167	-3.2914259031	-4.3218196126
C26	2.2975863710	-2.0174931198	4.0212563685
C27	1.1687777665	-2.5519414762	3.3984029049
C28	0.7723462364	-2.1017219021	2.1379094895
C29	1.5128227440	-1.1052853195	1.4829630853
C30	2.6491227030	-0.5700590806	2.1140333125
C31	3.0368098996	-1.0254856165	3.3746569742
H32	2.6003393879	-2.3704117815	5.0038574092
H33	0.5882339794	-3.3268581111	3.8923133562
H34	-0.0964388524	-2.5357650410	1.6495869984
H35	3.2313761395	0.2071744371	1.6289685981
H36	3.9178510679	-0.6015069265	3.8501830988
C37	-1.4281243836	1.3724813248	-0.8812243351
C38	-2.7766507469	1.4640518142	-1.6211623861
H39	-1.4686798583	1.8196548414	0.1174627206
H40	-3.3969525128	2.2466569707	-1.1608174581
H41	-0.5979367752	1.8072127485	-1.4371053617
C42	-4.9795637207	-2.2129589173	-0.7621109198
C43	-4.6476998328	-1.9051433232	-2.0847174304
C44	-3.9189343888	-0.7580980261	-2.3857446974
C45	-3.5062747735	0.1185976129	-1.3621173959
C46	-3.8367252229	-0.2146066900	-0.0267043712
C47	-4.5736844676	-1.3668640336	0.2648070821
H48	-5.5438047198	-3.1133253586	-0.5369681071
H49	-4.9553128228	-2.5688455993	-2.8884059250
H50	-3.6772852539	-0.5252228593	-3.4174567830
H51	-3.5744988104	0.4711332168	0.7755754997
H52	-4.8180918806	-1.6001534029	1.2973255466
C53	-2.5168454686	2.4692793529	-5.8375471407
C54	-3.5411567154	2.9840480930	-5.0421806761
C55	-3.6070938718	2.6573520528	-3.6871049634
C56	-2.6564459936	1.8142737472	-3.0964433428
C57	-1.6314625730	1.3045666780	-3.9067228261
C58	-1.5624737316	1.6278634892	-5.2629453115
H59	-2.4616193949	2.7220965077	-6.8931744910
H60	-4.2900851872	3.6431504170	-5.4744782213
H61	-4.4104274034	3.0634694337	-3.0751605516
H62	-0.8831580527	0.6450764445	-3.4740295250
H63	-0.7590406181	1.2202077396	-5.8718380308

3-Coordinated TS (complex1-> complex 2)

Gas phase energy (Lacvp*): -1854.917591 au
Gas phase energy (Lacv3p**+): -1855.233582au
Solvation energy: -0.02565851au
Total Gibbs free energy: -1855.009094au
Dispersion energy: -0.06114166au
ZPE: 807.7367968kJ/mol

Pd1	1.9003870000	0.6459960000	-0.1241540000

Cl2	1.5288570000	2.1094000000	-1.9592490000
P3	1.5833880000	-1.5349810000	0.4417500000
C4	5.3517470000	-4.0706800000	1.4263690000
C5	4.6697460000	-4.2707710000	0.2262540000
C6	3.5290460000	-3.5219850000	-0.0694800000
C7	3.0591400000	-2.5575300000	0.8350520000
C8	3.7579150000	-2.3522720000	2.0381410000
C9	4.8911430000	-3.1103330000	2.3305190000
H10	6.2374500000	-4.6569310000	1.6560740000
H11	5.0205110000	-5.0141980000	-0.4847050000
H12	3.0064700000	-3.6930380000	-1.0048440000
H13	3.4193290000	-1.6035250000	2.7468180000
H14	5.4174670000	-2.9450190000	3.2668430000
C15	-1.5727100000	-2.2149610000	3.7792900000
C16	-1.7178880000	-1.1872280000	2.8437260000
C17	-0.7454040000	-0.9878700000	1.8649180000
C18	0.3845450000	-1.8209600000	1.8054800000
C19	0.5226840000	-2.8529810000	2.7448720000
C20	-0.4522330000	-3.0446860000	3.7269490000
H21	-2.3279420000	-2.3656040000	4.5459370000
H22	-2.5865290000	-0.5352350000	2.8781860000
H23	-0.8587100000	-0.1806460000	1.1445940000
H24	1.3884740000	-3.5069470000	2.7155600000
H25	-0.3321390000	-3.8459860000	4.4514890000
C26	-0.3714800000	-3.6048130000	-3.2322440000
C27	-0.5664630000	-4.1269550000	-1.9506870000
C28	0.0128570000	-3.5064300000	-0.8451700000
C29	0.7996230000	-2.3535680000	-1.0115010000
C30	0.9891350000	-1.8314060000	-2.3002930000
C31	0.4052600000	-2.4587300000	-3.4032480000
H32	-0.8299770000	-4.0866030000	-4.0917240000
H33	-1.1761330000	-5.0156750000	-1.8093420000
H34	-0.1544310000	-3.9160860000	0.1466430000
H35	1.5705270000	-0.9246550000	-2.4465130000
H36	0.5519760000	-2.0386360000	-4.3943160000
C37	4.0635000000	1.7676290000	3.9703360000
C38	4.8006250000	1.4874190000	2.8173120000
C39	4.1580830000	1.0460920000	1.6557570000
C40	2.7664100000	0.9040190000	1.6500240000
C41	2.0207030000	1.1681850000	2.8018300000
C42	2.6767330000	1.6086840000	3.9588650000
H43	4.5673460000	2.1065350000	4.8716200000
H44	5.8812870000	1.6090200000	2.8151610000
H45	4.7413800000	0.8284780000	0.7654080000
H46	0.9429170000	1.0406790000	2.8105450000
H47	2.0946110000	1.8239570000	4.8519150000

