

ELECTRONIC SUPPLEMENTARY INFORMATION

Catalyst-Transfer Polymerization of Arylamines by Buchwald-Hartwig Cross-Coupling

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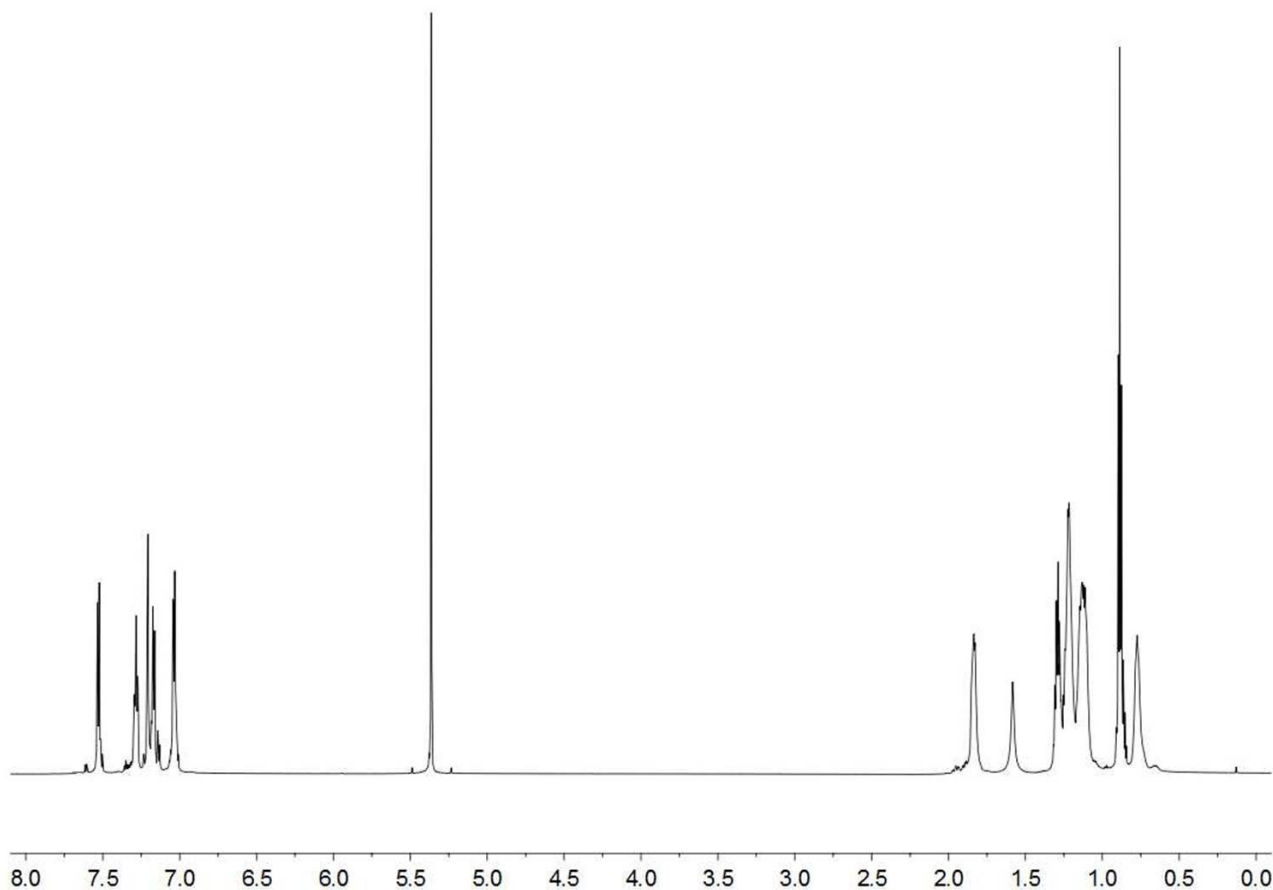


Figure S1. ¹H-NMR spectrum of **POLY-A** in CD₂Cl₂.

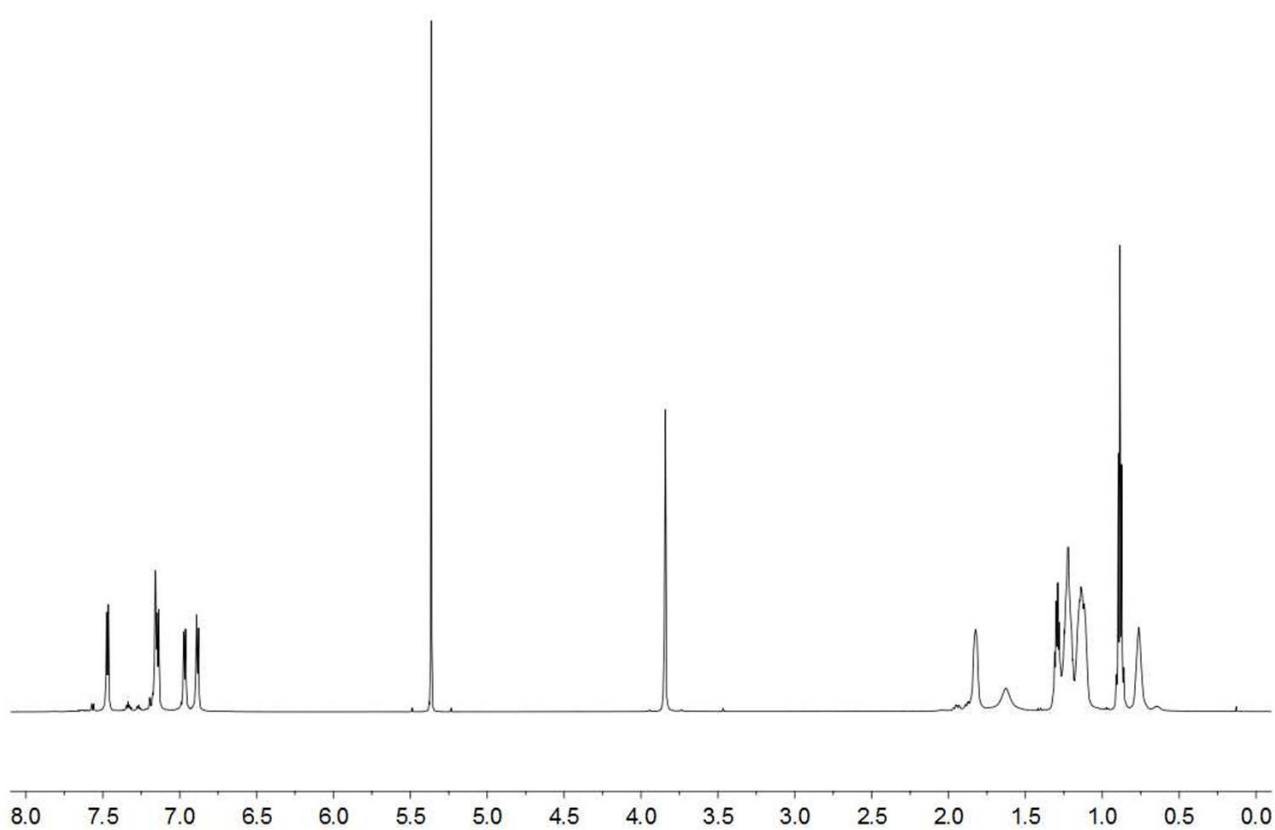


Figure S2. ^1H -NMR spectrum of **POLY-B** in CD_2Cl_2 .

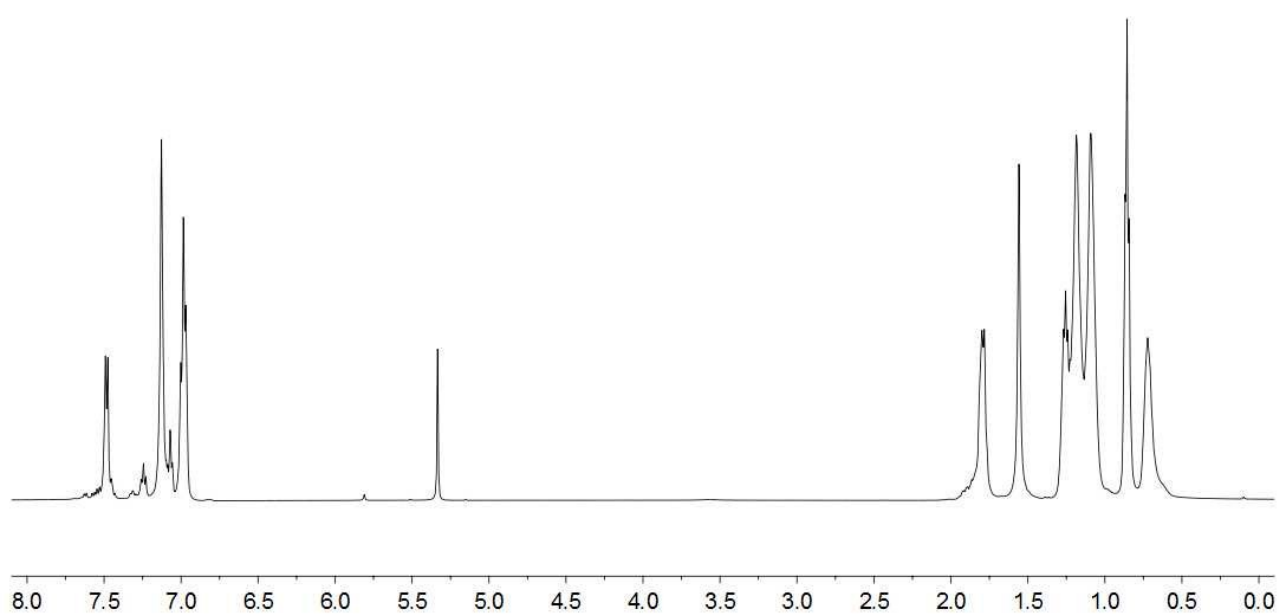
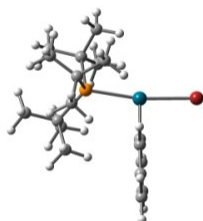


Figure S3. ^1H -NMR spectrum of **POLY-C** in CD_2Cl_2 .

XYZ Coordinates and Energies for Optimized Structures

Complex 1



P	-1.18249	3.17807	4.46448
C	-2.23868	2.14524	5.74234
C	-3.73183	2.17699	5.34518
C	-1.80571	0.66132	5.62194
C	-2.11882	2.59006	7.21316
H	-4.20112	3.14543	5.52363
H	-3.88855	1.89586	4.29992
H	-4.26397	1.44363	5.96245
H	-0.75905	0.48568	5.86212
H	-2.41096	0.06402	6.31513
H	-1.99407	0.24929	4.62043
H	-2.79159	1.97282	7.82165
H	-1.11275	2.45638	7.61446
H	-2.41049	3.63201	7.36101
C	0.56892	3.52878	5.22734
C	1.14724	2.20853	5.78515
C	1.53189	3.97071	4.10156
C	0.59132	4.59444	6.34269
H	0.63607	1.86008	6.68398
H	1.13248	1.40981	5.03762
H	2.19457	2.38211	6.05859
H	1.26559	4.92501	3.65067
H	2.53266	4.08365	4.53622
H	1.59224	3.23	3.30418
H	1.61049	4.65717	6.74374
H	0.33552	5.58863	5.97016
H	-0.07197	4.35898	7.17691
C	-2.08936	4.85663	4.10776
C	-1.13156	5.80746	3.35522
C	-3.27898	4.58118	3.15682
C	-2.61359	5.58523	5.36249
H	-0.32899	6.18655	3.99051
H	-0.69317	5.34114	2.46961
H	-1.70949	6.67649	3.01893
H	-4.10026	4.05276	3.63814
H	-3.67226	5.54265	2.80568
H	-2.97426	4.0014	2.28381
H	-3.07868	6.52816	5.04923
H	-3.37751	5.01336	5.89222
H	-1.82133	5.83452	6.07052
Pd	-1.20209	1.5757	2.69409
C	-0.1715	2.50304	1.26497
C	1.14933	2.09908	1.05086
C	-0.7617	3.45661	0.43535
C	1.89427	2.69369	0.02667
H	1.5949	1.31794	1.65741
C	-0.00598	4.04282	-0.58869
H	-1.80113	3.73867	0.55683
C	1.32257	3.67025	-0.79067

H	2.92117	2.3768	-0.13556
H	-0.47018	4.78606	-1.23177
H	1.90337	4.12514	-1.58774
Br	-1.62296	-0.45032	1.2536

Zero-point correction= 0.468848 (Hartree/Particle)

Thermal correction to Energy= 0.495634

Thermal correction to Enthalpy= 0.496578

Thermal correction to Gibbs Free Energy= 0.413234

Sum of electronic and zero-point Energies= -1185.519145

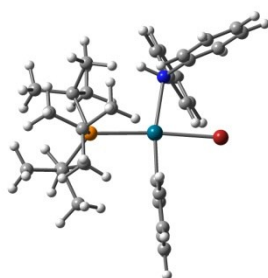
Sum of electronic and thermal Energies= -1185.492359

Sum of electronic and thermal Enthalpies= -1185.491415

Sum of electronic and thermal Free Energies= -1185.574760

E(RM062X) = -1185.98799337

Complex 2A



P	-1.33566	3.12458	4.4938
C	-2.04618	2.17118	6.07218
C	-3.58836	2.07362	6.03873
C	-1.51331	0.7199	5.98871
C	-1.69083	2.7584	7.45571
H	-4.07975	3.03057	6.22785
H	-3.95389	1.64486	5.10487
H	-3.89258	1.39647	6.84844
H	-0.42433	0.65679	6.02752
H	-1.90727	0.15549	6.84505
H	-1.85975	0.23166	5.07488
H	-2.16812	2.12773	8.21737
H	-0.62309	2.76473	7.67727
H	-2.08039	3.77104	7.59332
C	0.41064	3.83914	5.08015
C	1.25316	2.65705	5.61337
C	1.24128	4.41558	3.90897
C	0.34877	4.96063	6.14378
H	0.89554	2.25143	6.55997
H	1.29541	1.84606	4.88109
H	2.28051	3.00798	5.77748
H	0.74139	5.2095	3.35861
H	2.15787	4.84433	4.33803
H	1.53439	3.6477	3.19994
H	1.36916	5.15017	6.50456
H	-0.00809	5.89875	5.71034
H	-0.26515	4.7348	7.0131
C	-2.48871	4.66018	4.15041
C	-1.7601	5.64372	3.20997
C	-3.71999	4.1458	3.37183
C	-2.96203	5.45476	5.38568
H	-0.99389	6.22913	3.72407
H	-1.29879	5.13265	2.36206
H	-2.49625	6.35441	2.81188
H	-4.32318	3.43324	3.93152
H	-4.35442	5.00598	3.11525
H	-3.42256	3.64374	2.44819
H	-3.56908	6.30429	5.04348
H	-3.58927	4.86453	6.05489
H	-2.13363	5.86267	5.96774
C	0.36425	2.28133	1.6456
C	1.57605	1.57856	1.75721
C	0.33446	3.39107	0.78642
C	2.72593	2.00462	1.08724
H	1.6149	0.67727	2.36229
C	1.48106	3.81366	0.10123
H	-0.5938	3.93639	0.63542
C	2.68765	3.13055	0.25783
H	3.65408	1.44671	1.20185
H	1.42624	4.67909	-0.55751

H	3.58126	3.46012	-0.26749
Pd	-1.30206	1.57737	2.53367
Br	-0.89908	-0.19131	0.93187
N	-3.07692	0.75241	2.83316
C	-3.93647	1.00232	1.66712
C	-4.37547	-0.06466	0.88271
C	-4.31326	2.30608	1.34497
C	-5.19054	0.17223	-0.22399
H	-4.07761	-1.09233	1.1365
C	-5.12938	2.54311	0.23855
H	-3.96749	3.14712	1.96321
C	-5.56793	1.47649	-0.546
H	-5.53609	-0.66866	-0.84269
H	-5.42665	3.57114	-0.01497
H	-6.21064	1.66302	-1.41861
C	-2.918	-0.69657	3.02319
C	-3.82113	-1.58075	2.4324
C	-1.86428	-1.18752	3.79403
C	-3.6709	-2.95553	2.61301
H	-4.65221	-1.19334	1.82538
C	-1.71329	-2.56274	3.97398
H	-1.15227	-0.4908	4.25959
C	-2.61644	-3.44675	3.38375
H	-4.38309	-3.65249	2.14789
H	-0.88214	-2.94957	4.58146
H	-2.49816	-4.53076	3.52597
H	-3.49671	1.15145	3.64835

