Mechanistic Study on the Reductive Elimination of (Aryl)(fluoroaryl)palladium Complexes: A Key Step in Regiospecific Dehydrogenative Cross-coupling

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Theoretical calculations

All calculations were carried out with Gaussian 09 Rev. D.01. Program package[1] or Gaussian 16 Rev. B.01 Program package.[2] Geometry optimizations and energy calculations for the ground-state structures and the transition-state structures were carried out with the DFT methods using Becker's three-parameter hybrid functional B3LYP[3], and SDD (for Pd)[4] as well as the standard 6-31G(d,p) (for the other)[5] basis set. Frequency calculations for the optimized structures were performed at the same level to identify whether the obtained structures are the stable structures (without imaginary frequency) or the transition states (with sole imaginary frequency). The connection of the transition state with the reactant and product was examined by the intrinsic reaction coordinate (IRC)[6] technique. To evaluate precise energies, single-point calculations were performed using the same functional, and SDD (for Pd) as well as the standard 6-311+G(d,p) (for the other) basis sets. Solvation effects were considered by using the self-consistent reaction field (SCRF) method with IEF-PCM solvation model[7] of cyclopentylmethyl ether (ε = 4.74). The coordinates of the optimized geometries for the ground and transition states as well as their calculated parameters with atomic units are shown below.

Int1-α

Parameters:

Zero-point correction = 0.410571

Thermal correction to Energy = 0.439663

Thermal correction to Enthalpy = 0.440607

Thermal correction to Gibbs Free Energy= 0.351806

Sum of electronic and zero-point Energies = -1588.813566

Sum of electronic and thermal Energies = -1588.784475

Sum of electronic and thermal Enthalpies = -1588.783530

Sum of electronic and thermal Free Energies = -1588.872331

Coordinates:

C	-2.23087	3.24125	-0.53873
H	-3.02433	3.96091	-0.28810
C	-0.87020	3.85999	-0.24838
N	-2.43655	1.96551	0.20275
N	0.24283	2.94072	-0.60446
Pd	-0.46839	0.90322	0.09808
H	-2.32521	3.02017	-1.60476
C	-2.76100	2.22971	1.62548
H	-0.78056	4.09082	0.81612
H	-0.77614	4.81145	-0.79344
C	-3.56301	1.22218	-0.40848
C	1.35981	0.02651	0.06070
C	1.48793	3.38880	0.05750
C	0.45968	2.91703	-2.06969
C	-1.21524	-0.85597	0.75525
H	-0.44727	2.59569	-2.58319
H	0.74531	3.91346	-2.43865
H	1.24918	2.20362	-2.30496
H	1.75684	4.40804	-0.25681
H	1.35461	3.37054	1.14074
H	2.29944	2.70943	-0.20549
H	-4.48593	1.81892	-0.37486
H	-3.32550	0.98352	-1.44629
H	-3.71659	0.29070	0.13573

H	-1.95313	2.78368	2.10502
H	-3.69280	2.80802	1.70969
H	-2.87813	1.27712	2.14306
C	-1.73229	-1.85845	-0.13623
C	-1.31802	-1.08186	2.12078
C	-2.37081	-3.03420	0.39795
C	-1.64805	-1.73828	-1.55351
C	-1.94268	-2.24275	2.64707
C	-2.46388	-3.19833	1.80621
C	-2.89283	-4.00941	-0.49713
C	-2.16142	-2.70219	-2.39466
C	-2.79524	-3.85094	-1.86135
H	-0.90427	-0.36090	2.82014
H	-1.14615	-0.86589	-1.95959
H	-2.00326	-2.37164	3.72528
H	-2.94470	-4.08933	2.20268
H	-3.37303	-4.89147	-0.07937
H	-2.07558	-2.58565	-3.47168
H	-3.19796	-4.60671	-2.53014
C	1.96018	-0.44448	-1.10214
C	2.13317	-0.10150	1.21113
C	3.40712	-0.66462	1.22774
C	3.23107	-1.01542	-1.14137
C	3.96038	-1.12943	0.03792
F	1.66158	0.35151	2.40457
F	4.11303	-0.75900	2.37019
F	1.31096	-0.34721	-2.29660
F	3.76341	-1.45144	-2.29843
F	5.18927	-1.67301	0.02726