Chloride

Gas phase energy (Lacvp*): -460.2487411 au
Gas phase energy (Lacv3p**+): -460.3037263au
Solvation energy: -0.11572889au
Total Gibbs free energy: -460.4344782
Dispersion energy: 0 au
ΔG_{Therm}: -303.8462007KJ/mol

E-strain analysis

Cationic
TS for branched product, substrate
Gas phase energy (Lacvp*): -309.61526690653au

C1	-1.922606	0.520266	0.968131
C2	-0.589824	1.045612	0.942578
H3	-0.071439	1.105237	1.893616
H4	-2.307540	0.198323	1.933850
H5	-2.664977	0.998665	0.336928
C6	0.691796	4.116345	-1.774722
C7	1.279558	3.987501	-0.510876
C8	0.866648	2.968164	0.350584
C9	-0.150250	2.070505	-0.030993
C10	-0.729269	2.206398	-1.308504
C11	-0.311783	3.221441	-2.171526
H12	1.013577	4.904633	-2.446838
H13	2.056263	4.677002	-0.198330
H14	1.328432	2.868059	1.328606
H15	-1.500273	1.512535	-1.628421
H16	-0.764798	3.316219	-3.152852

Cationic
TS for branched product, complex
Gas phase energy (Lacvp*): -2430.75164451924au

C1	3.194529	-1.425701	1.352564
C2	2.112907	-1.744726	2.186096
C3	0.816154	-1.366976	1.820862
C4	0.587390	-0.704979	0.594502
C5	1.677054	-0.380059	-0.228564
C6	2.975491	-0.741404	0.151176
H7	4.203120	-1.696124	1.646671
H8	2.281635	-2.260251	3.126337
H9	-0.008432	-1.566357	2.499803
H10	1.520310	0.173053	-1.147959
H11	3.811105	-0.492765	-0.493700
Pd12	-1.390704	-1.228658	-0.143838
P13	-0.490215	-3.125976	-1.611815
P14	-3.871073	-1.775800	-0.201926
C15	4.149425	-3.516574	-2.277279
C16	3.395010	-2.614154	-3.037780
C17	2.016284	-2.501767	-2.830337
C18	1.378121	-3.300503	-1.865270
C19	2.136561	-4.200988	-1.104047
C20	3.518206	-4.305728	-1.310120
H21	5.217793	-3.608184	-2.443075
H22	3.876072	-2.004138	-3.795644
H23	1.440245	-1.808350	-3.434441
H24	1.659323	-4.830521	-0.361904
H25	4.094929	-5.012623	-0.722523
C26	-1.600671	-7.271838	0.308182
C27	-1.319325	-6.156691	1.105920
C28	-1.002786	-4.929810	0.509498
C29	-0.959679	-4.810444	-0.890550
C30	-1.243462	-5.931255	-1.686051
C31	-1.563241	-7.155856	-1.086708
H32	-1.848036	-8.222312	0.768963
H33	-1.350170	-6.238035	2.187409
H34	-0.792624	-4.066621	1.132805

H35	-1.233014	-5.854820	-2.766533
H36	-1.780601	-8.017167	-1.710042
C37	-2.008366	-3.047756	-6.057374
C38	-0.971510	-3.916701	-5.695133
C39	-0.510324	-3.950602	-4.374857
C40	-1.092102	-3.119037	-3.399918
C41	-2.121825	-2.243543	-3.773176
C42	-2.580247	-2.208814	-5.095753
H43	-2.361482	-3.021105	-7.082836
H44	-0.516583	-4.561803	-6.439515
H45	0.314036	-4.605460	-4.114750
H46	-2.564440	-1.591666	-3.029503
H47	-3.380421	-1.529970	-5.371108
C48	-5.906674	-4.678286	-3.291695
C49	-6.193652	-3.310452	-3.341838
C50	-5.600687	-2.429617	-2.427992
C51	-4.711182	-2.917132	-1.458500
C52	-4.429957	-4.292846	-1.405143
C53	-5.026435	-5.167268	-2.319138
H54	-6.369683	-5.358207	-3.998986
H55	-6.885934	-2.925271	-4.083386
H56	-5.848860	-1.375949	-2.469745
H57	-3.759583	-4.687575	-0.651080
H58	-4.803188	-6.227529	-2.266539
C59	-6.389822	2.184135	-0.499673
C60	-5.431079	1.867857	-1.470684
C61	-4.689670	0.686299	-1.363609
C62	-4.910052	-0.199031	-0.291123
C63	-5.868513	0.125123	0.679935
C64	-6.603006	1.314266	0.574141
H65	-6.961436	3.102522	-0.579009
H66	-5.257947	2.539773	-2.304845
H67	-3.939476	0.457187	-2.115723
H68	-6.047696	-0.538737	1.517291
H69	-7.340661	1.556049	1.332063
C70	-5.059288	-3.739257	3.895759
C71	-5.961279	-3.759433	2.824675
C72	-5.611388	-3.184731	1.597801
C73	-4.352483	-2.579793	1.435004
C74	-3.450374	-2.569266	2.509867
C75	-3.802654	-3.145355	3.736609
H76	-5.333342	-4.186718	4.845230
H77	-6.934943	-4.223405	2.941648
H78	-6.312742	-3.217508	0.771280
H79	-2.469674	-2.122705	2.383379
H80	-3.097799	-3.132399	4.561600