Zero-point correction= 0.672188 (Hartree/Particle)

Thermal correction to Energy= 0.710407

Thermal correction to Enthalpy= 0.711351

Thermal correction to Gibbs Free Energy= 0.601403

Sum of electronic and zero-point Energies= -1703.759692

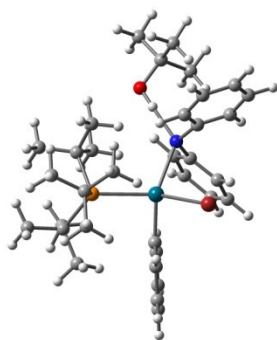
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Sum of electronic and thermal Enthalpies= -1703.720529

Sum of electronic and thermal Free Energies= -1703.830478

E(RM062X) = -1704.43188041

Complex 3A



P	-1.24908	3.28087	4.43345
C	-2.40987	2.35051	5.71515
C	-3.86731	2.49102	5.22652
C	-2.00837	0.85755	5.69911
C	-2.36554	2.83463	7.17404
H	-4.29741	3.44956	5.50559
H	-3.96965	2.4034	4.14724
H	-4.47414	1.71414	5.69786
H	-1.17667	0.65878	6.36867
H	-2.85232	0.25485	6.04402
H	-1.71827	0.50575	4.71035
H	-3.11296	2.26543	7.73466
H	-1.40117	2.64819	7.64033
H	-2.60716	3.88969	7.27752
C	0.47005	3.54988	5.33527
C	0.92433	2.19358	5.904
C	1.55539	3.9872	4.33339
C	0.41584	4.58616	6.46986
H	0.37464	1.91155	6.79822
H	0.83502	1.39662	5.16331
H	1.97826	2.2786	6.1795
H	1.28219	4.8441	3.72725
H	2.44455	4.25358	4.91214
H	1.82078	3.17484	3.66699
H	1.36547	4.5364	7.01003
H	0.31426	5.59983	6.08883
H	-0.38052	4.40433	7.18362
C	-2.02399	5.05353	4.10312
C	-0.94782	5.99033	3.52459
C	-3.11718	4.89919	3.02954
C	-2.62234	5.73489	5.34433
H	-0.20271	6.27165	4.26409
H	-0.44303	5.5561	2.66614
H	-1.4455	6.90587	3.19524
H	-3.98674	4.35822	3.3949
H	-3.45302	5.89555	2.73234
H	-2.73487	4.39145	2.14171
H	-2.96673	6.72917	5.04636
H	-3.48085	5.20296	5.74389
H	-1.89245	5.865	6.14005
C	0.27984	2.69617	1.56905
C	1.43691	1.9181	1.66657
C	0.32578	3.93253	0.92937
C	2.64831	2.40156	1.16576
H	1.40104	0.941	2.13244
C	1.54294	4.42058	0.44144
H	-0.5783	4.50803	0.78443
C	2.70673	3.66096	0.56544
H	3.5407	1.79586	1.24558

H	1.574	5.385	-0.04711
H	3.64472	4.03778	0.18284
Pd	-1.38637	1.85882	2.19979
Br	-1.55239	1.05398	-0.33422
N	-3.24845	0.33127	2.66792
C	-4.2526	0.44683	1.6263
C	-4.63199	-0.64056	0.84169
C	-4.83832	1.69774	1.41075
C	-5.58623	-0.46908	-0.16321
H	-4.17912	-1.60828	0.99648
C	-5.7996	1.85798	0.41821
H	-4.51319	2.54915	1.99379
C	-6.17642	0.77407	-0.37851
H	-5.86574	-1.31501	-0.77498
H	-6.24312	2.83055	0.25891
H	-6.91533	0.90086	-1.15609
C	-2.78358	-1.01332	2.97425
C	-3.47405	-1.76628	3.92663
C	-1.66902	-1.5498	2.33257
C	-3.03611	-3.04692	4.25771
H	-4.34993	-1.34624	4.40487
C	-1.24061	-2.83814	2.65874
H	-1.15664	-0.96802	1.58029
C	-1.91645	-3.58583	3.62293
H	-3.56868	-3.62005	5.00269
H	-0.37543	-3.25205	2.16143
H	-1.576	-4.57919	3.8765
H	-3.60714	0.74863	3.5222
O	-3.94599	1.14291	4.32925
C	-5.18645	0.52332	4.67893
C	-5.03058	-0.21624	6.0207
H	-5.22841	0.46014	6.82585
H	-5.72274	-1.03121	6.06126
H	-4.03229	-0.59151	6.10724
C	-6.27917	1.60048	4.81041
H	-7.238	1.15911	4.63507
H	-6.25295	2.01673	5.79577
H	-6.1058	2.37401	4.09173
C	-5.58547	-0.48151	3.58226
H	-6.15007	-1.27928	4.0178
H	-6.17989	0.01422	2.84347
H	-4.70368	-0.87765	3.12353

Zero-point correction= 0.795477 (Hartree/Particle)

Thermal correction to Energy= 0.841468

Thermal correction to Enthalpy= 0.842412

Thermal correction to Gibbs Free Energy= 0.717547

Sum of electronic and zero-point Energies= -1936.721514

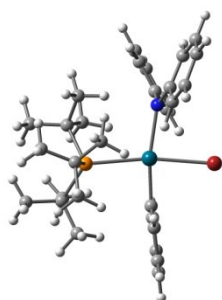
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Sum of electronic and thermal Enthalpies= -1936.674580

Sum of electronic and thermal Free Energies= -1936.799445

E(RM062X) = -1937.51699185

Complex 4A



P	-1.14404	3.56323	4.48486
C	-2.37013	2.90575	5.86735
C	-3.80704	3.09199	5.35308
C	-2.14102	1.38993	5.98438
C	-2.24891	3.55299	7.25364
H	-4.11201	4.13534	5.33245
H	-3.92677	2.64627	4.36654
H	-4.47719	2.5491	6.0211
H	-1.20116	1.13531	6.4651
H	-2.9599	0.95939	6.5636
H	-2.1739	0.93097	4.99985
H	-3.03672	3.13102	7.88442
H	-1.29748	3.3341	7.7339
H	-2.38716	4.63195	7.22799
C	0.6111	3.79031	5.34195
C	0.94917	2.48504	6.08343
C	1.73381	3.99506	4.305
C	0.66282	4.96749	6.33209
H	0.3592	2.35347	6.98629
H	0.81346	1.61614	5.43713
H	2.00165	2.52573	6.37671
H	1.53413	4.78425	3.58933
H	2.63939	4.2619	4.85869
H	1.93597	3.08207	3.75382
H	1.6073	4.90226	6.88043
H	0.65403	5.9264	5.81687
H	-0.14373	4.95814	7.05861
C	-1.75841	5.34132	3.9278
C	-0.617	6.04897	3.17861
C	-2.90444	5.16352	2.91445
C	-2.23597	6.24458	5.07494
H	0.18778	6.35806	3.84076
H	-0.20673	5.41755	2.39116
H	-1.02515	6.94846	2.7106
H	-3.78109	4.69355	3.34863
H	-3.1998	6.15468	2.55845
H	-2.58657	4.57486	2.05263
H	-2.48699	7.22265	4.65369
H	-3.13077	5.85763	5.55606
H	-1.4733	6.39707	5.83451
C	0.38651	2.19801	1.9552
C	1.12697	1.08716	2.37835
C	1.00227	3.18658	1.18681
C	2.48536	0.98471	2.06064
H	0.65111	0.2968	2.95034
C	2.36257	3.08682	0.88159
H	0.42625	4.01859	0.81034
C	3.10955	1.99254	1.32325
H	3.0491	0.12267	2.39162

H	2.83516	3.86225	0.29355
H	4.16154	1.92018	1.0852
Pd	-1.52292	2.05055	2.39895
Br	-2.07255	2.57968	-0.28863
N	-3.46955	0.66725	2.67782
C	-4.52715	0.87935	1.78204
C	-5.06704	-0.1084	0.92672
C	-5.18108	2.132	1.80208
C	-6.20469	0.14459	0.15994
H	-4.59724	-1.08035	0.87203
C	-6.31533	2.37559	1.04012
H	-4.75883	2.91238	2.41853
C	-6.84757	1.3817	0.20993
H	-6.59242	-0.63853	-0.47912
H	-6.78511	3.34969	1.08565
H	-7.72875	1.57282	-0.38565
C	-2.60415	-0.44497	2.48429
C	-2.19935	-1.21126	3.59859
C	-2.01825	-0.75478	1.23502
C	-1.22368	-2.19818	3.48009
H	-2.682	-1.02759	4.54743
C	-1.04748	-1.74888	1.12255
H	-2.31593	-0.18529	0.3663
C	-0.63135	-2.46946	2.24361
H	-0.9324	-2.76453	4.35503
H	-0.6056	-1.94986	0.1555
H	0.12813	-3.2334	2.15377

Zero-point correction= 0.658063 (Hartree/Particle)

Thermal correction to Energy= 0.695693

Thermal correction to Enthalpy= 0.696637

Thermal correction to Gibbs Free Energy= 0.589978

Sum of electronic and zero-point Energies= -1703.286935

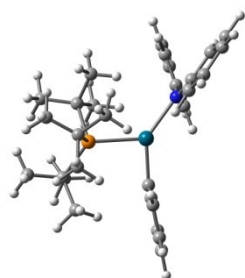
Sum of electronic and thermal Energies= -1703.249305

Sum of electronic and thermal Enthalpies= -1703.248361

Sum of electronic and thermal Free Energies= -1703.355020

E(RM062X) = -1703.94499815

Complex 5A



P	-0.97661	3.31755	4.27955
C	-1.94252	2.19691	5.57604
C	-3.41715	2.1507	5.13636
C	-1.37123	0.76808	5.47342
C	-1.88799	2.63041	7.04906
H	-3.92841	3.09584	5.30431
H	-3.50671	1.87079	4.08734
H	-3.92242	1.39032	5.73763
H	-0.43722	0.65828	6.01682
H	-2.09568	0.07231	5.90462
H	-1.21256	0.46647	4.44157
H	-2.53519	1.95159	7.61277
H	-0.88852	2.54402	7.4698
H	-2.25287	3.64248	7.2097
C	0.74157	3.77206	5.1255
C	1.40044	2.46242	5.59313
C	1.73093	4.42827	4.14074
C	0.59566	4.72481	6.32678
H	0.93527	2.06136	6.48992
H	1.3795	1.70283	4.81016
H	2.44676	2.67396	5.8294
H	1.31973	5.26834	3.59463
H	2.57573	4.79288	4.73359
H	2.11337	3.71254	3.42318
H	1.56207	4.76475	6.83839
H	0.3573	5.73806	6.00875
H	-0.1477	4.40617	7.04866
C	-1.95992	4.99966	4.08618
C	-1.03944	6.07537	3.48454
C	-3.0677	4.76125	3.04613
C	-2.57423	5.555	5.3808
H	-0.3107	6.45302	4.19734
H	-0.51692	5.70696	2.60207
H	-1.66691	6.91596	3.17578
H	-3.70122	3.90584	3.26276
H	-3.69702	5.65447	2.99233
H	-2.61958	4.6037	2.06547
H	-3.02013	6.52703	5.15
H	-3.36515	4.92029	5.77176
H	-1.835	5.70894	6.16296
C	0.71284	2.71304	1.57167
C	1.77931	1.84382	1.84152
C	0.98007	3.92884	0.93433
C	3.08957	2.19557	1.50491
H	1.59112	0.88628	2.31299
C	2.29075	4.28664	0.60448
H	0.16655	4.59761	0.68255
C	3.35072	3.42467	0.89477
H	3.90177	1.51361	1.71992
H	2.48192	5.23359	0.11678

H	4.36402	3.70121	0.63823
Pd	-1.12012	2.0564	1.94906
N	-3.04965	0.92498	2.10502
C	-4.20992	1.25165	1.43419
C	-5.3144	0.37366	1.23733
C	-4.32063	2.52687	0.81499
C	-6.44809	0.77376	0.53371
H	-5.2711	-0.63317	1.6235
C	-5.45799	2.915	0.12006
H	-3.4682	3.1853	0.86734
C	-6.55008	2.05055	-0.02236
H	-7.26016	0.06751	0.41171
H	-5.48726	3.89964	-0.32993
H	-7.43482	2.3542	-0.56333
C	-2.90841	-0.33368	2.71663
C	-3.83754	-0.85619	3.64351
C	-1.73749	-1.08665	2.48494
C	-3.59437	-2.05202	4.31483
H	-4.7388	-0.29637	3.85225
C	-1.49295	-2.27708	3.16646
H	-1.02902	-0.71536	1.75633
C	-2.41693	-2.77036	4.09037
H	-4.32084	-2.41784	5.02915
H	-0.58083	-2.82474	2.96845
H	-2.22819	-3.69479	4.61763

Zero-point correction= 0.657849 (Hartree/Particle)

Thermal correction to Energy= 0.693386

Thermal correction to Enthalpy= 0.694331

Thermal correction to Gibbs Free Energy= 0.591772

Sum of electronic and zero-point Energies= -1689.976628

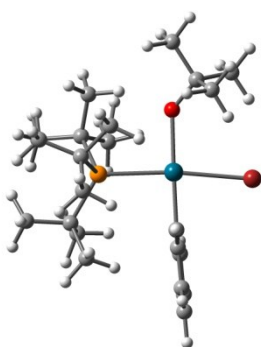
Sum of electronic and thermal Energies= -1689.941090

Sum of electronic and thermal Enthalpies= -1689.940146

Sum of electronic and thermal Free Energies= -1690.042704

E(RM062X) = -1690.63447671

Complex 2B



P	-1.33566	3.12458	4.4938
C	-2.04618	2.17118	6.07218
C	-3.58836	2.07362	6.03873
C	-1.51331	0.7199	5.98871
C	-1.69083	2.7584	7.45571
H	-4.07975	3.03057	6.22785
H	-3.95389	1.64486	5.10487
H	-3.89258	1.39647	6.84844
H	-0.42433	0.65679	6.02752
H	-1.90727	0.15549	6.84505
H	-1.85975	0.23166	5.07488
H	-2.16812	2.12773	8.21737
H	-0.62309	2.76473	7.67727
H	-2.08039	3.77104	7.59332
C	0.41064	3.83914	5.08015
C	1.25316	2.65705	5.61337
C	1.24128	4.41558	3.90897
C	0.34877	4.96063	6.14378
H	0.89554	2.25143	6.55997
H	1.29541	1.84606	4.88109
H	2.28051	3.00798	5.77748
H	0.74139	5.2095	3.35861
H	2.15787	4.84433	4.33803
H	1.53439	3.6477	3.19994
H	1.36916	5.15017	6.50456
H	-0.00809	5.89875	5.71034
H	-0.26515	4.7348	7.0131
C	-2.48871	4.66018	4.15041
C	-1.7601	5.64372	3.20997
C	-3.71999	4.1458	3.37183
C	-2.96203	5.45476	5.38568
H	-0.99389	6.22913	3.72407
H	-1.29879	5.13265	2.36206
H	-2.49625	6.35441	2.81188
H	-4.32318	3.43324	3.93152
H	-4.35442	5.00598	3.11525
H	-3.42256	3.64374	2.44819
H	-3.56908	6.30429	5.04348
H	-3.58927	4.86453	6.05489
H	-2.13363	5.86267	5.96774
C	0.36425	2.28133	1.6456
C	1.57605	1.57856	1.75721
C	0.33446	3.39107	0.78642
C	2.72593	2.00462	1.08724
H	1.6149	0.67727	2.36229
C	1.48106	3.81366	0.10123
H	-0.5938	3.93639	0.63542
C	2.68765	3.13055	0.25783

H	3.65408	1.44671	1.20185
H	1.42624	4.67909	-0.55751
H	3.58126	3.46012	-0.26749
Pd	-1.30206	1.57737	2.53367
O	-3.04107	0.76907	2.82711
C	-3.35493	-0.09808	1.73421
C	-4.81751	-0.56531	1.85329
H	-5.03866	-1.25037	1.06166
H	-4.96116	-1.051	2.79582
H	-5.46891	0.28082	1.78513
C	-3.16444	0.65928	0.40691
H	-3.22501	1.71255	0.58539
H	-2.20578	0.42184	-0.00481
H	-3.93016	0.36966	-0.28207
C	-2.42087	-1.32207	1.76545
H	-3.00523	-2.21467	1.84723
H	-1.8448	-1.35421	0.86433
H	-1.76359	-1.24776	2.6065
Br	-0.89908	-0.19131	0.93187