TS-α

Zero-point correction = 0.407771

Thermal correction to Energy = 0.436912

Thermal correction to Enthalpy = 0.437856

Thermal correction to Gibbs Free Energy = 0.348820

Sum of electronic and zero-point Energies = -1588.763413

Sum of electronic and thermal Energies= -1588.734272

Sum of electronic and thermal Enthalpies= -1588.733328

Sum of electronic and thermal Free Energies= -1588.822364

Imaginary frequency = 142.7330*i*

Coordinates:

C	-2.26610	3.32459	-0.44397
H	-2.95518	4.12585	-0.12736
C	-0.84241	3.88133	-0.46207
N	-2.40402	2.13422	0.42060
N	0.15173	2.90288	-0.95706
Pd	-0.42796	0.84850	0.04665
H	-2.56353	3.03510	-1.45571
C	-2.43754	2.50466	1.84707
H	-0.54507	4.17036	0.54962
H	-0.82661	4.79863	-1.07412
C	-3.63027	1.39184	0.08286
C	1.04008	-0.63390	0.20534
C	1.51197	3.32413	-0.57419
C	0.08289	2.76877	-2.42480
C	-0.49266	-1.14831	0.74673
H	-0.90816	2.43168	-2.73256
H	0.30250	3.72601	-2.92652
H	0.81098	2.02411	-2.75304
H	1.77762	4.29711	-1.01956
H	1.58188	3.40186	0.51267
H	2.23163	2.57627	-0.91438
H	-4.53546	1.99972	0.24855
H	-3.59825	1.08126	-0.96336
H	-3.69161	0.49541	0.70337
H	-1.52682	3.03645	2.12721
H	-3.30628	3.14447	2.07721
H	-2.49676	1.59741	2.45214
C	-1.46911	-1.86048	-0.08285
C	-0.51014	-1.43833	2.12637

C	-2.32043	-2.85462	0.51749
C	-1.70162	-1.55678	-1.45443
C	-1.35821	-2.40376	2.69301
C	-2.23195	-3.12449	1.90763
C	-3.28682	-3.52902	-0.28224
C	-2.66201	-2.21021	-2.19871
C	-3.45803	-3.22029	-1.61135
H	0.18857	-0.93329	2.77920
H	-1.10681	-0.78080	-1.92060
H	-1.30477	-2.58712	3.76299
H	-2.87754	-3.88404	2.34004
H	-3.90467	-4.28792	0.19155
H	-2.80377	-1.94829	-3.24348
H	-4.20474	-3.74006	-2.20507
C	1.67053	-1.31422	-0.87299
C	2.00119	-0.14311	1.14504
C	3.37003	-0.30887	1.04192
C	3.04253	-1.50337	-0.99540
C	3.91396	-1.00869	-0.03439
F	1.59657	0.58212	2.22693
F	4.19097	0.23300	1.96016
F	0.94004	-1.83742	-1.88295
F	3.53319	-2.16795	-2.05699
F	5.23983	-1.18824	-0.14034

Int2-α

Parameters:

Zero-point correction = 0.409038

Thermal correction to Energy = 0.438674

Thermal correction to Enthalpy = 0.439618

Thermal correction to Gibbs Free Energy= 0.348482

Sum of electronic and zero-point Energies = -1588.792702

Sum of electronic and thermal Energies= -1588.763066

Sum of electronic and thermal Enthalpies = -1588.762122

Sum of electronic and thermal Free Energies = -1588.853258

Coordinates:

C	3.46109	-2.14228	0.61966
H	3.95554	-2.82090	1.33603
C	2.56557	-2.96921	-0.30319
N	2.72492	-1.07486	1.32621
N	1.96816	-2.17016	-1.39238
Pd	1.2724	-0.10474	-0.34906
H	4.25536	-1.66930	0.03552
C	1.96087	-1.61825	2.46134
H	1.7457	-3.40553	0.27477
H	3.1537	-3.81093	-0.70919
C	3.65977	-0.04861	1.81843
C	-1.94553	0.56800	0.54737
C	0.81826	-2.88080	-1.97454
C	2.95181	-1.88544	-2.45020
C	-0.79426	1.45151	0.89034
H	3.80160	-1.33407	-2.04484
H	3.32317	-2.81323	-2.91904
H	2.48598	-1.26466	-3.21834
H	1.11099	-3.85181	-2.41013
H	0.06340	-3.05397	-1.20427
H	0.37440	-2.26772	-2.76234
H	4.39148	-0.46721	2.53120
H	4.19920	0.39230	0.97720
H	3.09668	0.74185	2.31900
H	1.25020	-2.37157	2.11944
H	2.62685	-2.07511	3.21389
H	1.39292	-0.81383	2.93164
C	0.20809	1.79509	-0.10787
C	-0.71716	1.98102	2.16136
C	1.14387	2.86968	0.21339
C	0.14999	1.31381	-1.48390
C	0.29311	2.92076	2.50212
C	1.18143	3.36243	1.55242

C	1.95330	3.41324	-0.79839
C	0.97725	1.93437	-2.45833
C	1.86747	2.95166	-2.11518
H	-1.45403	1.69563	2.90631
H	-0.73036	0.78192	-1.83709
H	0.32688	3.32015	3.51173
H	1.91217	4.12928	1.79913
H	2.64452	4.21210	-0.54174
H	0.87609	1.63274	-3.49776
H	2.48582	3.40592	-2.88517
C	-2.93691	0.98034	-0.35050
C	-2.12571	-0.68897	1.13322
C	-3.21068	-1.50591	0.82956
C	-4.03261	0.18370	-0.67189
C	-4.17220	-1.06604	-0.07558
F	-1.21449	-1.16940	1.99812
F	-3.33078	-2.71520	1.39692
F	-2.85243	2.18778	-0.93421
F	-4.95911	0.61787	-1.53755
F	-5.22182	-1.84099	-0.37261

Int1-β

Parameters:

Zero-point correction = 0.410324

Thermal correction to Energy = 0.439537

Thermal correction to Enthalpy = 0.440481

Thermal correction to Gibbs Free Energy = 0.350725

Sum of electronic and zero-point Energies = -1588.815773

Sum of electronic and thermal Energies = -1588.786560

Sum of electronic and thermal Enthalpies= -1588.785616

Sum of electronic and thermal Free Energies = -1588.875372

Coordinates:

C	0.66175	-4.06576	0.18283
H	0.36780	-5.08664	-0.10513
C	1.85900	-3.62534	-0.65105
N	-0.49169	-3.13522	0.04505
N	2.32563	-2.26602	-0.27687
Pd	0.41019	-1.08167	0.02964
H	0.93322	-4.09832	1.24100
C	-1.20706	-3.36513	-1.23173
H	1.59008	-3.60163	-1.71041
H	2.67178	-4.36041	-0.54124
C	-1.43633	-3.34997	1.16549
C	1.27176	0.74812	-0.01513
C	3.18476	-1.71817	-1.34871
C	3.09327	-2.29375	0.98844
C	-1.33001	-0.12680	0.33450
H	2.47919	-2.68682	1.79955
H	3.99591	-2.91562	0.88707
H	3.38416	-1.27655	1.25199
H	4.06419	-2.35779	-1.51754
H	2.61224	-1.63960	-2.27461
H	3.51971	-0.72025	-1.06347
H	-1.81372	-4.38334	1.16676
H	-0.93149	-3.14975	2.11235
H	-2.27358	-2.65941	1.06619
H	-0.53518	-3.21489	-2.07796
H	-1.61359	-4.38697	-1.27212
H	-2.02492	-2.64831	-1.31137
C	1.80828	1.34810	1.11859
C	1.38887	1.48615	-1.18840
C	1.99779	2.73780	-1.25143
C	2.42691	2.59689	1.11014
C	2.52133	3.29791	-0.08887
F	0.90237	0.98840	-2.35666
F	2.09347	3.40891	-2.41350
F	1.74752	0.70928	2.32029
F	2.93541	3.13089	2.23570
F	3.11765	4.50088	-0.12558
C	-1.70414	0.28992	1.64914