Cationic

TS for linear product, substrate

Gas phase energy (Lacvp*): -309.61929670152au

C1	15.173999	2.629242	-0.102148
C2	16.465824	2.258757	-0.565129
H3	17.325987	2.457330	0.062213
H4	14.495807	3.030776	-0.847767
H5	16.659765	2.372218	-1.625833
C6	14.377963	4.058841	3.876245
C7	15.484304	3.229149	3.649700
C8	15.750776	2.743855	2.367738
C9	14.907181	3.067743	1.281583
C10	13.797588	3.907365	1.527359

C11	13.539678	4.400615	2.807672
H12	16.146460	2.972039	4.469979
H13	16.626593	2.124554	2.211124
H14	13.146056	4.181972	0.703877
H15	12.688892	5.053574	2.971242
H16	14.179955	4.443657	4.870936

Cationic

TS for linear product, complex

Gas phase energy (Lacvp*): -2430.75823503729au

Pd1	14.775992	0.429347	-0.487518
P2	14.613402	-2.111896	-0.620596
P3	12.301325	0.955071	-0.959739
C4	18.011719	-4.609428	1.472494
C5	18.091803	-4.334624	0.103591
C6	17.090187	-3.586918	-0.527725
C7	15.990486	-3.119194	0.207348
C8	15.916451	-3.391240	1.583881
C9	16.923677	-4.131167	2.212219
H10	18.786407	-5.193519	1.958134
H11	18.931664	-4.701303	-0.477601
H12	17.172691	-3.375717	-1.586613
H13	15.068207	-3.050679	2.166780
H14	16.850021	-4.343554	3.273820
C15	10.895935	-3.894445	1.639160
C16	11.545736	-2.748060	2.110428
C17	12.636648	-2.222447	1.406667
C18	13.087737	-2.840463	0.228756
C19	12.429813	-3.986406	-0.242641
C20	11.339147	-4.510014	0.461905
H21	10.050817	-4.303608	2.182544
H22	11.202678	-2.256767	3.014653
H23	13.124531	-1.324205	1.770074
H24	12.749360	-4.465446	-1.159607
H25	10.838274	-5.398286	0.090844
C26	14.548894	-3.601308	-5.071030
C27	14.745349	-4.529608	-4.041296
C28	14.773465	-4.106929	-2.707688
C29	14.598468	-2.746311	-2.393074
C30	14.409592	-1.821123	-3.431312
C31	14.383050	-2.246662	-4.764605
H32	14.530184	-3.932203	-6.104035
H33	14.881507	-5.580503	-4.274156
H34	14.951212	-4.833832	-1.922797
H35	14.279131	-0.770642	-3.194751
H36	14.232832	-1.522920	-5.558755
C37	9.879398	-1.848027	-3.872627
C38	10.526824	-0.714163	-4.374406
C39	11.243334	0.127577	-3.515405
C40	11.320984	-0.161630	-2.143299
C41	10.669382	-1.301243	-1.642538
C42	9.951491	-2.136989	-2.505732
H43	9.319383	-2.495958	-4.538556
H44	10.466477	-0.473989	-5.430886
H45	11.715373	1.014236	-3.920643
H46	10.706043	-1.535580	-0.586214
H47	9.448074	-3.010062	-2.104409
C48	12.023957	5.094067	-3.192706
C49	12.982061	4.141906	-3.561566
C50	13.058174	2.923745	-2.876419