Zero-point correction= 0.594373 (Hartree/Particle)

Thermal correction to Energy= 0.628285

Thermal correction to Enthalpy= 0.629229

Thermal correction to Gibbs Free Energy= 0.532069

Sum of electronic and zero-point Energies= -1418.479828

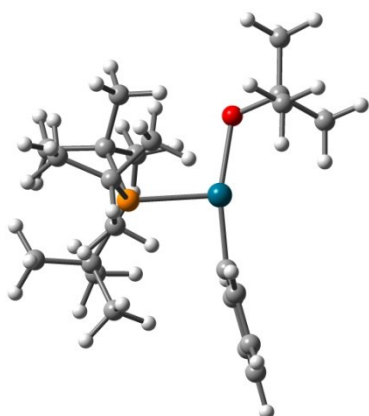
Sum of electronic and thermal Energies= -1418.445916

Sum of electronic and thermal Enthalpies= -1418.444972

Sum of electronic and thermal Free Energies= -1418.542132

E(RM062X) = -1419.07420096

Complex 3B



P	-1.33566	3.12458	4.4938
C	-2.04618	2.17118	6.07218
C	-3.58836	2.07362	6.03873
C	-1.51331	0.7199	5.98871
C	-1.69083	2.7584	7.45571
H	-4.07975	3.03057	6.22785
H	-3.95389	1.64486	5.10487
H	-3.89258	1.39647	6.84844
H	-0.42433	0.65679	6.02752
H	-1.90727	0.15549	6.84505
H	-1.85975	0.23166	5.07488
H	-2.16812	2.12773	8.21737
H	-0.62309	2.76473	7.67727
H	-2.08039	3.77104	7.59332
C	0.41064	3.83914	5.08015
C	1.25316	2.65705	5.61337
C	1.24128	4.41558	3.90897
C	0.34877	4.96063	6.14378
H	0.89554	2.25143	6.55997
H	1.29541	1.84606	4.88109
H	2.28051	3.00798	5.77748
H	0.74139	5.2095	3.35861
H	2.15787	4.84433	4.33803
H	1.53439	3.6477	3.19994
H	1.36916	5.15017	6.50456
H	-0.00809	5.89875	5.71034
H	-0.26515	4.7348	7.0131
C	-2.48871	4.66018	4.15041
C	-1.7601	5.64372	3.20997
C	-3.71999	4.1458	3.37183
C	-2.96203	5.45476	5.38568
H	-0.99389	6.22913	3.72407
H	-1.29879	5.13265	2.36206
H	-2.49625	6.35441	2.81188
H	-4.32318	3.43324	3.93152
H	-4.35442	5.00598	3.11525
H	-3.42256	3.64374	2.44819
H	-3.56908	6.30429	5.04348
H	-3.58927	4.86453	6.05489
H	-2.13363	5.86267	5.96774
C	0.36425	2.28133	1.6456
C	1.57605	1.57856	1.75721
C	0.33446	3.39107	0.78642
C	2.72593	2.00462	1.08724
H	1.6149	0.67727	2.36229
C	1.48106	3.81366	0.10123

H	-0.5938	3.93639	0.63542
C	2.68765	3.13055	0.25783
H	3.65408	1.44671	1.20185
H	1.42624	4.67909	-0.55751
H	3.58126	3.46012	-0.26749
Pd	-1.30206	1.57737	2.53367
O	-3.04107	0.76907	2.82711
C	-3.35493	-0.09808	1.73421
C	-4.81751	-0.56531	1.85329
H	-5.03866	-1.25037	1.06166
H	-4.96116	-1.051	2.79582
H	-5.46891	0.28082	1.78513
C	-3.16444	0.65928	0.40691
H	-3.22501	1.71255	0.58539
H	-2.20578	0.42184	-0.00481
H	-3.93016	0.36966	-0.28207
C	-2.42087	-1.32207	1.76545
H	-3.00523	-2.21467	1.84723
H	-1.8448	-1.35421	0.86433
H	-1.76359	-1.24776	2.6065

Zero-point correction= 0.594464 (Hartree/Particle)

Thermal correction to Energy= 0.626203

Thermal correction to Enthalpy= 0.627147

Thermal correction to Gibbs Free Energy= 0.534824

Sum of electronic and zero-point Energies= -1405.167122

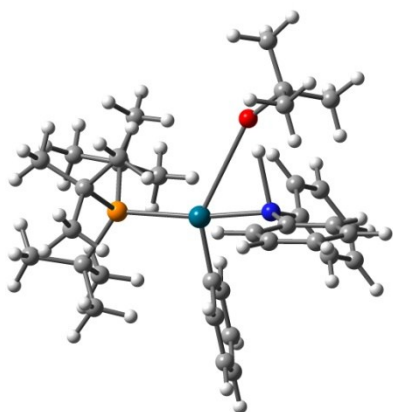
Sum of electronic and thermal Energies= -1405.135383

Sum of electronic and thermal Enthalpies= -1405.134439

Sum of electronic and thermal Free Energies= -1405.226763

E(RM062X) = -1405.76158641

Complex 4B



P	-2.67406	2.11114	5.27829
C	-2.34602	0.63941	6.61121
C	-3.16936	-0.59954	6.19326
C	-0.85053	0.25805	6.50029
C	-2.69041	1.0126	8.06615
H	-4.24715	-0.45584	6.33678
H	-2.9854	-0.90154	5.15203
H	-2.86269	-1.43935	6.83988
H	-0.17694	1.06105	6.81688
H	-0.66656	-0.61388	7.15073
H	-0.5912	-0.02263	5.46819
H	-2.52417	0.12292	8.69754
H	-2.05014	1.81234	8.4583
H	-3.73857	1.3126	8.18766
C	-2.04731	3.84241	6.07135
C	-0.62965	3.62604	6.64557
C	-1.93399	4.89656	4.94668
C	-2.97524	4.37822	7.1823
H	-0.62524	2.9802	7.53092
H	0.05509	3.21242	5.89422
H	-0.23504	4.60873	6.9536
H	-2.90174	5.17204	4.51628
H	-1.49405	5.80894	5.38426
H	-1.2793	4.55471	4.1388
H	-2.50756	5.28264	7.60785
H	-3.95901	4.67502	6.79724
H	-3.12191	3.66596	8.00267
C	-4.64379	2.24573	4.92407
C	-4.91879	3.5765	4.19149
C	-5.01238	1.10644	3.94602
C	-5.51824	2.15553	6.18976
H	-4.80078	4.45118	4.84144
H	-4.27296	3.69408	3.30923
H	-5.96474	3.56394	3.84185
H	-4.88269	0.10844	4.37469
H	-6.07351	1.22005	3.66598
H	-4.4107	1.16884	3.02602
H	-6.57386	2.26956	5.88923
H	-5.42615	1.18525	6.69359
H	-5.29318	2.94581	6.91538
C	-0.44578	2.67286	2.72136
C	0.84357	2.71873	3.28821
C	-0.81079	3.61682	1.74211
C	1.75226	3.71947	2.89146
H	1.1489	1.97824	4.02849
C	0.10451	4.61313	1.34833
H	-1.79814	3.5843	1.28116

C	1.3852	4.67032	1.92409
H	2.7478	3.74738	3.33866
H	-0.18958	5.34096	0.58963
H	2.09111	5.44363	1.61841
Pd	-1.68517	1.19325	3.23683
O	-2.79869	-2.02371	2.73686
C	-3.43066	-3.01723	1.82418
C	-4.16181	-3.98994	2.75539
H	-4.66093	-4.77984	2.17558
H	-3.44953	-4.45968	3.44843
H	-4.92088	-3.45531	3.34429
C	-4.41443	-2.29259	0.8895
H	-4.91825	-3.007	0.22
H	-5.18058	-1.76907	1.47962
H	-3.887	-1.55273	0.2691
C	-2.33015	-3.73394	1.02263
H	-2.76214	-4.50334	0.36443
H	-1.77986	-3.01735	0.3943
H	-1.61834	-4.21933	1.70544
N	-1.03776	0.02288	1.62276
C	-1.51229	0.26522	0.30833
C	-0.97273	-0.38092	-0.83987
C	-2.65568	1.08682	0.11527
C	-1.54639	-0.1977	-2.10664
H	-0.10992	-1.03716	-0.73207
C	-3.22052	1.26536	-1.15331
H	-3.09367	1.5729	0.99039
C	-2.66979	0.62907	-2.28123
H	-1.10997	-0.71229	-2.96489
H	-4.09754	1.90631	-1.26113
H	-3.10818	0.77065	-3.26934
C	0.30026	-0.46009	1.81474
C	0.53556	-1.44569	2.80385
C	1.4118	0.05999	1.10715
C	1.83706	-1.89392	3.07545
H	-0.32005	-1.8603	3.33781
C	2.70946	-0.39845	1.37651
H	1.25164	0.8367	0.35962
C	2.93262	-1.37709	2.36185
H	1.99362	-2.65616	3.84061
H	3.55209	0.0217	0.82463
H	3.94333	-1.72972	2.56982
H	-2.23715	-1.36304	2.22408

Zero-point correction= 0.796265 (Hartree/Particle)

Thermal correction to Energy= 0.839653

Thermal correction to Enthalpy= 0.840597

Thermal correction to Gibbs Free Energy= 0.721088

Sum of electronic and zero-point Energies= -1923.438381

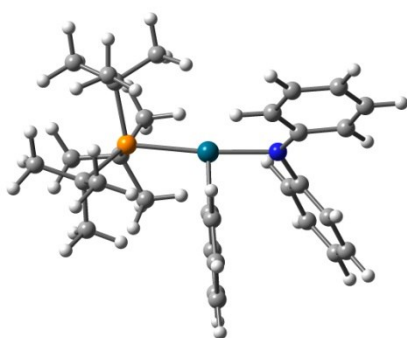
Sum of electronic and thermal Energies= -1923.394992

Sum of electronic and thermal Enthalpies= -1923.394048

Sum of electronic and thermal Free Energies= -1923.513557

E(RM062X) = -1924.23464526

Complex 5B



P	-3.11197	0.88719	5.30578
C	-2.24782	-0.36319	6.52561
C	-2.44581	-1.8044	6.00282
C	-0.72215	-0.10716	6.47531
C	-2.72874	-0.29778	7.98991
H	-3.47828	-2.16818	6.10227
H	-2.13088	-1.90397	4.95023
H	-1.80646	-2.47662	6.60251
H	-0.42994	0.89056	6.82671
H	-0.226	-0.84739	7.12874
H	-0.33524	-0.2448	5.45189
H	-2.20757	-1.0863	8.56262
H	-2.48763	0.66064	8.47283
H	-3.80874	-0.47744	8.09492
C	-3.26081	2.62001	6.17282
C	-1.90185	2.99699	6.80262
C	-3.55444	3.694	5.0985
C	-4.3495	2.69226	7.26528
H	-1.64262	2.37497	7.67113
H	-1.08318	2.95187	6.06817
H	-1.97125	4.03981	7.16065
H	-4.52987	3.571	4.61165
H	-3.55913	4.67997	5.59752
H	-2.77629	3.71023	4.3219
H	-4.30394	3.6936	7.73024
H	-5.36449	2.57375	6.85881
H	-4.20884	1.95256	8.06649
C	-4.90971	0.23953	4.90462
C	-5.73594	1.36902	4.24966
C	-4.79265	-0.87018	3.83051
C	-5.69324	-0.30749	6.11543
H	-6.01963	2.163	4.95497
H	-5.20844	1.82228	3.3944
H	-6.67287	0.92775	3.86506
H	-4.2	-1.73667	4.14929
H	-5.80877	-1.23206	3.58977
H	-4.36059	-0.47389	2.8937
H	-6.70845	-0.58358	5.77704
H	-5.2403	-1.21479	6.54138
H	-5.8061	0.43176	6.92132
C	-0.88205	2.33517	3.18145
C	0.31075	2.43056	3.92215
C	-1.23579	3.37642	2.30365
C	1.13046	3.56818	3.79883
H	0.6111	1.62597	4.5987
C	-0.41234	4.51232	2.18856
H	-2.14155	3.30769	1.69279
C	0.77014	4.61437	2.93674
H	2.05406	3.62898	4.38445

H	-0.70188	5.3162	1.50313
H	1.4081	5.49846	2.84358
Pd	-1.9686	0.65694	3.24301
N	-1.17639	-0.02503	1.4425
C	-1.67812	0.39174	0.20959
C	-1.09915	0.02888	-1.0412
C	-2.90061	1.12162	0.16086
C	-1.70354	0.39202	-2.25085
H	-0.17968	-0.5618	-1.0567
C	-3.49145	1.48431	-1.05239
H	-3.37948	1.38387	1.11297
C	-2.8989	1.12838	-2.27683
H	-1.22981	0.08672	-3.19026
H	-4.4302	2.04874	-1.04086
H	-3.36189	1.41161	-3.2263
C	0.15686	-0.47612	1.56069
C	0.42198	-1.59579	2.38821
C	1.26155	0.17113	0.95024
C	1.73101	-2.04558	2.60259
H	-0.42789	-2.1067	2.85341
C	2.56805	-0.28683	1.16256
H	1.08405	1.04802	0.32095
C	2.81466	-1.39692	1.9881
H	1.90434	-2.91511	3.24499
H	3.40385	0.23666	0.68659
H	3.83709	-1.75071	2.1497

Zero-point correction= 0.657285 (Hartree/Particle)

Thermal correction to Energy= 0.692975

Thermal correction to Enthalpy= 0.693919

Thermal correction to Gibbs Free Energy= 0.590957

Sum of electronic and zero-point Energies= -1689.991407

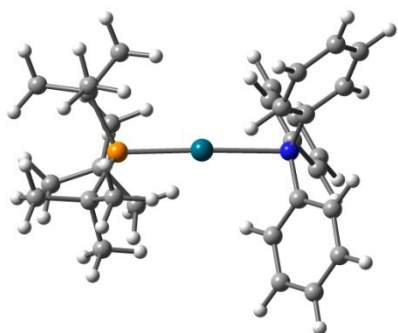
Sum of electronic and thermal Energies= -1689.955717

Sum of electronic and thermal Enthalpies= -1689.954773

Sum of electronic and thermal Free Energies= -1690.057735

E(RM062X) = -1690.64869201

Complex 6



P	-3.36744	1.0665	5.26249
C	-2.26993	2.02865	6.55728
C	-1.00583	1.19072	6.82483
C	-1.78878	3.33774	5.90068
C	-2.96588	2.35124	7.88647
H	-1.21497	0.28786	7.3944
H	-0.50323	0.9218	5.89336
H	-0.31637	1.79987	7.41514
H	-2.58088	4.0681	5.77364
H	-1.028	3.78266	6.54827
H	-1.33225	3.13963	4.93171
H	-2.23313	2.81045	8.55639
H	-3.77991	3.06241	7.75793
H	-3.35895	1.46541	8.38013
C	-5.13064	1.90015	5.19673
C	-4.94939	3.42396	5.08822
C	-5.81628	1.4528	3.89048
C	-6.03927	1.59193	6.39514
H	-4.61036	3.86824	6.0206
H	-4.25128	3.68812	4.29202
H	-5.91962	3.8647	4.84581
H	-6.02514	0.38868	3.85732
H	-6.76855	1.98329	3.80415
H	-5.20566	1.71266	3.02341
H	-6.9601	2.17321	6.29027
H	-6.32162	0.54228	6.44182
H	-5.57919	1.86686	7.34261
C	-3.57949	-0.77792	5.86403
C	-4.73154	-1.42676	5.07774
C	-2.30811	-1.54901	5.45709
C	-3.83535	-0.94442	7.36725
H	-5.70839	-1.05368	5.37362
H	-4.60333	-1.28338	4.00336
H	-4.71328	-2.5013	5.27678
H	-1.39556	-1.14512	5.88417
H	-2.41351	-2.58494	5.7913
H	-2.19858	-1.5467	4.37189
H	-4.02273	-2.0022	7.5727
H	-2.97583	-0.64325	7.96241
H	-4.70368	-0.38089	7.70414
C	-0.23232	1.00613	3.0109
C	0.33697	-0.21529	3.42385
C	0.45823	2.20066	3.28281
C	1.53905	-0.2292	4.12841
H	-0.16192	-1.14699	3.19928
C	1.66728	2.16774	3.98032
H	0.0594	3.15043	2.96213
C	2.21503	0.95992	4.41545
H	1.94551	-1.17755	4.45431