C	-2.23267	0.08932	-0.69439
C	-3.51422	0.67151	-0.46891
C	-4.44736	0.88533	-1.52096
C	-3.88019	1.05736	0.86167
C	-5.68030	1.44747	-1.27168
C	-5.15885	1.63537	1.08614
C	-6.04131	1.82655	0.04550
C	-2.93670	0.85260	1.90443
H	-1.97549	-0.17604	-1.71807
H	-0.99807	0.16916	2.46619
H	-3.19891	1.15941	2.91515
H	-4.16848	0.59839	-2.53238
H	-5.42951	1.92765	2.09817
H	-6.38144	1.60505	-2.08672
H	-7.01565	2.27029	0.22985

TS-β

Parameters:

Zero-point correction = 0.407844

Thermal correction to Energy = 0.437117

Thermal correction to Enthalpy = 0.438061

Thermal correction to Gibbs Free Energy= 0.347833

Sum of electronic and zero-point Energies= -1588.776393

Sum of electronic and thermal Energies= -1588.747120

Sum of electronic and thermal Enthalpies = -1588.746176

Sum of electronic and thermal Free Energies = -1588.836404

Imaginary Frequency = 249.2575*i*

Coordinates:

C	0.21605	4.17962	0.21136
H	0.71461	5.13173	-0.03544
C	-0.97845	3.98964	-0.72286
N	1.16789	3.04984	0.14894
N	-1.75600	2.76784	-0.41194
Pd	-0.18362	1.10266	0.03721
H	-0.13161	4.26401	1.24470
C	2.01031	3.12143	-1.05864
H	-0.63124	3.90534	-1.75620
H	-1.61943	4.88511	-0.67294
C	2.03025	3.03451	1.34358
C	-0.88137	-0.83244	0.10190
C	-2.60518	2.39931	-1.56095
C	-2.61120	2.96570	0.77529
C	0.86430	-0.67635	0.34065
H	-2.00523	3.21971	1.64610
H	-3.34789	3.76876	0.60847
H	-3.14322	2.03749	0.99291
H	-3.33744	3.18933	-1.79466
H	-1.98066	2.22341	-2.43911
H	-3.14533	1.47859	-1.33013
H	2.64573	3.94649	1.41564
H	1.41373	2.95248	2.24146
H	2.69184	2.16678	1.29965
H	1.39208	3.11532	-1.95794
H	2.63161	4.03257	-1.06273
H	2.66409	2.24749	-1.09250
C	-1.68808	-1.17266	1.21944
C	-1.34713	-1.42852	-1.09939
C	-2.41421	-2.30855	-1.17757
C	-2.76116	-2.05039	1.17646
C	-3.12986	-2.64213	-0.02874
F	-0.73736	-1.12961	-2.27578
F	-2.78542	-2.82715	-2.36252
F	-1.44561	-0.59728	2.42888
F	-3.47328	-2.31063	2.28825
F	-4.16381	-3.49727	-0.08798
C	1.36978	-0.90255	1.67270
C	1.72265	-0.99631	-0.72307
C	3.03646	-1.48864	-0.51763
C	3.90286	-1.79689	-1.60559
C	3.51960	-1.68110	0.81825

C	5.17845	-2.26764	-1.38224
C	4.83585	-2.16981	1.01555
C	5.65151	-2.45731	-0.05974
C	2.64006	-1.37295	1.89445
H	1.38076	-0.88588	-1.74426
H	0.72722	-0.70120	2.51936
H	2.99078	-1.51905	2.91387
H	3.53825	-1.65480	-2.62010
H	5.19375	-2.31473	2.03209
H	5.82748	-2.49844	-2.22235
H	6.65852	-2.83027	0.10330