C51	12.167308	2.638355	-1.824153
C52	11.210896	3.597770	-1.458782
C53	11.143813	4.820856	-2.140460
H54	11.966844	6.040566	-3.719270
H55	13.669746	4.347270	-4.375368
H56	13.815485	2.197195	-3.160071
H57	10.518297	3.400024	-0.649125
H58	10.400762	5.555594	-1.848616
C59	9.508280	1.332044	2.794078
C60	8.941315	1.224903	1.517868
C61	9.762167	1.104614	0.390827
C62	11.161219	1.090149	0.535102
C63	11.724007	1.195112	1.816340
C64	10.899572	1.317485	2.941804
H65	8.869156	1.425479	3.665804
H66	7.863043	1.233481	1.398105
H67	9.312181	1.010492	-0.591289
H68	12.801058	1.189425	1.937633
H69	11.345812	1.405318	3.926774
C70	19.469725	-0.991472	-0.459490
C71	18.815491	-0.720285	0.749087
C72	17.558302	-0.106649	0.747655
C73	16.940298	0.247093	-0.469250
C74	17.594036	-0.053698	-1.681718
C75	18.849867	-0.672214	-1.674394
H76	20.453224	-1.449061	-0.454303
H77	19.282623	-0.983909	1.692210
H78	17.070530	0.106124	1.692800
H79	17.141104	0.222970	-2.629110
H80	19.348415	-0.885928	-2.614665

Cationic
square planar pre-insertion complex, substrate
Gas phase energy (Lacvp*): -309.63812694065au

C1	14.730415	2.947844	0.208259
C2	15.378736	2.538821	-0.923572
H3	16.456232	2.439081	-0.956287
H4	13.662910	3.144966	0.123363
H5	14.863388	2.579692	-1.876398
C6	16.314363	3.973975	4.039829
C7	17.187794	3.581995	3.020658
C8	16.694565	3.228806	1.769723
C9	15.309813	3.262829	1.513439
C10	14.443515	3.666007	2.548766
C11	14.939362	4.015987	3.801221
H12	18.258291	3.553528	3.203562
H13	17.386869	2.929224	0.990459
H14	13.373573	3.710505	2.359814
H15	14.257512	4.328344	4.587334
H16	16.706362	4.251198	5.014738

Cationic
square planar pre-insertion complex, complex
Gas phase energy (Lacvp*): -2430.78951564941au

Pd1	14.602716	0.263885	-0.548253
P2	14.571814	-2.131127	-0.668281
P3	12.153288	0.793795	-1.261288
C4	17.999365	-4.648325	1.228500
C5	18.179573	-4.019707	-0.005856

C6	17.152227	-3.265649	-0.568944
C7	15.921183	-3.131471	0.094741
C8	15.747097	-3.765540	1.334148
C9	16.781254	-4.517490	1.894566
H10	18.800707	-5.238897	1.663571
H11	19.123289	-4.117092	-0.535570
H12	17.311749	-2.786707	-1.529449
H13	14.803773	-3.689157	1.864415
H14	16.625866	-5.008368	2.851605
C15	10.896153	-3.937587	1.534928
C16	11.519478	-2.780976	2.007408
C17	12.598565	-2.233266	1.310581
C18	13.069270	-2.834414	0.133066
C19	12.437293	-3.996639	-0.335223
C20	11.359327	-4.541900	0.363510
H21	10.055481	-4.364863	2.074320
H22	11.164402	-2.298518	2.913751
H23	13.071934	-1.328926	1.682556
H24	12.772352	-4.473607	-1.250097
H25	10.878992	-5.441692	-0.011878
C26	14.576427	-3.483733	-5.110505
C27	14.822619	-4.416817	-4.100896
C28	14.833193	-4.019372	-2.765096
C29	14.583173	-2.677901	-2.422562
C30	14.347692	-1.748795	-3.444779
C31	14.343323	-2.149106	-4.780981
H32	14.575142	-3.796302	-6.151174
H33	15.016616	-5.455598	-4.353755
H34	15.055948	-4.749588	-1.993032
H35	14.173965	-0.707376	-3.190848
H36	14.160160	-1.417498	-5.563114
C37	9.593042	-2.044291	-3.939220
C38	10.175031	-0.907308	-4.497715
C39	10.932853	-0.042278	-3.707693
C40	11.125166	-0.306573	-2.343009
C41	10.534587	-1.454703	-1.789110
C42	9.772861	-2.312092	-2.581824
H43	8.996643	-2.712083	-4.554956
H44	10.029989	-0.679993	-5.550640
H45	11.349686	0.849724	-4.161532
H46	10.649391	-1.674589	-0.733771
H47	9.315785	-3.189221	-2.131772
C48	12.069118	4.849375	-3.562332
C49	12.876647	3.795677	-3.995259
C50	12.892879	2.593549	-3.288732
C51	12.088634	2.415359	-2.147303
C52	11.281539	3.481606	-1.724228
C53	11.276762	4.689263	-2.426336
H54	12.061347	5.789699	-4.106317
H55	13.499628	3.911114	-4.878117
H56	13.536887	1.786847	-3.634305
H57	10.650761	3.375328	-0.847808
H58	10.647159	5.505329	-2.081898
C59	9.530149	1.504543	2.513292
C60	8.915909	1.309518	1.274361
C61	9.687568	1.082212	0.135149
C62	11.089377	1.044979	0.221945
C63	11.695641	1.236853	1.472811
C64	10.921541	1.468452	2.611324
H65	8.925209	1.680502	3.398699