H	2.17676	3.09978	4.18628
H	3.1475	0.94416	4.9606
Pd	-2.28813	1.0116	3.01574
N	-1.06908	0.90368	1.27319
C	-0.89945	2.05231	0.47063
C	-0.29149	2.02364	-0.80084
C	-1.38724	3.29343	0.93015
C	-0.16258	3.18795	-1.55665
H	0.06188	1.09126	-1.21148
C	-1.24045	4.45188	0.17476
H	-1.91105	3.32754	1.87732
C	-0.62201	4.41365	-1.07658
H	0.301	3.12815	-2.5319
H	-1.62712	5.38532	0.56057
H	-0.51599	5.31231	-1.66621
C	-0.76607	-0.38812	0.74459
C	-1.77241	-1.3561	0.67266
C	0.54391	-0.73954	0.38873
C	-1.48179	-2.64785	0.23096
H	-2.77481	-1.08049	0.97242
C	0.83185	-2.0259	-0.06096
H	1.3296	-0.00323	0.49203
C	-0.18069	-2.98495	-0.14196
H	-2.26936	-3.38622	0.17799
H	1.8458	-2.28455	-0.33211
H	0.0448	-3.98463	-0.48448

Zero-point correction= 0.658689 (Hartree/Particle)

Thermal correction to Energy= 0.694589

Thermal correction to Enthalpy= 0.695533

Thermal correction to Gibbs Free Energy= 0.589327

Sum of electronic and zero-point Energies= -1690.016973

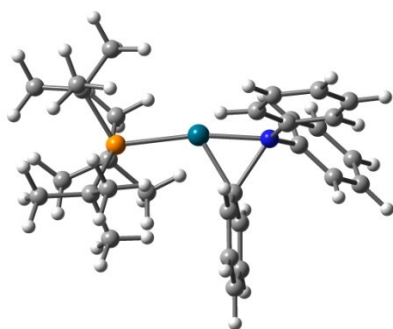
Sum of electronic and thermal Energies= -1689.981073

Sum of electronic and thermal Enthalpies= -1689.980129

Sum of electronic and thermal Free Energies= -1690.086335

E(RM062X) = -1690.67566210

Complex 5-TS



P	-3.11197	0.88719	5.30578
C	-2.24782	-0.36319	6.52561
C	-2.44581	-1.8044	6.00282
C	-0.72215	-0.10716	6.47531
C	-2.72874	-0.29778	7.98991
H	-3.47828	-2.16818	6.10227
H	-2.13088	-1.90397	4.95023
H	-1.80646	-2.47662	6.60251
H	-0.42994	0.89056	6.82671
H	-0.226	-0.84739	7.12874
H	-0.33524	-0.2448	5.45189
H	-2.20757	-1.0863	8.56262
H	-2.48763	0.66064	8.47283
H	-3.80874	-0.47744	8.09492
C	-3.26081	2.62001	6.17282
C	-1.90185	2.99699	6.80262
C	-3.55444	3.694	5.0985
C	-4.3495	2.69226	7.26528
H	-1.64262	2.37497	7.67113
H	-1.08318	2.95187	6.06817
H	-1.97125	4.03981	7.16065
H	-4.52987	3.571	4.61165
H	-3.55913	4.67997	5.59752
H	-2.77629	3.71023	4.3219
H	-4.30394	3.6936	7.73024
H	-5.36449	2.57375	6.85881
H	-4.20884	1.95256	8.06649
C	-4.90971	0.23953	4.90462
C	-5.73594	1.36902	4.24966
C	-4.79265	-0.87018	3.83051
C	-5.69324	-0.30749	6.11543
H	-6.01963	2.163	4.95497
H	-5.20844	1.82228	3.3944
H	-6.67287	0.92775	3.86506
H	-4.2	-1.73667	4.14929
H	-5.80877	-1.23206	3.58977
H	-4.36059	-0.47389	2.8937
H	-6.70845	-0.58358	5.77704
H	-5.2403	-1.21479	6.54138
H	-5.8061	0.43176	6.92132
C	-0.88205	2.33517	3.18145
C	0.31075	2.43056	3.92215
C	-1.23579	3.37642	2.30365
C	1.13046	3.56818	3.79883
H	0.6111	1.62597	4.5987
C	-0.41234	4.51232	2.18856
H	-2.14155	3.30769	1.69279
C	0.77014	4.61437	2.93674
H	2.05406	3.62898	4.38445
H	-0.70188	5.3162	1.50313

H	1.4081	5.49846	2.84358
Pd	-1.9686	0.65694	3.24301
N	-1.17639	-0.02503	1.4425
C	-1.67812	0.39174	0.20959
C	-1.09915	0.02888	-1.0412
C	-2.90061	1.12162	0.16086
C	-1.70354	0.39202	-2.25085
H	-0.17968	-0.5618	-1.0567
C	-3.49145	1.48431	-1.05239
H	-3.37948	1.38387	1.11297
C	-2.8989	1.12838	-2.27683
H	-1.22981	0.08672	-3.19026
H	-4.4302	2.04874	-1.04086
H	-3.36189	1.41161	-3.2263
C	0.15686	-0.47612	1.56069
C	0.42198	-1.59579	2.38821
C	1.26155	0.17113	0.95024
C	1.73101	-2.04558	2.60259
H	-0.42789	-2.1067	2.85341
C	2.56805	-0.28683	1.16256
H	1.08405	1.04802	0.32095
C	2.81466	-1.39692	1.9881
H	1.90434	-2.91511	3.24499
H	3.40385	0.23666	0.68659
H	3.83709	-1.75071	2.1497

Zero-point correction= 0.656527 (Hartree/Particle)

Thermal correction to Energy= 0.691551

Thermal correction to Enthalpy= 0.692495

Thermal correction to Gibbs Free Energy= 0.592263

Sum of electronic and zero-point Energies= -1689.967921

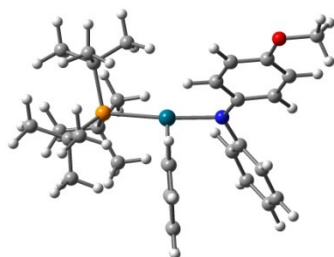
Sum of electronic and thermal Energies= -1689.932897

Sum of electronic and thermal Enthalpies= -1689.931953

Sum of electronic and thermal Free Energies= -1690.032185

E(RM062X) = -1690.62444791

Complex 5-OMe



P	-3.19883	0.86206	5.31067
C	-2.35063	-0.39477	6.53729
C	-2.62358	-1.83186	6.05803
C	-0.82548	-0.19732	6.43142
C	-2.79665	-0.25805	7.99961
H	-3.65579	-2.13999	6.20267
H	-2.35588	-1.9604	5.00767
H	-1.99335	-2.50441	6.64511
H	-0.49843	0.81307	6.65652
H	-0.34465	-0.87562	7.14138
H	-0.4782	-0.45449	5.42966
H	-2.33065	-1.06167	8.57643
H	-2.47847	0.685	8.4389
H	-3.87517	-0.34771	8.11598
C	-3.27532	2.61831	6.14667
C	-1.88362	2.9531	6.71214
C	-3.56914	3.67019	5.06024
C	-4.32527	2.73352	7.2619
H	-1.61489	2.33382	7.56418
H	-1.11237	2.86429	5.94589
H	-1.90174	3.99127	7.05262
H	-4.56775	3.58983	4.64458
H	-3.47978	4.65879	5.51864
H	-2.84451	3.60778	4.25168
H	-4.23123	3.72397	7.71555
H	-5.33913	2.64623	6.87616
H	-4.19066	1.99324	8.04735
C	-5.01626	0.25322	4.94038
C	-5.80016	1.3996	4.2788
C	-4.93656	-0.87647	3.89241
C	-5.78982	-0.23674	6.17263
H	-6.04753	2.19367	4.97871
H	-5.25439	1.82346	3.43408
H	-6.73965	0.99065	3.89897
H	-4.37874	-1.74345	4.2301
H	-5.95487	-1.20295	3.66541
H	-4.49827	-0.51797	2.95603
H	-6.81125	-0.47683	5.86431
H	-5.35937	-1.13878	6.60163
H	-5.8483	0.51963	6.95263
C	-0.81456	2.10441	3.18972
C	0.41704	2.00961	3.84279
C	-1.12952	3.25993	2.47003
C	1.31	3.08534	3.81221
H	0.69761	1.10154	4.35738
C	-0.23077	4.33134	2.43808
H	-2.06335	3.33271	1.92899
C	0.98672	4.25023	3.11504
H	2.25874	3.0045	4.32524
H	-0.48395	5.22221	1.87945
H	1.67941	5.07935	3.08918

Pd	-2.0334	0.54904	3.158
N	-1.11504	0.00889	1.36705
C	-1.68133	0.36417	0.14138
C	-1.16083	-0.0657	-1.10328
C	-2.88574	1.10509	0.10851
C	-1.80524	0.24033	-2.2983
H	-0.25831	-0.65931	-1.12215
C	-3.52338	1.40348	-1.09178
H	-3.31514	1.43638	1.04632
C	-2.99086	0.97914	-2.3113
H	-1.38076	-0.11348	-3.22874
H	-4.4427	1.9738	-1.0726
C	0.25593	-0.2934	1.48404
C	0.66367	-1.22572	2.45709
C	1.26001	0.37239	0.75357
C	2.01272	-1.47946	2.69363
H	-0.10192	-1.74196	3.02272
C	2.60751	0.10981	0.98745
H	0.97401	1.11505	0.02158
C	2.99742	-0.8161	1.95833
H	2.29491	-2.19997	3.44957
H	3.35813	0.64356	0.42007
H	4.04416	-1.01436	2.13856
O	-3.64674	1.28905	-3.54364
C	-3.30486	0.30796	-4.52623
H	-3.93302	0.42831	-5.38404
H	-2.28158	0.43214	-4.81325
H	-3.44415	-0.67067	-4.11663

Zero-point correction= 0.690426 (Hartree/Particle)

Thermal correction to Energy= 0.728662

Thermal correction to Enthalpy= 0.729606

Thermal correction to Gibbs Free Energy= 0.620795

Sum of electronic and zero-point Energies= -1804.428383

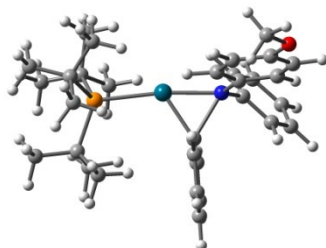
Sum of electronic and thermal Energies= -1804.390147

Sum of electronic and thermal Enthalpies= -1804.389203

Sum of electronic and thermal Free Energies= -1804.498013

E(RM062X) = -1805.11880857

Complex 5-OMe-TS



P	-3.11197	0.88719	5.30578
C	-2.24782	-0.36319	6.52561
C	-2.44581	-1.8044	6.00282
C	-0.72215	-0.10716	6.47531
C	-2.72874	-0.29778	7.98991
H	-3.47828	-2.16818	6.10227
H	-2.13088	-1.90397	4.95023
H	-1.80646	-2.47662	6.60251
H	-0.42994	0.89056	6.82671
H	-0.226	-0.84739	7.12874
H	-0.33524	-0.2448	5.45189
H	-2.20757	-1.0863	8.56262
H	-2.48763	0.66064	8.47283
H	-3.80874	-0.47744	8.09492
C	-3.26081	2.62001	6.17282
C	-1.90185	2.99699	6.80262
C	-3.55444	3.694	5.0985
C	-4.3495	2.69226	7.26528
H	-1.64262	2.37497	7.67113
H	-1.08318	2.95187	6.06817
H	-1.97125	4.03981	7.16065
H	-4.52987	3.571	4.61165
H	-3.55913	4.67997	5.59752
H	-2.77629	3.71023	4.3219
H	-4.30394	3.6936	7.73024
H	-5.36449	2.57375	6.85881
H	-4.20884	1.95256	8.06649
C	-4.90971	0.23953	4.90462
C	-5.73594	1.36902	4.24966
C	-4.79265	-0.87018	3.83051
C	-5.69324	-0.30749	6.11543
H	-6.01963	2.163	4.95497
H	-5.20844	1.82228	3.3944
H	-6.67287	0.92775	3.86506
H	-4.2	-1.73667	4.14929
H	-5.80877	-1.23206	3.58977
H	-4.36059	-0.47389	2.8937
H	-6.70845	-0.58358	5.77704
H	-5.2403	-1.21479	6.54138
H	-5.8061	0.43176	6.92132
C	-0.91783	2.04824	2.97005
C	0.27497	2.14363	3.71075
C	-1.27158	3.0895	2.09225
C	1.09467	3.28126	3.58743
H	0.57532	1.33905	4.3873
C	-0.44813	4.22539	1.97716
H	-2.17733	3.02076	1.48139
C	0.73435	4.32744	2.72534
H	2.01827	3.34206	4.17305
H	-0.73766	5.02928	1.29173
H	1.37232	5.21154	2.63218
Pd	-1.9686	0.65694	3.24301

N	-1.14061	0.26189	1.6539
C	-1.64234	0.67866	0.42099
C	-1.06337	0.31581	-0.8298
C	-2.86483	1.40855	0.37226
C	-1.66776	0.67895	-2.03945
H	-0.14389	-0.27488	-0.8453
C	-3.45567	1.77124	-0.84099
H	-3.3437	1.67079	1.32437
C	-2.86311	1.4153	-2.06543
H	-1.19403	0.37365	-2.97886
H	-4.39442	2.33566	-0.82946
C	0.19264	-0.1892	1.77209
C	0.45776	-1.30887	2.59961
C	1.29734	0.45805	1.16164
C	1.76679	-1.75865	2.81399
H	-0.39211	-1.81978	3.06481
C	2.60383	0.00009	1.37396
H	1.11983	1.33494	0.53235
C	2.85044	-1.10999	2.1995
H	1.94012	-2.62819	3.45639
H	3.43964	0.52359	0.89799
H	3.87287	-1.46378	2.3611
O	-3.4685	1.78564	-3.30691
C	-3.21117	0.77378	-4.28406
H	-3.83558	0.93539	-5.13781
H	-2.18388	0.81697	-4.58021
H	-3.4215	-0.18815	-3.86531

Zero-point correction= 0.688594 (Hartree/Particle)

Thermal correction to Energy= 0.726615

Thermal correction to Enthalpy= 0.727560

Thermal correction to Gibbs Free Energy= 0.619268

Sum of electronic and zero-point Energies= -1804.405796

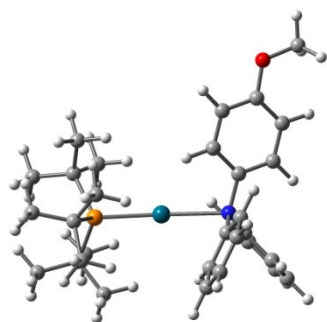
Sum of electronic and thermal Energies= -1804.367774

Sum of electronic and thermal Enthalpies= -1804.366830

Sum of electronic and thermal Free Energies= -1804.475122

E(RM062X) = -1805.09438962

Complex 6-OMe



P	-3.36744	1.0665	5.26249
C	-2.26993	2.02865	6.55728
C	-1.00583	1.19072	6.82483
C	-1.78878	3.33774	5.90068
C	-2.96588	2.35124	7.88647
H	-1.21497	0.28786	7.3944
H	-0.50323	0.9218	5.89336
H	-0.31637	1.79987	7.41514
H	-2.58088	4.0681	5.77364
H	-1.028	3.78266	6.54827
H	-1.33225	3.13963	4.93171
H	-2.23313	2.81045	8.55639
H	-3.77991	3.06241	7.75793
H	-3.35895	1.46541	8.38013
C	-5.13064	1.90015	5.19673
C	-4.94939	3.42396	5.08822
C	-5.81628	1.4528	3.89048
C	-6.03927	1.59193	6.39514
H	-4.61036	3.86824	6.0206
H	-4.25128	3.68812	4.29202
H	-5.91962	3.8647	4.84581
H	-6.02514	0.38868	3.85732
H	-6.76855	1.98329	3.80415
H	-5.20566	1.71266	3.02341
H	-6.9601	2.17321	6.29027
H	-6.32162	0.54228	6.44182
H	-5.57919	1.86686	7.34261
C	-3.57949	-0.77792	5.86403
C	-4.73154	-1.42676	5.07774
C	-2.30811	-1.54901	5.45709
C	-3.83535	-0.94442	7.36725
H	-5.70839	-1.05368	5.37362
H	-4.60333	-1.28338	4.00336
H	-4.71328	-2.5013	5.27678
H	-1.39556	-1.14512	5.88417
H	-2.41351	-2.58494	5.7913
H	-2.19858	-1.5467	4.37189
H	-4.02273	-2.0022	7.5727
H	-2.97583	-0.64325	7.96241
H	-4.70368	-0.38089	7.70414
C	-0.23232	1.00613	3.0109
C	0.33697	-0.21529	3.42385
C	0.45823	2.20066	3.28281
C	1.53905	-0.2292	4.12841
H	-0.16192	-1.14699	3.19928
C	1.66728	2.16774	3.98032
H	0.0594	3.15043	2.96213
C	2.21503	0.95992	4.41545
H	1.94551	-1.17755	4.45431

H	2.17676	3.09978	4.18628
H	3.1475	0.94416	4.9606
Pd	-2.28813	1.0116	3.01574
N	-1.06908	0.90368	1.27319
C	-0.89945	2.05231	0.47063
C	-0.29149	2.02364	-0.80084
C	-1.38724	3.29343	0.93015
C	-0.16258	3.18795	-1.55665
H	0.06188	1.09126	-1.21148
C	-1.24045	4.45188	0.17476
H	-1.91105	3.32754	1.87732
C	-0.62201	4.41365	-1.07658
H	0.301	3.12815	-2.5319
H	-1.62712	5.38532	0.56057
C	-0.76607	-0.38812	0.74459
C	-1.77241	-1.3561	0.67266
C	0.54391	-0.73954	0.38873
C	-1.48179	-2.64785	0.23096
H	-2.77481	-1.08049	0.97242
C	0.83185	-2.0259	-0.06096
H	1.3296	-0.00323	0.49203
C	-0.18069	-2.98495	-0.14196
H	-2.26936	-3.38622	0.17799
H	1.8458	-2.28455	-0.33211
H	0.0448	-3.98463	-0.48448
O	-0.48164	5.60349	-1.85726
C	-0.4899	5.26636	-3.24693
H	-0.58236	6.15882	-3.82991
H	0.42336	4.7689	-3.49869
H	-1.31688	4.6191	-3.45201

Zero-point correction= 0.691280 (Hartree/Particle)

Thermal correction to Energy= 0.729861

Thermal correction to Enthalpy= 0.730805

Thermal correction to Gibbs Free Energy= 0.618245

Sum of electronic and zero-point Energies= -1804.456739

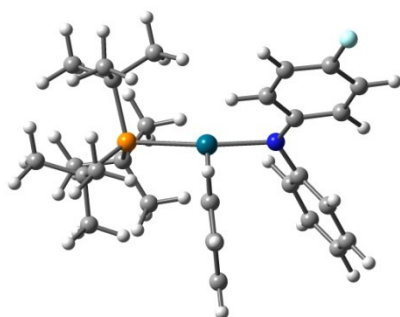
Sum of electronic and thermal Energies= -1804.418158

Sum of electronic and thermal Enthalpies= -1804.417213

Sum of electronic and thermal Free Energies= -1804.529773

E(RM062X) = -1805.14801840

Complex 5-F



P	-3.19883	0.86206	5.31067
C	-2.35063	-0.39477	6.53729
C	-2.62358	-1.83186	6.05803
C	-0.82548	-0.19732	6.43142
C	-2.79665	-0.25805	7.99961
H	-3.65579	-2.13999	6.20267
H	-2.35588	-1.9604	5.00767
H	-1.99335	-2.50441	6.64511
H	-0.49843	0.81307	6.65652
H	-0.34465	-0.87562	7.14138
H	-0.4782	-0.45449	5.42966
H	-2.33065	-1.06167	8.57643
H	-2.47847	0.685	8.4389
H	-3.87517	-0.34771	8.11598
C	-3.27532	2.61831	6.14667
C	-1.88362	2.9531	6.71214
C	-3.56914	3.67019	5.06024
C	-4.32527	2.73352	7.2619
H	-1.61489	2.33382	7.56418
H	-1.11237	2.86429	5.94589
H	-1.90174	3.99127	7.05262
H	-4.56775	3.58983	4.64458
H	-3.47978	4.65879	5.51864
H	-2.84451	3.60778	4.25168
H	-4.23123	3.72397	7.71555
H	-5.33913	2.64623	6.87616
H	-4.19066	1.99324	8.04735
C	-5.01626	0.25322	4.94038
C	-5.80016	1.3996	4.2788
C	-4.93656	-0.87647	3.89241
C	-5.78982	-0.23674	6.17263
H	-6.04753	2.19367	4.97871
H	-5.25439	1.82346	3.43408
H	-6.73965	0.99065	3.89897
H	-4.37874	-1.74345	4.2301
H	-5.95487	-1.20295	3.66541
H	-4.49827	-0.51797	2.95603
H	-6.81125	-0.47683	5.86431
H	-5.35937	-1.13878	6.60163
H	-5.8483	0.51963	6.95263
C	-0.81456	2.10441	3.18972
C	0.41704	2.00961	3.84279
C	-1.12952	3.25993	2.47003
C	1.31	3.08534	3.81221
H	0.69761	1.10154	4.35738
C	-0.23077	4.33134	2.43808
H	-2.06335	3.33271	1.92899
C	0.98672	4.25023	3.11504
H	2.25874	3.0045	4.32524
H	-0.48395	5.22221	1.87945

H	1.67941	5.07935	3.08918
Pd	-2.0334	0.54904	3.158
N	-1.11504	0.00889	1.36705
C	-1.68133	0.36417	0.14138
C	-1.16083	-0.0657	-1.10328
C	-2.88574	1.10509	0.10851
C	-1.80524	0.24033	-2.2983
H	-0.25831	-0.65931	-1.12215
C	-3.52338	1.40348	-1.09178
H	-3.31514	1.43638	1.04632
C	-2.99086	0.97914	-2.3113
H	-1.38076	-0.11348	-3.22874
H	-4.4427	1.9738	-1.0726
C	0.25593	-0.2934	1.48404
C	0.66367	-1.22572	2.45709
C	1.26001	0.37239	0.75357
C	2.01272	-1.47946	2.69363
H	-0.10192	-1.74196	3.02272
C	2.60751	0.10981	0.98745
H	0.97401	1.11505	0.02158
C	2.99742	-0.8161	1.95833
H	2.29491	-2.19997	3.44957
H	3.35813	0.64356	0.42007
H	4.04416	-1.01436	2.13856
F	-3.61005	1.27171	-3.4747

Zero-point correction= 0.648775 (Hartree/Particle)

Thermal correction to Energy= 0.685377

Thermal correction to Enthalpy= 0.686321

Thermal correction to Gibbs Free Energy= 0.581288

Sum of electronic and zero-point Energies= -1789.220297

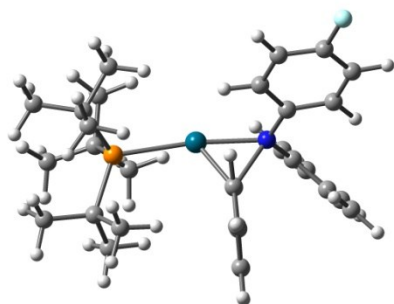
Sum of electronic and thermal Energies= -1789.183695

Sum of electronic and thermal Enthalpies= -1789.182751

Sum of electronic and thermal Free Energies= -1789.287784

E(RM062X) = -1789.86907201

Complex 5-F-TS



P	-3.11197	0.88719	5.30578
C	-2.24782	-0.36319	6.52561
C	-2.44581	-1.8044	6.00282
C	-0.72215	-0.10716	6.47531
C	-2.72874	-0.29778	7.98991
H	-3.47828	-2.16818	6.10227
H	-2.13088	-1.90397	4.95023
H	-1.80646	-2.47662	6.60251
H	-0.42994	0.89056	6.82671
H	-0.226	-0.84739	7.12874
H	-0.33524	-0.2448	5.45189
H	-2.20757	-1.0863	8.56262
H	-2.48763	0.66064	8.47283
H	-3.80874	-0.47744	8.09492
C	-3.26081	2.62001	6.17282
C	-1.90185	2.99699	6.80262
C	-3.55444	3.694	5.0985
C	-4.3495	2.69226	7.26528
H	-1.64262	2.37497	7.67113
H	-1.08318	2.95187	6.06817
H	-1.97125	4.03981	7.16065
H	-4.52987	3.571	4.61165
H	-3.55913	4.67997	5.59752
H	-2.77629	3.71023	4.3219
H	-4.30394	3.6936	7.73024
H	-5.36449	2.57375	6.85881
H	-4.20884	1.95256	8.06649
C	-4.90971	0.23953	4.90462
C	-5.73594	1.36902	4.24966
C	-4.79265	-0.87018	3.83051
C	-5.69324	-0.30749	6.11543
H	-6.01963	2.163	4.95497
H	-5.20844	1.82228	3.3944
H	-6.67287	0.92775	3.86506
H	-4.2	-1.73667	4.14929
H	-5.80877	-1.23206	3.58977
H	-4.36059	-0.47389	2.8937
H	-6.70845	-0.58358	5.77704
H	-5.2403	-1.21479	6.54138
H	-5.8061	0.43176	6.92132
C	-0.88205	2.33517	3.18145
C	0.31075	2.43056	3.92215
C	-1.23579	3.37642	2.30365
C	1.13046	3.56818	3.79883
H	0.6111	1.62597	4.5987
C	-0.41234	4.51232	2.18856
H	-2.14155	3.30769	1.69279
C	0.77014	4.61437	2.93674
H	2.05406	3.62898	4.38445
H	-0.70188	5.3162	1.50313

H	1.4081	5.49846	2.84358
Pd	-1.9686	0.65694	3.24301
N	-1.17639	-0.02503	1.4425
C	-1.67812	0.39174	0.20959
C	-1.09915	0.02888	-1.0412
C	-2.90061	1.12162	0.16086
C	-1.70354	0.39202	-2.25085
H	-0.17968	-0.5618	-1.0567
C	-3.49145	1.48431	-1.05239
H	-3.37948	1.38387	1.11297
C	-2.8989	1.12838	-2.27683
H	-1.22981	0.08672	-3.19026
H	-4.4302	2.04874	-1.04086
C	0.15686	-0.47612	1.56069
C	0.42198	-1.59579	2.38821
C	1.26155	0.17113	0.95024
C	1.73101	-2.04558	2.60259
H	-0.42789	-2.1067	2.85341
C	2.56805	-0.28683	1.16256
H	1.08405	1.04802	0.32095
C	2.81466	-1.39692	1.9881
H	1.90434	-2.91511	3.24499
H	3.40385	0.23666	0.68659
H	3.83709	-1.75071	2.1497
F	-3.47041	1.47799	-3.44885

Zero-point correction= 0.647307 (Hartree/Particle)

Thermal correction to Energy= 0.683497

Thermal correction to Enthalpy= 0.684441

Thermal correction to Gibbs Free Energy= 0.580595

Sum of electronic and zero-point Energies= -1789.196350

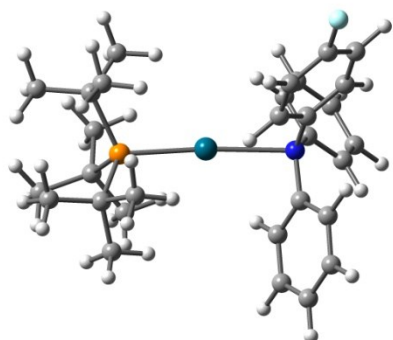
Sum of electronic and thermal Energies= -1789.160160

Sum of electronic and thermal Enthalpies= -1789.159216

Sum of electronic and thermal Free Energies= -1789.263062

E(RM062X) = -1789.84365703

Complex 6-F



P	-3.28482	1.07661	5.43407
C	-2.18731	2.03877	6.72885
C	-0.92322	1.20084	6.9964
C	-1.70616	3.34786	6.07226
C	-2.88327	2.36136	8.05804
H	-1.13235	0.29797	7.56597
H	-0.42062	0.93191	6.06493
H	-0.23375	1.80998	7.58671
H	-2.49826	4.07822	5.94521
H	-0.94538	3.79277	6.71985
H	-1.24963	3.14974	5.10328
H	-2.15052	2.82056	8.72796
H	-3.69729	3.07252	7.9295
H	-3.27633	1.47553	8.5517
C	-5.04802	1.91027	5.3683
C	-4.86677	3.43407	5.25979
C	-5.73366	1.46292	4.06205
C	-5.95665	1.60204	6.56671
H	-4.52774	3.87836	6.19217
H	-4.16866	3.69824	4.46359
H	-5.83701	3.87482	5.01738
H	-5.94252	0.3988	4.02889
H	-6.68593	1.9934	3.97572
H	-5.12304	1.72278	3.19499
H	-6.87748	2.18333	6.46184
H	-6.239	0.5524	6.6134
H	-5.49657	1.87697	7.51419
C	-3.49688	-0.76781	6.0356
C	-4.64893	-1.41664	5.24931
C	-2.22549	-1.5389	5.62867
C	-3.75273	-0.9343	7.53882
H	-5.62577	-1.04356	5.54519
H	-4.52072	-1.27326	4.17493
H	-4.63066	-2.49119	5.44836
H	-1.31294	-1.135	6.05575
H	-2.3309	-2.57483	5.96287
H	-2.11596	-1.53658	4.54346
H	-3.94012	-1.99209	7.74427
H	-2.89321	-0.63313	8.13399
H	-4.62107	-0.37077	7.87571
C	-0.26663	0.86054	2.81645
C	0.26555	-0.41038	3.11316
C	0.48072	2.00279	3.15471
C	1.48857	-0.52546	3.77084
H	-0.27812	-1.30184	2.83545
C	1.7097	1.86905	3.80366
H	0.1107	2.98935	2.92284
C	2.22165	0.61076	4.12429

H	1.86644	-1.5113	4.00774
H	2.26334	2.76191	4.06247
H	3.17014	0.51666	4.6327
Pd	-2.20551	1.02172	3.18731
N	-0.98646	0.91379	1.44477
C	-0.81684	2.06242	0.6422
C	-0.20887	2.03376	-0.62927
C	-1.30462	3.30354	1.10173
C	-0.07996	3.19806	-1.38508
H	0.1445	1.10138	-1.0399
C	-1.15783	4.462	0.34633
H	-1.82843	3.33765	2.04889
C	-0.53939	4.42376	-0.90501
H	0.38362	3.13827	-2.36033
H	-1.5445	5.39543	0.73214
C	-0.61553	-0.40148	1.0295
C	-1.58095	-1.41244	1.00076
C	0.71886	-0.72549	0.74562
C	-1.22552	-2.72146	0.67167
H	-2.60327	-1.15571	1.24481
C	1.07169	-2.02988	0.40806
H	1.47164	0.04808	0.81657
C	0.10007	-3.03289	0.36938
H	-1.98191	-3.49329	0.65098
H	2.10387	-2.26703	0.19156
H	0.37574	-4.04597	0.11403
F	-0.40688	5.54704	-1.64202

Zero-point correction= 0.649923 (Hartree/Particle)

Thermal correction to Energy= 0.685826

Thermal correction to Enthalpy= 0.686770

Thermal correction to Gibbs Free Energy= 0.581980

Sum of electronic and zero-point Energies= -1789.245060

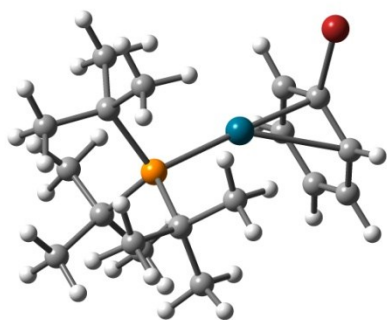
Sum of electronic and thermal Energies= -1789.209157

Sum of electronic and thermal Enthalpies= -1789.208213

Sum of electronic and thermal Free Energies= -1789.313004

E(RM062X) = -1789.89498319

Complex 7



H	-4.13963	3.28885	2.43429
H	-4.40332	4.61705	5.92066
H	-4.76716	2.91154	6.15188
H	-3.21122	3.5634	6.68055

Zero-point correction= 0.466102 (Hartree/Particle)

Thermal correction to Energy= 0.493638

Thermal correction to Enthalpy= 0.494582

Thermal correction to Gibbs Free Energy= 0.407450

Sum of electronic and zero-point Energies= -1185.484148

Sum of electronic and thermal Energies= -1185.456612

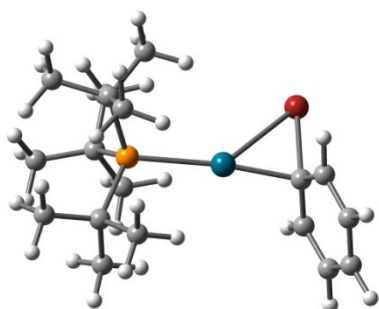
Sum of electronic and thermal Enthalpies= -1185.455667