H66	7.832549	1.335000	1.193301
H67	9.197234	0.929173	-0.821532
H68	12.778559	1.199471	1.560543
H69	11.406246	1.613405	3.573350
C70	19.134947	-0.116708	1.094101
C71	18.051697	-0.204312	1.969570
C72	16.740005	-0.143170	1.482485
C73	16.510921	0.006697	0.111893
C74	17.594990	0.080054	-0.771033
C75	18.903683	0.027152	-0.276416
H76	20.151436	-0.166828	1.474614
H77	18.220486	-0.322573	3.037318
H78	15.911118	-0.220169	2.181931
H79	17.434860	0.188032	-1.841718
H80	19.741009	0.094896	-0.967340

Neutral via **3**

TS for branched product, substrate

Gas phase energy (Lacvp*): -309.61276158374au

C1	-1.028194	-3.316130	-0.759132
C2	0.204186	-2.942471	-1.402325
H3	-0.969432	-3.901614	0.156584
H4	1.108322	-3.392872	-1.003519
H5	-1.900844	-3.532309	-1.367246
C6	0.438592	-2.452541	-5.676494
C7	1.536435	-2.928542	-4.950671
C8	1.451559	-3.062829	-3.561889
C9	0.267126	-2.734071	-2.876679
C10	-0.828532	-2.248813	-3.616142
C11	-0.742521	-2.111826	-5.003987
H12	0.502281	-2.345109	-6.754549
H13	2.455433	-3.194134	-5.463322
H14	2.307210	-3.429337	-3.001543
H15	-1.743837	-1.972895	-3.101679
H16	-1.596168	-1.738522	-5.560612

Neutral via **3**

TS for branched product, komplex

Gas phase energy (Lacvp*): -1854.87380081521au

Pd1	-1.346996	-1.333907	-0.145357
P2	-1.797698	1.048672	0.611874
Cl3	-3.697513	-1.926717	0.246828
C4	1.572995	4.269896	-0.038112
C5	1.651693	3.367887	1.029831
C6	0.643375	2.418591	1.226393
C7	-0.466332	2.371469	0.365523
C8	-0.535985	3.272852	-0.708858
C9	0.480319	4.215174	-0.910127
H10	2.355455	5.007164	-0.188639
H11	2.498341	3.399383	1.708637
H12	0.722643	1.717872	2.050484
H13	-1.385536	3.249924	-1.382143
H14	0.410770	4.909366	-1.741979
C15	-2.894841	1.332623	5.179538
C16	-2.288560	2.427161	4.552914
C17	-1.944750	2.360209	3.197171
C18	-2.203258	1.193046	2.458090
C19	-2.816410	0.097148	3.088930
C20	-3.159068	0.171468	4.444619

H21	-3.160233	1.385595	6.230911
H22	-2.082570	3.333090	5.114905
H23	-1.466276	3.211572	2.726286
H24	-3.043704	-0.796563	2.517427
H25	-3.635201	-0.679658	4.920997
C26	-5.476994	2.993904	-1.569049
C27	-4.865910	1.848356	-2.089266
C28	-3.779376	1.266709	-1.423651
C29	-3.294056	1.835117	-0.237029
C30	-3.914472	2.980745	0.286319
C31	-5.001821	3.557542	-0.378215
H32	-6.323768	3.439805	-2.081495
H33	-5.240905	1.396112	-3.001797
H34	-3.331597	0.356006	-1.804010
H35	-3.561238	3.417119	1.214300
H36	-5.479421	4.440112	0.035887
C37	3.197892	0.178960	-0.004485
C38	2.481972	0.432329	-1.181465
C39	1.287965	-0.250427	-1.439333
C40	0.790145	-1.186846	-0.514465
C41	1.522912	-1.441337	0.666136
C42	2.712192	-0.751436	0.925146
H43	4.131183	0.699634	0.185547
H44	2.851679	1.159386	-1.897429
H45	0.753965	-0.070952	-2.366240
H46	1.171254	-2.190662	1.370148
H47	3.266321	-0.952225	1.837315

Neutral via **3**

TS for linear product, substrate

Gas phase energy (Lacvp*): -309.61873806255au

C1	-0.216008	0.106267	3.272933
C2	-1.527573	-0.254116	2.834927
H3	-1.976796	-1.168787	3.204219
H4	-2.243222	0.553174	2.714054
H5	-0.022592	1.159641	3.460899
C6	2.554554	-2.535976	5.239609
C7	1.318599	-3.031105	4.806743
C8	0.408822	-2.190103	4.160602
C9	0.716884	-0.830723	3.929179
C10	1.967887	-0.346450	4.374935
C11	2.872852	-1.189084	5.021025
H12	3.258780	-3.190364	5.743555
H13	1.059268	-4.071363	4.978650
H14	-0.547902	-2.596007	3.848869
H15	2.229142	0.686450	4.173443
H16	3.829691	-0.796158	5.349889

Neutral via **3**

TS for linear product, complex

Gas phase energy (Lacvp*): -1854.88162963451au

Pd1	0.113035	0.307182	1.107501
Cl2	1.955221	1.894452	1.583712
P3	0.520923	0.616588	-1.346134
C4	0.568004	5.152532	-2.553624
C5	-0.057541	4.734891	-1.373943
C6	-0.048881	3.381573	-1.015560
C7	0.577369	2.437611	-1.842658

C8	1.209198	2.860050	-3.022645
C9	1.204337	4.214166	-3.375336
H10	0.569164	6.203211	-2.826521
H11	-0.536231	5.459871	-0.723548
H12	-0.496102	3.062220	-0.080965
H13	1.714104	2.141630	-3.659221
H14	1.701058	4.534765	-4.285785
C15	4.659516	-1.084680	-2.795356
C16	4.488167	-0.633345	-1.481937
C17	3.249191	-0.137259	-1.058412
C18	2.168490	-0.090382	-1.955397
C19	2.344248	-0.539632	-3.275658
C20	3.585956	-1.035554	-3.691596
H21	5.621219	-1.470865	-3.118732
H22	5.316835	-0.663707	-0.781727
H23	3.126218	0.230212	-0.045286
H24	1.517852	-0.516743	-3.977165
H25	3.710712	-1.381729	-4.713081
C26	-2.624053	-1.224660	-4.320102
C27	-1.700866	-2.046683	-3.662320
C28	-0.761201	-1.491490	-2.787991
C29	-0.725539	-0.103060	-2.572247
C30	-1.656852	0.716170	-3.229451
C31	-2.602649	0.156160	-4.097666
H32	-3.352293	-1.656954	-4.999229
H33	-1.713135	-3.119728	-3.825757
H34	-0.057448	-2.139894	-2.277414
H35	-1.640678	1.789058	-3.074746
H36	-3.314149	0.801469	-4.603680
C37	-3.151218	-2.939961	-0.367035
C38	-3.551261	-1.597778	-0.319918
C39	-2.763878	-0.651908	0.343800
C40	-1.558940	-1.033146	0.970533
C41	-1.164231	-2.389147	0.916081
C42	-1.951556	-3.330530	0.242777
H43	-3.768537	-3.673976	-0.875086
H44	-4.473907	-1.287732	-0.800564
H45	-3.091348	0.382588	0.388178
H46	-0.251614	-2.706037	1.410780
H47	-1.634153	-4.368635	0.205023

Neutral via **3**

square planar pre-insertion complex, substrate

Gas phase energy (Lacvp*): -309.63900634152au

C	0.311158	0.266385	3.483225
C	-0.932405	0.696502	3.103155
H	-1.796739	0.040720	3.089467
H	-1.116955	1.761503	2.995647
H	1.091599	1.021475	3.539728
C	1.610800	-3.592999	4.801876
C	0.251115	-3.374736	4.563630
C	-0.195310	-2.131720	4.125088
C	0.712505	-1.077955	3.918008
C	2.077313	-1.310534	4.168777
C	2.524174	-2.556347	4.602330
H	1.955176	-4.565945	5.143478
H	-0.464027	-4.178338	4.718899
H	-1.254141	-1.979350	3.942462
H	2.786967	-0.500961	4.014345

H	3.583141	-2.717277	4.786970

Neutral via **3**

square planar pre-insertion complex, complex

Gas phase energy (Lacvp*): -1854.91117969156au

Pd	0.095659	0.551967	0.979407
Cl	1.538187	2.512617	1.437210
P	0.472213	0.738259	-1.345322
C	0.389650	5.145262	-2.794754
C	-0.389818	4.743724	-1.709108
C	-0.338468	3.424697	-1.260142
C	0.482984	2.490497	-1.905522
C	1.264297	2.899471	-2.995450
C	1.218447	4.222630	-3.434391
H	0.358322	6.177059	-3.135604
H	-1.024714	5.461447	-1.196560
H	-0.915374	3.124740	-0.391020
H	1.915972	2.190863	-3.497755
H	1.834627	4.532152	-4.274700
C	4.698048	-0.830985	-2.473864
C	4.471263	-0.190457	-1.254382
C	3.194673	0.260740	-0.920818
C	2.127124	0.075825	-1.814719
C	2.362405	-0.561404	-3.043267
C	3.642462	-1.013311	-3.367365
H	5.693937	-1.185423	-2.727998
H	5.290729	-0.039289	-0.556473
H	3.025038	0.775680	0.021417
H	1.550377	-0.709926	-3.747574
H	3.811639	-1.507713	-4.320764
C	-2.523542	-1.333389	-4.252598
C	-1.654664	-2.096566	-3.469179
C	-0.756577	-1.475160	-2.603885
C	-0.702996	-0.073424	-2.514608
C	-1.580790	0.685022	-3.303317
C	-2.485369	0.057309	-4.162774
H	-3.225521	-1.820296	-4.924549
H	-1.679661	-3.181756	-3.523160
H	-0.104434	-2.086370	-1.989030
H	-1.559759	1.768577	-3.254296
H	-3.156422	0.662978	-4.766656
C	-2.438824	-3.530773	0.402422
C	-3.085077	-2.296822	0.295535
C	-2.362237	-1.105914	0.423956
C	-0.983357	-1.132188	0.676802
C	-0.341071	-2.373981	0.787501
C	-1.064997	-3.565084	0.647932
H	-3.000638	-4.455464	0.295227
H	-4.155468	-2.257596	0.103698
H	-2.883050	-0.156655	0.319621
H	0.726993	-2.424307	0.986370
H	-0.549335	-4.519451	0.735289