Sum of electronic and thermal Free Energies= -1185.542800

E(RM062X) = -1185.95024944

C	-0.88848	-0.02041	0.08645
C	0.38085	0.55813	-0.04894
C	0.51952	1.89162	-0.4391
C	-0.6167	2.67801	-0.65265
C	-1.89808	2.1318	-0.52594
C	-2.03729	0.76575	-0.17694
H	-0.99718	-1.07697	0.30104
H	1.25971	-0.05347	0.13398
H	1.50868	2.32114	-0.56434
H	-0.51448	3.72112	-0.93788
H	-2.77866	2.71719	-0.76357
Br	-3.73083	-0.12787	-0.53758
Pd	-2.25294	1.18801	1.93638
P	-2.48833	1.64121	4.2267
C	-3.55556	0.25372	5.08341
C	-5.03135	0.40802	4.65319
C	-3.09943	-1.11228	4.51462
C	-3.49939	0.20272	6.62355
H	-5.52188	1.27119	5.10693
H	-5.13093	0.47721	3.56597
H	-5.58298	-0.48232	4.97941
H	-2.08391	-1.38331	4.80087
H	-3.76828	-1.89399	4.89718
H	-3.15456	-1.1174	3.42184
H	-4.17773	-0.58335	6.97991
H	-2.5037	-0.04337	6.9989
H	-3.81458	1.13889	7.08947
C	-0.75701	1.71597	5.11916
C	-0.18419	0.28611	5.23685
C	0.22267	2.47875	4.19405
C	-0.73789	2.36603	6.51741
H	-0.70646	-0.32646	5.97397
H	-0.19779	-0.23313	4.27414
H	0.86149	0.35663	5.56098
H	-0.01586	3.53659	4.08939
H	1.23194	2.41201	4.62063
H	0.24001	2.03679	3.19367
H	0.2772	2.29616	6.92965
H	-0.99551	3.42685	6.489
H	-1.40924	1.87144	7.22241
C	-3.38662	3.35031	4.49045
C	-2.40774	4.49338	4.14392
C	-4.52518	3.44956	3.4459
C	-3.9678	3.60971	5.89459
H	-1.62364	4.62769	4.8912
H	-1.93999	4.33881	3.1672
H	-2.9715	5.43333	4.09774
H	-5.33123	2.73637	3.61348
H	-4.96097	4.4558	3.49376

Complex 7-TS



H	-4.40332	4.61705	5.92066
H	-4.76716	2.91154	6.15188
H	-3.21122	3.5634	6.68055

Zero-point correction= 0.466202 (Hartree/Particle)

Thermal correction to Energy= 0.492926

Thermal correction to Enthalpy= 0.493870

Thermal correction to Gibbs Free Energy= 0.409668

Sum of electronic and zero-point Energies= -1185.480333

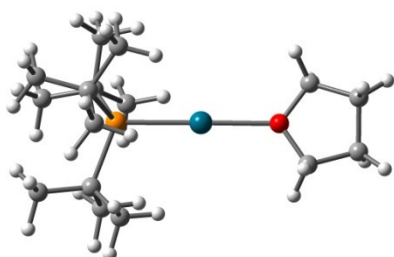
Sum of electronic and thermal Energies= -1185.453608

Sum of electronic and thermal Enthalpies= -1185.452664

Sum of electronic and thermal Free Energies= -1185.536866

E(RM062X) = -1185.94653446

C	-0.88848	-0.02041	0.08645
C	0.38085	0.55813	-0.04894
C	0.51952	1.89162	-0.4391
C	-0.6167	2.67801	-0.65265
C	-1.89808	2.1318	-0.52594
C	-2.03729	0.76575	-0.17694
H	-0.99718	-1.07697	0.30104
H	1.25971	-0.05347	0.13398
H	1.50868	2.32114	-0.56434
H	-0.51448	3.72112	-0.93788
H	-2.77866	2.71719	-0.76357
Br	-3.73083	-0.12787	-0.53758
Pd	-2.25294	1.18801	1.93638
P	-2.48833	1.64121	4.2267
C	-3.55556	0.25372	5.08341
C	-5.03135	0.40802	4.65319
C	-3.09943	-1.11228	4.51462
C	-3.49939	0.20272	6.62355
H	-5.52188	1.27119	5.10693
H	-5.13093	0.47721	3.56597
H	-5.58298	-0.48232	4.97941
H	-2.08391	-1.38331	4.80087
H	-3.76828	-1.89399	4.89718
H	-3.15456	-1.1174	3.42184
H	-4.17773	-0.58335	6.97991
H	-2.5037	-0.04337	6.9989
H	-3.81458	1.13889	7.08947
C	-0.75701	1.71597	5.11916
C	-0.18419	0.28611	5.23685
C	0.22267	2.47875	4.19405
C	-0.73789	2.36603	6.51741
H	-0.70646	-0.32646	5.97397
H	-0.19779	-0.23313	4.27414
H	0.86149	0.35663	5.56098
H	-0.01586	3.53659	4.08939
H	1.23194	2.41201	4.62063
H	0.24001	2.03679	3.19367
H	0.2772	2.29616	6.92965
H	-0.99551	3.42685	6.489
H	-1.40924	1.87144	7.22241
C	-3.38662	3.35031	4.49045
C	-2.40774	4.49338	4.14392
C	-4.52518	3.44956	3.4459
C	-3.9678	3.60971	5.89459
H	-1.62364	4.62769	4.8912
H	-1.93999	4.33881	3.1672
H	-2.9715	5.43333	4.09774
H	-5.33123	2.73637	3.61348
H	-4.96097	4.4558	3.49376
H	-4.13963	3.28885	2.43429

^tBu₃PPd-THF

H	0.14042	1.77508	-1.09321
H	1.60463	1.85052	-0.04245

Zero-point correction= 0.494631 (Hartree/Particle)

Thermal correction to Energy= 0.520772

Thermal correction to Enthalpy= 0.521716

Sum of electronic and Gibbs Free Energy= 0.438018

Sum of electronic and zero-point Energies= -1173.132907

Sum of electronic and thermal Energies= -1173.106767

Sum of electronic and thermal Enthalpies= -1173.105823

Sum of electronic and thermal Free Energies= -1173.189521

E(RM062X) = -1173.62753830

P	-3.28279	0.8255	5.29337
C	-2.80625	-0.60061	6.5437
C	-3.29299	-1.93814	5.9585
C	-1.26781	-0.69015	6.5867
C	-3.35581	-0.44586	7.96845
H	-4.37374	-2.04786	6.0032
H	-2.96442	-2.05725	4.92459
H	-2.85424	-2.74805	6.54704
H	-0.80081	0.1812	7.03454
H	-0.98933	-1.56403	7.18255
H	-0.86628	-0.81419	5.57963
H	-3.08876	-1.33772	8.54321
H	-2.9277	0.41235	8.48265
H	-4.4399	-0.35046	7.98728
C	-3.10786	2.5326	6.23301
C	-1.743	2.55709	6.94219
C	-3.05351	3.64791	5.17
C	-4.21181	2.84381	7.25294
H	-1.70554	1.89871	7.80638
H	-0.93842	2.28982	6.25493
H	-1.56066	3.57535	7.29537
H	-3.98999	3.77626	4.63664
H	-2.82137	4.59148	5.67188
H	-2.26922	3.43967	4.44018
H	-3.95921	3.77676	7.76562
H	-5.18092	2.98604	6.77854
H	-4.31151	2.06622	8.00788
C	-5.16388	0.59665	4.80614
C	-5.64929	1.89526	4.13895
C	-5.23498	-0.4934	3.71824
C	-6.11123	0.23911	5.95925
H	-5.76709	2.71079	4.84774
H	-4.96836	2.20807	3.34542
H	-6.62713	1.70445	3.68929
H	-4.96742	-1.4799	4.08332
H	-6.26125	-0.54091	3.34348
H	-4.57253	-0.2449	2.88725
H	-7.13419	0.20867	5.57238
H	-5.89428	-0.7402	6.38074
H	-6.08216	0.97164	6.76354
Pd	-1.87486	0.76689	3.33566
O	-0.7425	0.71975	1.76114
C	-0.24362	-0.47425	1.15169
C	-0.29015	1.87416	1.04792
C	0.60481	-0.09609	-0.05772
H	0.35043	-1.01347	1.93357
H	-1.13526	-1.09002	0.8674
C	0.57468	1.42468	-0.12492
H	-1.20493	2.4265	0.71163
H	0.28112	2.50307	1.77807
H	0.18643	-0.54739	-0.99059
H	1.65065	-0.47195	0.06018

Bromo-benzene

C	4.37447	-1.52326	2.55321
C	5.01312	-0.65147	1.64759
C	5.12724	-2.33645	3.39793
C	6.39728	-0.58574	1.57861
C	6.52259	-2.27838	3.33565
H	4.65156	-3.00919	4.09799
C	7.1271	-1.4108	2.43356
H	6.8982	0.07914	0.88887
H	7.1262	-2.8995	3.97975
Br	9.09099	-1.344	2.35947
H	4.42251	-0.03241	1.00506
H	3.30583	-1.56058	2.59199

Zero-point correction= 0.091706 (Hartree/Particle)

Thermal correction to Energy= 0.097374

Thermal correction to Enthalpy= 0.098319

Thermal correction to Gibbs Free Energy= 0.060789

Sum of electronic and zero-point Energies= -244.565839

Sum of electronic and thermal Energies= -244.560170

Sum of electronic and thermal Enthalpies= -244.559226

Sum of electronic and thermal Free Energies= -244.596755

E(RM062X) = -244.65754413

THF

O	-0.60985	0.71067	1.59986
C	-0.17484	-0.51319	0.91275
C	-0.05457	1.90232	0.94319
C	0.42686	-0.0188	-0.40114
H	0.56404	-1.01094	1.54001
H	-1.04586	-1.15061	0.79128
C	1.00346	1.35356	-0.012
H	-0.86307	2.40612	0.41465
H	0.34061	2.55247	1.71836
H	-0.35234	0.10182	-1.15415
H	1.18304	-0.69682	-0.78918
H	1.1592	2.00191	-0.8707
H	1.95434	1.22711	0.506

Zero-point correction= 0.118366 (Hartree/Particle)

Thermal correction to Energy= 0.123174

Thermal correction to Enthalpy= 0.124118

Thermal correction to Gibbs Free Energy= 0.090479

Sum of electronic and zero-point Energies= -232.218915

Sum of electronic and thermal Energies= -232.214107

Sum of electronic and thermal Enthalpies= -232.213163

Sum of electronic and thermal Free Energies= -232.246803

E(RM062X) = -232.33728115

Bromide

Zero-point correction= 0.000000 (Hartree/Particle)

Thermal correction to Energy= 0.001416

Thermal correction to Enthalpy= 0.002360

Thermal correction to Gibbs Free Energy= -0.016176

Sum of electronic and zero-point Energies= -13.283035

Sum of electronic and thermal Energies= -13.281619

Sum of electronic and thermal Enthalpies= -13.280675

Sum of electronic and thermal Free Energies= -13.299211

E(RM062X) = -13.28303509

Tert-Butylate

O	-3.04107	0.76907	2.82711
C	-3.35493	-0.09808	1.73421
C	-4.81751	-0.56531	1.85329
H	-5.03866	-1.25037	1.06166
H	-4.96116	-1.051	2.79582
H	-5.46891	0.28082	1.78513
C	-3.16444	0.65928	0.40691
H	-3.22501	1.71255	0.58539
H	-2.20578	0.42184	-0.00481
H	-3.93016	0.36966	-0.28207
C	-2.42087	-1.32207	1.76545
H	-3.00523	-2.21467	1.84723
H	-1.8448	-1.35421	0.86433
H	-1.76359	-1.24776	2.6065

Zero-point correction= 0.122659 (Hartree/Particle)

Thermal correction to Energy= 0.128921

Thermal correction to Enthalpy= 0.129865

Thermal correction to Gibbs Free Energy= 0.094027

Sum of electronic and zero-point Energies= -232.903790

Sum of electronic and thermal Energies= -232.897528

Sum of electronic and thermal Enthalpies= -232.896584

Sum of electronic and thermal Free Energies= -232.932422

E(RM062X) = -233.02644879

Tert-Butanol

O	-3.04107	0.76907	2.82711
C	-3.35493	-0.09808	1.73421
C	-4.81751	-0.56531	1.85329
H	-5.03866	-1.25037	1.06166
H	-4.96116	-1.051	2.79582
H	-5.46891	0.28082	1.78513
C	-3.16444	0.65928	0.40691
H	-3.22501	1.71255	0.58539
H	-2.20578	0.42184	-0.00481
H	-3.93016	0.36966	-0.28207
C	-2.42087	-1.32207	1.76545
H	-3.00523	-2.21467	1.84723
H	-1.8448	-1.35421	0.86433
H	-1.76359	-1.24776	2.6065
H	-2.0878	0.83964	2.91605

Zero-point correction= 0.137172 (Hartree/Particle)

Thermal correction to Energy= 0.143762

Thermal correction to Enthalpy= 0.144706

Thermal correction to Gibbs Free Energy= 0.108297

Sum of electronic and zero-point Energies= -233.425121

Sum of electronic and thermal Energies= -233.418532

Sum of electronic and thermal Enthalpies= -233.417588

Sum of electronic and thermal Free Energies= -233.453996

E(RM062X) = -233.56229366

Diphenyl-amine

C	-1.66667	0.61699	0.
C	-0.27151	0.61699	0.
C	0.42603	1.82474	0.
C	-0.27162	3.03325	-0.0012
C	-1.66645	3.03317	-0.00168
C	-2.36405	1.82496	-0.00068
H	-2.21643	-0.33533	0.00045
H	0.278	-0.33553	0.00132
H	0.27858	3.98539	-0.00126
H	-2.21657	3.98545	-0.00263
H	-3.46365	1.82515	-0.00086
N	1.89603	1.82485	0.00085
H	2.22893	1.35382	0.81774
C	2.38677	1.1314	-1.19882
C	2.80169	-0.19801	-1.11535
C	2.43752	1.8024	-2.4206
C	3.26787	-0.856	-2.25331
H	2.76229	-0.7265	-0.15182
C	2.90289	1.14405	-3.5592
H	2.11037	2.85013	-2.4866
C	3.31817	-0.1849	-3.47573
H	3.59553	-1.90367	-2.18747
H	2.9424	1.67323	-4.52247
H	3.68572	-0.70392	-4.37285

Zero-point correction= 0.201432 (Hartree/Particle)

Thermal correction to Energy= 0.211346

Thermal correction to Enthalpy= 0.212290

Thermal correction to Gibbs Free Energy= 0.164939

Sum of electronic and zero-point Energies= -518.235584

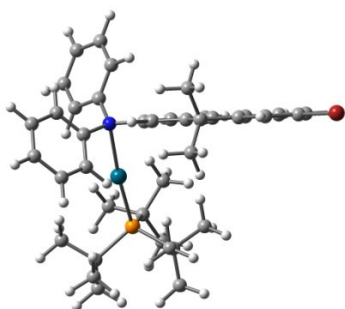
Sum of electronic and thermal Energies= -518.225671

Sum of electronic and thermal Enthalpies= -518.224727

Sum of electronic and thermal Free Energies= -518.272078

E(RM062X) = -518.43701678

Complex 8



P	-3.61787	-0.40414	5.12231
C	-3.66101	-2.02511	6.2176
C	-4.58747	-3.04168	5.52828
C	-2.25156	-2.64845	6.19149
C	-4.11354	-1.83333	7.67188
H	-5.63591	-2.76218	5.59112
H	-4.31546	-3.17054	4.47875
H	-4.4709	-4.00649	6.02865
H	-1.50608	-2.04484	6.69958
H	-2.29544	-3.62023	6.6915
H	-1.92497	-2.80095	5.16164
H	-4.17046	-2.81553	8.15092
H	-3.40938	-1.23288	8.24456
H	-5.09601	-1.37077	7.74441
C	-2.84778	1.03137	6.20172
C	-1.5552	0.50924	6.85259
C	-2.41474	2.15948	5.24406
C	-3.76488	1.6032	7.29196
H	-1.74524	-0.19772	7.65634
H	-0.90237	0.04205	6.113
H	-1.02187	1.36081	7.28306
H	-3.24857	2.63962	4.74167
H	-1.8887	2.92206	5.82557
H	-1.73402	1.7719	4.48454
H	-3.19812	2.33444	7.87609
H	-4.62707	2.11844	6.87287
H	-4.12385	0.8365	7.97582
C	-5.4648	0.08654	4.69829
C	-5.47889	1.53612	4.1817
C	-5.92009	-0.78849	3.51312
C	-6.46857	-0.04255	5.85282
H	-5.30115	2.26425	4.96906
H	-4.74145	1.67952	3.38994
H	-6.46786	1.7383	3.76197
H	-5.97174	-1.84593	3.75298
H	-6.9187	-0.46292	3.20807
H	-5.24087	-0.66209	2.66857
H	-7.44258	0.318	5.5081
H	-6.59883	-1.07436	6.17267
H	-6.18271	0.55214	6.71848
Pd	-2.3454	-0.78844	3.10991
N	-1.19814	-1.21806	1.21075
C	-1.61456	-0.2758	0.19198
C	-1.99708	-0.71182	-1.07725
C	-1.61831	1.09332	0.48641
C	-2.40014	0.2162	-2.0405
H	-1.99003	-1.76723	-1.3087
C	-2.00375	2.0133	-0.48288
H	-1.32653	1.41931	1.47742
C	-2.40254	1.57812	-1.7505