Neutral via **2**

TS for branched product, substrate

Gas phase energy (Lacvp*): -309.61616977590au

C1	-1.222848	1.619356	-1.059146
C2	-2.503526	1.528650	-1.693574

H3	-1.184071	2.050658	-0.060427
H4	-3.346434	1.942059	-1.150857
H5	-0.357260	1.850593	-1.674104
C6	-2.992347	1.828861	-5.957328
C7	-3.973825	2.319883	-5.088866
C8	-3.811629	2.193078	-3.706508
C9	-2.661201	1.585619	-3.168633
C10	-1.685635	1.085059	-4.052717
C11	-1.849943	1.208273	-5.434126
H12	-3.118940	1.920533	-7.031244
H13	-4.864493	2.796059	-5.485991
H14	-4.578805	2.568907	-3.035491
H15	-0.810822	0.580145	-3.654830
H16	-1.091871	0.813631	-6.103032

Neutral via **2**

TS for branched product, complex

Gas phase energy (Lacvp*): -1854.86759055109au

Pd1	-1.213965	-0.486921	-0.838605
P2	1.183817	-0.579739	-0.279958
Cl3	-1.369291	-2.971653	-0.806342
C4	3.059717	3.731552	-0.353099
C5	3.306330	2.849163	-1.409753
C6	2.786486	1.548106	-1.380321
C7	2.014076	1.117377	-0.289964
C8	1.757644	2.014603	0.763104
C9	2.282955	3.310744	0.733685
H10	3.465601	4.737788	-0.375918
H11	3.905346	3.167413	-2.257224
H12	2.992072	0.871151	-2.201899
H13	1.156367	1.699902	1.610392
H14	2.084884	3.989531	1.557308
C15	3.815173	-3.133289	-3.207160
C16	4.417178	-2.484729	-2.120696
C17	3.640639	-1.723709	-1.241440
C18	2.256001	-1.603185	-1.448262
C19	1.652785	-2.261959	-2.529258
C20	2.435579	-3.023612	-3.407346
H21	4.418643	-3.727428	-3.886330
H22	5.486165	-2.575516	-1.955115
H23	4.113594	-1.231816	-0.397998
H24	0.576827	-2.216987	-2.651673
H25	1.960889	-3.539720	-4.235531
C26	2.144721	-2.358173	3.960166
C27	1.021523	-2.782368	3.241681
C28	0.734207	-2.234222	1.985312
C29	1.579599	-1.252541	1.442544
C30	2.709655	-0.829281	2.163004
C31	2.988459	-1.381227	3.418771
H32	2.362403	-2.784884	4.934380
H33	0.364926	-3.542327	3.652937
H34	-0.127704	-2.576918	1.421292
H35	3.364700	-0.064411	1.760143
H36	3.862129	-1.047459	3.970217
C37	-5.841185	-1.589473	-0.724771
C38	-5.191228	-1.683382	-1.962286
C39	-3.948541	-1.069125	-2.154648
C40	-3.344709	-0.374644	-1.097261
C41	-4.011304	-0.250643	0.135326
C42	-5.250727	-0.873817	0.324649

H43	-6.805628	-2.066544	-0.580844
H44	-5.645908	-2.241225	-2.775198
H45	-3.447837	-1.147779	-3.112971
H46	-3.563774	0.316950	0.946735
H47	-5.753596	-0.795805	1.284016

Neutral via **2**

TS for linear product, substrate

Gas phase energy (Lacvp*): -309.61938381914au

C1	-0.325954	-1.377608	-2.196583
H2	-0.023010	-2.275858	-1.664224
C3	-1.722888	-1.093266	-2.242968
H4	-2.134026	-0.655634	-3.144966
H5	-2.391372	-1.780263	-1.737465
C6	2.400702	-0.193477	-5.318586
C7	1.260088	0.578486	-5.061046
C8	0.374088	0.211569	-4.046147
C9	0.608710	-0.937062	-3.258155
C10	1.760678	-1.704386	-3.531440
C11	2.644327	-1.337285	-4.549929
H12	3.087609	0.092776	-6.108513
H13	1.060893	1.467378	-5.651593
H14	-0.500847	0.824804	-3.860371
H15	1.955551	-2.596532	-2.946488
H16	3.522060	-1.946312	-4.742092