H	-2.70482	-0.13139	-3.01715
H	-2.00586	3.06756	-0.24569
H	-2.71395	2.29339	-2.49765
C	0.16293	-1.13219	1.68318
C	0.50911	-1.82	2.86137
C	1.12897	-0.38207	1.00163
C	1.79909	-1.75182	3.37359
H	-0.249	-2.39897	3.37063
C	2.41158	-0.30143	1.52995
H	0.87512	0.13436	0.08659
C	2.7533	-0.97834	2.70974
H	2.04433	-2.28347	4.28267
C	4.1629	-0.69849	3.01571
C	4.67017	0.15258	2.01488
C	4.97671	-1.12306	4.06289
C	5.98703	0.5881	2.05242
C	6.30472	-0.68987	4.11057
H	4.59987	-1.77814	4.8358
C	6.78092	0.15229	3.11179
H	6.38914	1.24237	1.29173
H	6.95405	-1.00408	4.91325
C	3.60089	0.47694	0.97676
C	4.00651	-0.03128	-0.41916
H	4.89667	0.4947	-0.76682
H	4.21906	-1.09977	-0.39296
H	3.20091	0.14814	-1.13232
C	3.30265	1.98694	0.92996
H	2.48829	2.18566	0.23162
H	3.01483	2.35271	1.91542
H	4.18418	2.53576	0.59571
Br	8.64829	0.75729	3.19465
C	-1.78232	-2.54144	1.11779
C	-3.15582	-2.68668	1.33486
C	-1.00973	-3.65342	0.77923
C	-3.74962	-3.94078	1.22235
H	-3.73922	-1.81468	1.60296
C	-1.60791	-4.91144	0.68346
H	0.04976	-3.53682	0.59956
C	-2.97635	-5.05982	0.90215
H	-4.81084	-4.04625	1.39615
H	-1.0032	-5.76967	0.42742
H	-3.43634	-6.03415	0.82438

Zero-point correction= 0.792265 (Hartree/Particle)

Thermal correction to Energy= 0.837663

Thermal correction to Enthalpy= 0.838607

Thermal correction to Gibbs Free Energy= 0.710547

Sum of electronic and zero-point Energies= -2050.058846

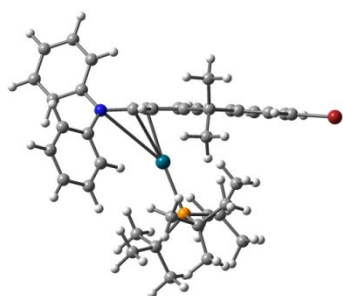
Sum of electronic and thermal Energies= -2050.013448

Sum of electronic and thermal Enthalpies= -2050.012504

Sum of electronic and thermal Free Energies= -2050.143099

E(RM062X) = -2050.85111054

Complex 8-TS



P	-2.51926	0.11796	4.22553
C	-3.30891	-0.81249	5.75104
C	-4.69957	-1.32818	5.34119
C	-2.45226	-2.06559	6.01928
C	-3.43853	0.01187	7.0391
H	-5.43346	-0.531	5.25344
H	-4.65695	-1.87755	4.39916
H	-5.0498	-2.01579	6.11548
H	-1.44103	-1.8317	6.33678
H	-2.9301	-2.64693	6.81293
H	-2.39359	-2.68503	5.12288
H	-3.95542	-0.59404	7.78937
H	-2.46854	0.28275	7.45146
H	-4.01639	0.92305	6.89321
C	-1.00881	1.19065	4.87169
C	-0.11619	0.27508	5.72833
C	-0.15574	1.59672	3.65227
C	-1.379	2.44378	5.67602
H	-0.56742	0.01899	6.68399
H	0.12991	-0.64257	5.18982
H	0.81907	0.80268	5.9334
H	-0.61256	2.38541	3.06138
H	0.8126	1.96379	4.00777
H	0.02775	0.73705	3.00572
H	-0.45801	2.90484	6.04557
H	-1.88928	3.18466	5.06278
H	-2.00651	2.21814	6.53583
C	-3.8584	1.33949	3.49609
C	-3.14068	2.31719	2.54885
C	-4.82073	0.51508	2.61996
C	-4.65757	2.13813	4.53452
H	-2.55524	3.06028	3.08491
H	-2.48631	1.7882	1.85153
H	-3.897	2.8503	1.96646
H	-5.45322	-0.1544	3.1944
H	-5.47269	1.20585	2.07732
H	-4.26768	-0.07895	1.89078
H	-5.32142	2.83083	4.00856
H	-5.28118	1.49673	5.1543
H	-4.01523	2.72493	5.18852
Pd	-1.59502	-1.45083	2.57889
N	-1.09157	-2.19344	0.05056
C	-1.98429	-1.13203	-0.27445
C	-2.6227	-1.09048	-1.52066
C	-2.2243	-0.10886	0.65338
C	-3.49345	-0.04592	-1.82469
H	-2.43468	-1.87229	-2.24286
C	-3.08683	0.9375	0.33612
H	-1.73053	-0.14223	1.61756
C	-3.72814	0.97582	-0.90286
H	-3.9787	-0.02509	-2.79014

H	-3.26244	1.71705	1.06538
H	-4.39771	1.78743	-1.14673
C	0.04018	-1.91432	0.86621
C	0.33171	-2.73328	1.98296
C	0.8417	-0.80408	0.57545
C	1.40731	-2.41378	2.83211
H	-0.23044	-3.64535	2.13115
C	1.88746	-0.47991	1.42994
H	0.6116	-0.19693	-0.29061
C	2.16867	-1.2678	2.5562
H	1.67191	-3.07653	3.64468
C	3.25204	-0.63124	3.31441
C	3.62708	0.54602	2.63773
C	3.8444	-0.97002	4.52818
C	4.5957	1.38947	3.16171
C	4.81766	-0.12364	5.06773
H	3.55692	-1.86491	5.06285
C	5.17097	1.03188	4.37971
H	4.89056	2.29764	2.65514
H	5.28723	-0.35921	6.0103
C	2.8235	0.72133	1.35355
C	3.73575	0.643	0.11414
H	4.43507	1.48024	0.10835
H	4.30317	-0.28744	0.11338
H	3.13538	0.68774	-0.79551
C	2.034	2.04268	1.3543
H	1.4259	2.1155	0.45142
H	1.37669	2.09676	2.22217
H	2.71704	2.89296	1.37715
Br	6.52711	2.21845	5.16366
C	-1.37322	-3.53187	-0.3363
C	-2.6888	-4.01378	-0.35362
C	-0.32403	-4.38802	-0.69674
C	-2.94587	-5.32741	-0.73921
H	-3.5001	-3.35936	-0.069
C	-0.58868	-5.70477	-1.06393
H	0.69043	-4.01452	-0.6884
C	-1.90028	-6.18144	-1.09286
H	-3.96522	-5.68628	-0.75025
H	0.23058	-6.35349	-1.33939
H	-2.10422	-7.201	-1.3852

Zero-point correction= 0.792886 (Hartree/Particle)

Thermal correction to Energy= 0.837349

Thermal correction to Enthalpy= 0.838293

Thermal correction to Gibbs Free Energy= 0.713509

Sum of electronic and zero-point Energies= -2050.061186

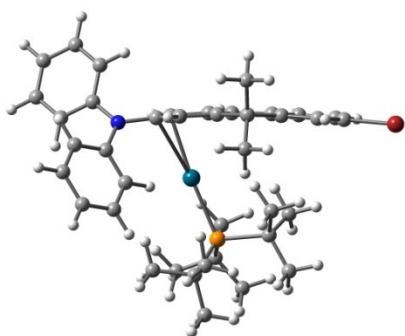
Sum of electronic and thermal Energies= -2050.016723

Sum of electronic and thermal Enthalpies= -2050.015779

Sum of electronic and thermal Free Energies= -2050.140563

E(RM062X) = -2050.85407233

Complex 9



P	-1.95613	-0.12144	5.42839
C	-2.07511	-1.54578	6.76486
C	-3.15612	-2.54007	6.30691
C	-0.74487	-2.32407	6.74296
C	-2.38229	-1.08922	8.19793
H	-4.16108	-2.13557	6.39488
H	-2.98755	-2.85391	5.27483
H	-3.09862	-3.42673	6.94357
H	0.0989	-1.74149	7.0992
H	-0.84714	-3.19917	7.39106
H	-0.52299	-2.66449	5.73035
H	-2.50031	-1.97618	8.82787
H	-1.5744	-0.49539	8.62106
H	-3.30211	-0.51108	8.26233
C	-0.95417	1.36029	6.21542
C	0.32728	0.79546	6.8525
C	-0.48825	2.27614	5.0659
C	-1.71287	2.18948	7.26112
H	0.13292	0.24241	7.76808
H	0.86418	0.15156	6.15351
H	0.97995	1.63445	7.10749
H	-1.30696	2.76902	4.55111
H	0.1606	3.05102	5.48416
H	0.08287	1.70427	4.33292
H	-1.02668	2.92929	7.68417
H	-2.5491	2.73247	6.82481
H	-2.09086	1.57939	8.0792
C	-3.7713	0.51001	5.05673
C	-3.67844	1.8586	4.3212
C	-4.41211	-0.47317	4.05657
C	-4.68307	0.6703	6.28154
H	-3.36115	2.67031	4.97093
H	-2.99885	1.79692	3.46936
H	-4.67276	2.10859	3.94183
H	-4.55268	-1.47018	4.46228
H	-5.39364	-0.08383	3.77148
H	-3.79639	-0.55269	3.15926
H	-5.63992	1.08527	5.95024
H	-4.89222	-0.2806	6.76729
H	-4.26589	1.35015	7.02216
Pd	-0.90285	-0.94438	3.42091
N	-1.1383	-1.24047	1.11169
C	-1.55472	-0.29821	0.09292
C	-1.93725	-0.73423	-1.17631
C	-1.55847	1.07091	0.38735
C	-2.34031	0.19379	-2.13955
H	-1.93019	-1.78964	-1.40776
C	-1.94391	1.99089	-0.58193
H	-1.26669	1.3969	1.37836
C	-2.3427	1.55572	-1.84955

H	-2.64498	-0.1538	-3.11621
H	-1.94602	3.04516	-0.34474
H	-2.65411	2.27098	-2.5967
C	0.22276	-1.1546	1.58413
C	0.56895	-1.8424	2.76231
C	1.18881	-0.40448	0.90258
C	1.85893	-1.77423	3.27453
H	-0.18916	-2.42137	3.27157
C	2.47142	-0.32384	1.43089
H	0.93496	0.11195	-0.01246
C	2.81313	-1.00075	2.61068
H	2.10417	-2.30588	4.18361
C	4.22274	-0.7209	2.91665
C	4.73001	0.13017	1.91582
C	5.03655	-1.14546	3.96384
C	6.04687	0.5657	1.95336
C	6.36456	-0.71228	4.01151
H	4.65971	-1.80055	4.73675
C	6.84075	0.12989	3.01273
H	6.44898	1.21996	1.19267
H	7.01389	-1.02648	4.8142
C	3.66073	0.45453	0.87771
C	4.06634	-0.05368	-0.51821
H	4.95651	0.47229	-0.86588
H	4.2789	-1.12218	-0.49201
H	3.26075	0.12573	-1.23138
C	3.36249	1.96453	0.83091
H	2.54813	2.16325	0.13256
H	3.07467	2.3303	1.81636
H	4.24402	2.51335	0.49665
Br	8.70812	0.73488	3.0956
C	-1.72248	-2.56385	1.01873
C	-3.09598	-2.70908	1.2358
C	-0.94989	-3.67583	0.68017
C	-3.68979	-3.96319	1.1233
H	-3.67938	-1.83709	1.50391
C	-1.54808	-4.93385	0.5844
H	0.1096	-3.55922	0.50051
C	-2.91651	-5.08222	0.8031
H	-4.751	-4.06866	1.2971
H	-0.94336	-5.79208	0.32836
H	-3.3765	-6.05656	0.72532

Zero-point correction= 0.792304 (Hartree/Particle)

Thermal correction to Energy= 0.837522

Thermal correction to Enthalpy= 0.838466

Thermal correction to Gibbs Free Energy= 0.712136

Sum of electronic and zero-point Energies= -2050.066987

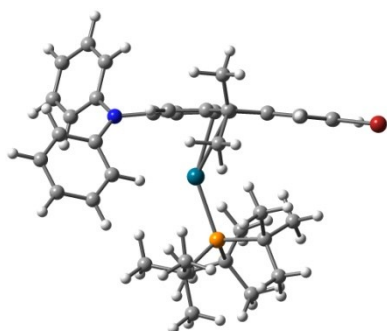
Sum of electronic and thermal Energies= -2050.021769

Sum of electronic and thermal Enthalpies= -2050.020824

Sum of electronic and thermal Free Energies= -2050.147154

E(RM062X) = -2050.85929032

Complex 10



P	-0.5755	0.33008	5.39598
C	-1.29494	-0.68347	6.90315
C	-2.71808	-1.1462	6.5448
C	-0.45168	-1.96663	7.03904
C	-1.33114	0.05734	8.24679
H	-3.43824	-0.33189	6.55219
H	-2.7425	-1.63364	5.56866
H	-3.03747	-1.87641	7.29297
H	0.58123	-1.77221	7.30999
H	-0.89497	-2.58979	7.82092
H	-0.45895	-2.52726	6.10291
H	-1.8165	-0.58679	8.98621
H	-0.33306	0.28323	8.61706
H	-1.89649	0.98636	8.19426
C	0.99314	1.33096	6.01826
C	1.91402	0.34554	6.75976
C	1.78228	1.80024	4.77865
C	0.69797	2.53544	6.92182
H	1.51383	0.03585	7.72227
H	2.10817	-0.53933	6.14989
H	2.87094	0.8417	6.94205
H	1.3091	2.63388	4.26777
H	2.77749	2.12583	5.09854
H	1.9089	0.98139	4.06859
H	1.6488	2.95475	7.26456
H	0.16908	3.32381	6.38881
H	0.11691	2.26556	7.80131
C	-1.92793	1.62051	4.82741
C	-1.24551	2.64481	3.90361
C	-2.95751	0.87247	3.95925
C	-2.64751	2.36402	5.96066
H	-0.6137	3.34069	4.45028
H	-0.64465	2.15071	3.13607
H	-2.0227	3.2283	3.40269
H	-3.56988	0.17846	4.52633
H	-3.62478	1.60879	3.5018
H	-2.46105	0.31738	3.16185
H	-3.32563	3.10139	5.52066
H	-3.24776	1.69491	6.57418
H	-1.95544	2.89525	6.61141
Pd	0.2166	-1.1444	3.60009
N	-1.09157	-2.19344	0.05056
C	-1.98429	-1.13203	-0.27445
C	-2.6227	-1.09048	-1.52066
C	-2.2243	-0.10886	0.65338
C	-3.49345	-0.04592	-1.82469
H	-2.43468	-1.87229	-2.24286
C	-3.08683	0.9375	0.33612
H	-1.73053	-0.14223	1.61756
C	-3.72814	0.97582	-0.90286