Neutral via **2**

TS for linear product, complex

Gas phase energy (Lacvp*): -1854.86886391799au

Pd1	-0.452792	0.116686	-0.596014
P2	1.688060	-0.465803	0.526502
Cl3	-0.539367	2.129098	0.842201
C4	3.840077	-4.336951	-1.061875
C5	2.568602	-4.408066	-0.475839
C6	1.951312	-3.247306	0.001406
C7	2.599054	-2.001989	-0.098718
C8	3.871353	-1.937147	-0.684041
C9	4.488376	-3.101652	-1.162777
H10	4.320030	-5.237404	-1.431657
H11	2.061860	-5.363937	-0.387317
H12	0.972344	-3.312280	0.467752
H13	4.382217	-0.984966	-0.767121
H14	5.475146	-3.039376	-1.610841
C15	1.300513	-1.417883	5.117632
C16	2.313284	-2.022573	4.364361
C17	2.431178	-1.748035	2.996766
C18	1.533849	-0.862747	2.372680
C19	0.521740	-0.252671	3.131600
C20	0.409470	-0.534165	4.499090
H21	1.208291	-1.633529	6.177634
H22	3.010696	-2.707806	4.836360
H23	3.214145	-2.230017	2.422200
H24	-0.155026	0.451500	2.660200
H25	-0.375539	-0.056787	5.076818
C26	4.899760	2.923774	0.129229
C27	3.932186	2.732475	-0.863896
C28	2.971842	1.724539	-0.724242
C29	2.983345	0.895191	0.408195
C30	3.950648	1.090902	1.405014

C31	4.906049	2.104294	1.263847
H32	5.638093	3.712541	0.024450
H33	3.913618	3.374081	-1.738852
H34	2.206130	1.595806	-1.481736
H35	3.953248	0.469070	2.293467
H36	5.646928	2.256469	2.042455
C37	-4.842138	2.052176	-0.957528
C38	-4.652632	0.897995	-0.188649
C39	-3.471977	0.155922	-0.312708
C40	-2.462292	0.578901	-1.193235
C41	-2.661303	1.729381	-1.974792
C42	-3.843888	2.465813	-1.849069
H43	-5.759116	2.625137	-0.863191
H44	-5.420637	0.573114	0.506962
H45	-3.334553	-0.739965	0.285479
H46	-1.887747	2.074416	-2.652760
H47	-3.980827	3.365900	-2.440852

Neutral via **2**
square planar pre-insertion complex,substrate
Gas phase energy (Lacvp*): -309.63568983949au

C1	-1.941205	1.556276	-0.370821
C2	-2.451974	1.305750	-1.630489
H3	-2.615653	1.568627	0.480100
H4	-3.499366	1.028676	-1.691404
H5	-0.978275	2.034231	-0.232301
C6	-0.784053	2.065748	-5.501709
C7	-1.966378	1.336480	-5.358518
C8	-2.484302	1.095730	-4.089091
C9	-1.826878	1.568847	-2.938050
C10	-0.642070	2.307487	-3.096830
C11	-0.127536	2.550807	-4.367930
H12	-0.379599	2.260478	-6.491738
H13	-2.486570	0.959544	-6.235274
H14	-3.405210	0.528392	-3.975376
H15	-0.127017	2.704263	-2.228722
H16	0.788310	3.126264	-4.472686

Neutral via **2**
square planar pre-insertion complex,complex
Gas phase energy (Lacvp*): -1854.88945040165au

Pd1	-1.583217	-0.656456	-0.652667
P2	0.985150	-0.461184	-0.465911
Cl3	-1.229901	-3.020045	-0.655646
C4	2.937239	3.752687	-0.925879
C5	3.197472	2.767996	-1.878843
C6	2.641053	1.492820	-1.748344
C7	1.817323	1.182242	-0.657156
C8	1.567100	2.181596	0.301131
C9	2.121327	3.454277	0.168502
H10	3.369234	4.744415	-1.030927
H11	3.839039	2.988070	-2.728621
H12	2.852328	0.737768	-2.498490
H13	0.952316	1.956903	1.169837
H14	1.918614	4.211541	0.921531
C15	3.041559	-3.039402	-3.734581
C16	3.637113	-2.936791	-2.476793
C17	3.034534	-2.175539	-1.474710
C18	1.825838	-1.511003	-1.722988

C19	1.225543	-1.630540	-2.985419
C20	1.835571	-2.383989	-3.987587
H21	3.510993	-3.636304	-4.512551
H22	4.571100	-3.453850	-2.271346
H23	3.502723	-2.108577	-0.497395
H24	0.272363	-1.146160	-3.178545
H25	1.359357	-2.471458	-4.960699
C26	2.599666	-1.879726	3.673341
C27	1.373589	-2.338898	3.190990
C28	0.895016	-1.912060	1.950633
C29	1.643760	-1.014081	1.173395
C30	2.879366	-0.558439	1.665674
C31	3.352450	-0.989370	2.905287
H32	2.967017	-2.211803	4.640920
H33	0.781387	-3.035383	3.778778
H34	-0.049074	-2.292750	1.574071
H35	3.472917	0.141542	1.085584
H36	4.309769	-0.625478	3.270219
C37	-6.290327	-1.744649	-0.345308
C38	-5.580517	-2.049675	-1.509525
C39	-4.219477	-1.745394	-1.609909
C40	-3.561716	-1.121188	-0.544481
C41	-4.268312	-0.816491	0.622127
C42	-5.630345	-1.132946	0.720048
H43	-7.346524	-1.989807	-0.267673
H44	-6.082729	-2.539951	-2.341082
H45	-3.670619	-2.022751	-2.505460
H46	-3.770234	-0.351449	1.469871
H47	-6.169458	-0.901416	1.636349