H	-3.9787	-0.02509	-2.79014
H	-3.26244	1.71705	1.06538
H	-4.39771	1.78743	-1.14673
C	0.04018	-1.91432	0.86621
C	0.33171	-2.73328	1.98296
C	0.8417	-0.80408	0.57545
C	1.40731	-2.41378	2.83211
H	-0.23044	-3.64535	2.13115
C	1.88746	-0.47991	1.42994
H	0.6116	-0.19693	-0.29061
C	2.16867	-1.2678	2.5562
H	1.67191	-3.07653	3.64468
C	3.25204	-0.63124	3.31441
C	3.62708	0.54602	2.63773
C	3.8444	-0.97002	4.52818
C	4.5957	1.38947	3.16171
C	4.81766	-0.12364	5.06773
H	3.55692	-1.86491	5.06285
C	5.17097	1.03188	4.37971
H	4.89056	2.29764	2.65515
H	5.28723	-0.35921	6.0103
C	2.8235	0.72133	1.35355
C	3.73575	0.643	0.11414
H	4.43507	1.48024	0.10835
H	4.30317	-0.28744	0.11338
H	3.13538	0.68774	-0.79551
C	2.034	2.04268	1.3543
H	1.4259	2.1155	0.45142
H	1.37669	2.09676	2.22217
H	2.71704	2.89296	1.37715
Br	6.52711	2.21845	5.16366
C	-1.37322	-3.53187	-0.3363
C	-2.6888	-4.01378	-0.35362
C	-0.32403	-4.38802	-0.69674
C	-2.94587	-5.32741	-0.73921
H	-3.5001	-3.35936	-0.069
C	-0.58868	-5.70477	-1.06393
H	0.69043	-4.01452	-0.6884
C	-1.90029	-6.18144	-1.09286
H	-3.96522	-5.68628	-0.75025
H	0.23058	-6.35349	-1.33939
H	-2.10422	-7.201	-1.3852

Zero-point correction= 0.792477 (Hartree/Particle)

Thermal correction to Energy= 0.837713

Thermal correction to Enthalpy= 0.838658

Thermal correction to Gibbs Free Energy= 0.712788

Sum of electronic and zero-point Energies= -2050.067181

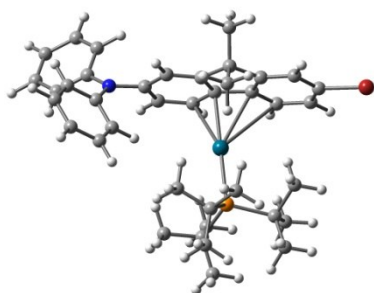
Sum of electronic and thermal Energies= -2050.021944

Sum of electronic and thermal Enthalpies= -2050.021000

Sum of electronic and thermal Free Energies= -2050.146870

E(RM062X) = -2050.85965785

Complex 10-TS



P	-0.44131	1.29564	5.46987
C	-1.68607	0.12905	6.42383
C	-2.84119	-0.23354	5.47292
C	-0.94944	-1.1928	6.72266
C	-2.26027	0.70192	7.72753
H	-3.50884	0.60253	5.28016
H	-2.46448	-0.61415	4.52111
H	-3.43059	-1.02589	5.94138
H	-0.15134	-1.0809	7.45018
H	-1.67334	-1.90696	7.12555
H	-0.52312	-1.6081	5.8077
H	-2.98844	-0.00837	8.13084
H	-1.49047	0.84325	8.48398
H	-2.76929	1.65176	7.57596
C	0.76474	2.11571	6.77776
C	1.30886	1.00527	7.69299
C	1.98132	2.66773	6.00644
C	0.15038	3.22376	7.64378
H	0.55953	0.62731	8.38431
H	1.70783	0.1742	7.10794
H	2.12634	1.42278	8.28655
H	1.73184	3.5026	5.35958
H	2.72205	3.01501	6.73277
H	2.43652	1.8843	5.39652
H	0.89959	3.55307	8.37012
H	-0.13803	4.09506	7.05903
H	-0.72086	2.88036	8.19898
C	-1.47087	2.72131	4.62007
C	-0.51334	3.85344	4.20915
C	-2.04575	2.15314	3.30796
C	-2.60104	3.31193	5.47434
H	-0.14743	4.42272	5.06003
H	0.33876	3.46999	3.64652
H	-1.06119	4.54219	3.56084
H	-2.7484	1.33969	3.46598
H	-2.57006	2.95685	2.78226
H	-1.2413	1.78834	2.66564
H	-3.05014	4.14829	4.93043
H	-3.39119	2.59004	5.66949
H	-2.24002	3.6921	6.42852
Pd	0.90968	0.01342	3.92315
N	-0.96202	-2.49361	-0.05021
C	-1.97606	-1.5318	-0.31231
C	-2.66877	-1.54013	-1.53025
C	-2.28107	-0.55185	0.64438
C	-3.65659	-0.59034	-1.7802
H	-2.42996	-2.28847	-2.2727
C	-3.25889	0.40406	0.37726
H	-1.74695	-0.53889	1.58652
C	-3.95498	0.38948	-0.83234
H	-4.18351	-0.60967	-2.72367

H	-3.48209	1.15571	1.12121
H	-4.71647	1.12909	-1.03195
C	0.16133	-2.10455	0.73919
C	0.51705	-2.85163	1.8674
C	0.86581	-0.93326	0.41219
C	1.56485	-2.44194	2.69362
H	-0.04099	-3.74622	2.10518
C	1.89389	-0.50954	1.23811
H	0.58163	-0.36933	-0.4673
C	2.25449	-1.26292	2.38351
H	1.84241	-3.03653	3.55381
C	3.37243	-0.5757	3.05405
C	3.67356	0.59299	2.32572
C	4.0543	-0.87481	4.23312
C	4.64559	1.47459	2.77718
C	5.03255	0.00884	4.6956
H	3.82798	-1.77125	4.79409
C	5.30305	1.16197	3.96649
H	4.8829	2.37895	2.23499
H	5.56576	-0.19551	5.61119
C	2.79872	0.71037	1.07959
C	3.65056	0.59376	-0.20081
H	4.34561	1.43191	-0.26631
H	4.22135	-0.33481	-0.20043
H	3.00639	0.60867	-1.081
C	1.99408	2.02112	1.07088
H	1.32607	2.04896	0.20841
H	1.39626	2.09245	1.98115
H	2.66487	2.88003	1.01554
Br	6.65212	2.41317	4.65197
C	-1.11983	-3.85498	-0.42382
C	-2.38345	-4.46088	-0.42354
C	0.0034	-4.6157	-0.7793
C	-2.5176	-5.80001	-0.78342
H	-3.25208	-3.88414	-0.13965
C	-0.1386	-5.95792	-1.12131
H	0.97887	-4.15031	-0.78288
C	-1.39855	-6.55816	-1.13004
H	-3.49871	-6.25338	-0.77806
H	0.73678	-6.5317	-1.39148
H	-1.50634	-7.59799	-1.40143

Zero-point correction= 0.792509 (Hartree/Particle)

Thermal correction to Energy= 0.836885

Thermal correction to Enthalpy= 0.837830

Thermal correction to Gibbs Free Energy= 0.714165

Sum of electronic and zero-point Energies= -2050.066028

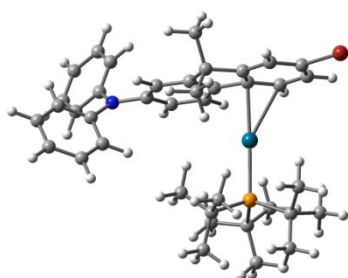
Sum of electronic and thermal Energies= -2050.021651

Sum of electronic and thermal Enthalpies= -2050.020707

Sum of electronic and thermal Free Energies= -2050.144371

E(RM062X) = -2050.85853686

Complex 11



P	-0.03388	1.97499	5.77044
C	-1.01424	0.71328	6.89446
C	-2.01084	-0.05584	6.00953
C	-0.00213	-0.33205	7.40336
C	-1.76734	1.32655	8.08283
H	-2.85365	0.55587	5.69766
H	-1.52122	-0.46465	5.12398
H	-2.40717	-0.89262	6.59065
H	0.75239	0.0886	8.06052
H	-0.54809	-1.09783	7.96165
H	0.50506	-0.81028	6.56388
H	-2.32822	0.53322	8.58607
H	-1.091	1.76217	8.81569
H	-2.47851	2.09116	7.77452
C	0.85082	3.28156	6.93656
C	1.61544	2.50055	8.02019
C	1.92282	4.01494	6.10436
C	-0.07194	4.3112	7.60189
H	0.95685	2.03579	8.75008
H	2.25185	1.7348	7.57159
H	2.26245	3.20081	8.5551
H	1.49945	4.74199	5.41732
H	2.59165	4.54986	6.7865
H	2.52297	3.30366	5.53461
H	0.5251	4.92436	8.28376
H	-0.52427	4.98244	6.87375
H	-0.86703	3.84672	8.18158
C	-1.32469	2.93374	4.66043
C	-0.61201	4.15578	4.05465
C	-1.69939	2.02036	3.47777
C	-2.59757	3.39792	5.38095
H	-0.4471	4.9444	4.78484
H	0.34785	3.87821	3.61204
H	-1.24472	4.56609	3.26299
H	-2.29118	1.15996	3.77397
H	-2.29084	2.60223	2.76481
H	-0.80443	1.66046	2.96792
H	-3.2058	3.97692	4.67954
H	-3.20341	2.56129	5.72364
H	-2.3796	4.03463	6.23637
Pd	1.75047	0.868	4.49865
N	-1.09157	-2.19344	0.05056
C	-1.98429	-1.13203	-0.27445
C	-2.6227	-1.09048	-1.52066
C	-2.2243	-0.10886	0.65338
C	-3.49345	-0.04592	-1.82469
H	-2.43468	-1.87229	-2.24286
C	-3.08683	0.9375	0.33612
H	-1.73053	-0.14223	1.61756
C	-3.72814	0.97582	-0.90286
H	-3.9787	-0.02509	-2.79014

H	-3.26244	1.71705	1.06538
H	-4.39771	1.78743	-1.14673
C	0.04018	-1.91432	0.86621
C	0.33171	-2.73328	1.98296
C	0.8417	-0.80408	0.57545
C	1.40731	-2.41378	2.83211
H	-0.23044	-3.64535	2.13115
C	1.88746	-0.47991	1.42994
H	0.6116	-0.19693	-0.29061
C	2.16867	-1.2678	2.5562
H	1.67191	-3.07653	3.64468
C	3.25204	-0.63124	3.31441
C	3.62708	0.54602	2.63773
C	3.8444	-0.97002	4.52818
C	4.5957	1.38947	3.16171
C	4.81766	-0.12364	5.06773
H	3.55692	-1.86491	5.06285
C	5.17097	1.03188	4.37971
H	4.89056	2.29764	2.65515
H	5.28723	-0.35921	6.0103
C	2.8235	0.72133	1.35355
C	3.73575	0.643	0.11414
H	4.43507	1.48024	0.10835
H	4.30317	-0.28744	0.11338
H	3.13538	0.68774	-0.79551
C	2.034	2.04268	1.3543
H	1.4259	2.1155	0.45142
H	1.37669	2.09676	2.22217
H	2.71704	2.89296	1.37715
Br	6.52711	2.21845	5.16366
C	-1.37322	-3.53187	-0.3363
C	-2.6888	-4.01378	-0.35362
C	-0.32403	-4.38802	-0.69674
C	-2.94587	-5.32741	-0.73921
H	-3.5001	-3.35936	-0.069
C	-0.58868	-5.70477	-1.06393
H	0.69043	-4.01452	-0.6884
C	-1.90029	-6.18144	-1.09286
H	-3.96522	-5.68628	-0.75025
H	0.23058	-6.35349	-1.33939
H	-2.10422	-7.201	-1.3852

Zero-point correction= 0.792363 (Hartree/Particle)

Thermal correction to Energy= 0.837872

Thermal correction to Enthalpy= 0.838817

Thermal correction to Gibbs Free Energy= 0.710121

Sum of electronic and zero-point Energies= -2050.065026

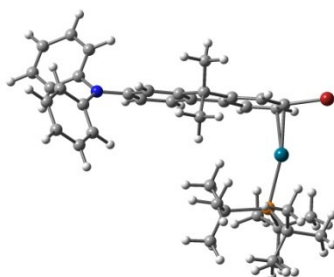
Sum of electronic and thermal Energies= -2050.019516

Sum of electronic and thermal Enthalpies= -2050.018572

Sum of electronic and thermal Free Energies= -2050.147268

E(RM062X) = -2050.85738878

Complex 12



P	1.06863	2.81853	6.90925
C	0.08827	1.55682	8.03327
C	-0.90833	0.7877	7.14834
C	1.10038	0.51149	8.54218
C	-0.66483	2.1701	9.22164
H	-1.75114	1.39942	6.83647
H	-0.41871	0.3789	6.26279
H	-1.30466	-0.04907	7.72946
H	1.8549	0.93215	9.19933
H	0.55442	-0.25429	9.10046
H	1.60757	0.03326	7.70269
H	-1.22571	1.37676	9.72488
H	0.01151	2.60572	9.9545
H	-1.376	2.9347	8.91333
C	1.95333	4.1251	8.07537
C	2.71795	3.3441	9.159
C	3.02533	4.85849	7.24317
C	1.03057	5.15475	8.7407
H	2.05936	2.87933	9.88889
H	3.35436	2.57835	8.7104
H	3.36496	4.04436	9.69392
H	2.60196	5.58554	6.55613
H	3.69416	5.39341	7.92532
H	3.62548	4.1472	6.67342
H	1.62761	5.7679	9.42258
H	0.57824	5.82598	8.01256
H	0.23548	4.69027	9.3204
C	-0.22218	3.77728	5.79924
C	0.4905	4.99933	5.19347
C	-0.59688	2.86391	4.61658
C	-1.49506	4.24146	6.51977
H	0.65541	5.78795	5.92365
H	1.45036	4.72176	4.75085
H	-0.14221	5.40964	4.4018
H	-1.18867	2.00351	4.91278
H	-1.18833	3.44577	3.90362
H	0.29808	2.50401	4.10673
H	-2.10329	4.82047	5.81835
H	-2.1009	3.40484	6.86245
H	-1.27709	4.87817	7.37518
Pd	2.85298	1.71155	5.63747
N	-1.09157	-2.19344	0.05056
C	-1.98429	-1.13203	-0.27445
C	-2.6227	-1.09048	-1.52066
C	-2.2243	-0.10886	0.65338
C	-3.49345	-0.04592	-1.82469
H	-2.43468	-1.87229	-2.24286
C	-3.08683	0.9375	0.33612
H	-1.73053	-0.14223	1.61756
C	-3.72814	0.97582	-0.90286
H	-3.9787	-0.02509	-2.79014

H	-3.26244	1.71705	1.06538
H	-4.39771	1.78743	-1.14673
C	0.04018	-1.91432	0.86621
C	0.33171	-2.73328	1.98296
C	0.8417	-0.80408	0.57545
C	1.40731	-2.41378	2.83211
H	-0.23044	-3.64535	2.13115
C	1.88746	-0.47991	1.42994
H	0.6116	-0.19693	-0.29061
C	2.16867	-1.2678	2.5562
H	1.67191	-3.07653	3.64468
C	3.25204	-0.63124	3.31441
C	3.62708	0.54602	2.63773
C	3.8444	-0.97002	4.52818
C	4.5957	1.38947	3.16171
C	4.81766	-0.12364	5.06773
H	3.55692	-1.86491	5.06285
C	5.17097	1.03188	4.37971
H	4.89056	2.29764	2.65515
H	5.28723	-0.35921	6.0103
C	2.8235	0.72133	1.35355
C	3.73575	0.643	0.11414
H	4.43507	1.48024	0.10835
H	4.30317	-0.28744	0.11338
H	3.13538	0.68774	-0.79551
C	2.034	2.04268	1.3543
H	1.4259	2.1155	0.45142
H	1.37669	2.09676	2.22217
H	2.71704	2.89296	1.37715
Br	6.52711	2.21845	5.16366
C	-1.37322	-3.53187	-0.3363
C	-2.6888	-4.01378	-0.35362
C	-0.32403	-4.38802	-0.69674
C	-2.94587	-5.32741	-0.73921
H	-3.5001	-3.35936	-0.069
C	-0.58868	-5.70477	-1.06393
H	0.69043	-4.01452	-0.6884
C	-1.90029	-6.18144	-1.09286
H	-3.96522	-5.68628	-0.75025
H	0.23058	-6.35349	-1.33939
H	-2.10422	-7.201	-1.3852

Zero-point correction= 0.792462 (Hartree/Particle)

Thermal correction to Energy= 0.837834

Thermal correction to Enthalpy= 0.838779

Thermal correction to Gibbs Free Energy= 0.711856

Sum of electronic and zero-point Energies= -2050.065315

Sum of electronic and thermal Energies= -2050.019943

Sum of electronic and thermal Enthalpies= -2050.018998

Sum of electronic and thermal Free Energies= -2050.145920

E(RM062X) = -2050.85777691