Int2-β

Parameters:

Zero-point correction = 0.409035

Thermal correction to Energy = 0.438673

Thermal correction to Enthalpy = 0.439617

Thermal correction to Gibbs Free Energy = 0.348473

Sum of electronic and zero-point Energies= -1588.792705

Sum of electronic and thermal Energies= -1588.763067

Sum of electronic and thermal Enthalpies = -1588.762122

Sum of electronic and thermal Free Energies = -1588.853266

Coordinates:

C	2.49831	3.17957	-0.59915
H	3.12512	3.86919	-1.20211
C	1.09134	3.75330	-0.46596
N	2.48289	1.82055	-1.18961
N	0.22256	2.90983	0.39091
Pd	0.75709	0.71133	-0.14103
H	2.96725	3.09962	0.39363
C	2.25611	1.86730	-2.64844
H	0.61595	3.81223	-1.45722
H	1.14768	4.78926	-0.07192
C	3.75980	1.13087	-0.91377
C	-1.70125	-0.92333	0.24790
C	-1.19256	3.25327	0.13716
C	0.52588	3.11502	1.82340
C	-0.23263	-1.02051	0.58501
H	1.57170	2.85323	2.03007
H	0.34731	4.16787	2.12715
H	-0.11326	2.44965	2.41712
H	-1.39169	4.32516	0.343748
H	-1.43727	3.03822	-0.91200
H	-1.83199	2.64365	0.784607
H	4.61598	1.66208	-1.37778
H	3.91316	1.07170	0.17218
H	3.71202	0.10676	-1.30678
H	1.29153	2.34155	-2.87024
H	3.06360	2.42766	-3.16434
H	2.22679	0.84057	-3.03619
C	-2.5711	-0.08681	0.97623
C	-2.31921	-1.66735	-0.77794
C	-3.67504	-1.53714	-1.10043
C	-3.92562	0.06364	0.67980
C	-4.49132	-0.67169	-0.36772
F	-1.61363	-2.56254	-1.50948
F	-4.20487	-2.27248	-2.09783
F	-2.08251	0.68430	1.98828
F	-4.68644	0.91878	1.39286
F	-5.79788	-0.54346	-0.66576
C	0.14878	-1.20745	1.97971
C	0.76700	-1.36391	-0.42074
C	2.00604	-2.02033	-0.02728
C	2.91350	-2.52128	-0.99075
C	2.32010	-2.18076	1.36139
C	4.11315	-3.12100	-0.61107
C	3.54489	-2.79120	1.72314
C	4.43550	-3.24977	0.75575
C	1.36027	-1.74197	2.33970
H	0.44375	-1.54875	-1.44932

H	-0.57167	-0.93775	2.75411
H	1.60427	-1.86738	3.39870
H	2.65696	-2.42651	-2.05111
H	3.77815	-2.90843	2.78595
H	4.80119	-3.49571	-1.37300
H	5.37543	-3.71978	1.05469

Int1_1-pyr

Parameters:

Zero-point correction = 0.469863

Thermal correction to Energy = 0.502293

Thermal correction to Enthalpy = 0.503237

Thermal correction to Gibbs Free Energy = 0.407374

Sum of electronic and zero-point Energies = -1818.682951

Sum of electronic and thermal Energies = -1818.650521

Sum of electronic and thermal Enthalpies = -1818.649577

Sum of electronic and thermal Free Energies = -1818.745440

Coordinates:

C	-1.78407	-3.89950	-0.61042
H	-1.82170	-4.97045	-0.36188
C	-3.15626	-3.27706	-0.39132
N	-0.72541	-3.22100	0.18872
N	-3.17066	-1.83172	-0.74057
Pd	-1.20789	-1.03803	0.06897
H	-1.49931	-3.82500	-1.66281
C	-0.79161	-3.63767	1.61076
H	-3.44747	-3.36622	0.65827
H	-3.90573	-3.82558	-0.98171
C	0.60403	-3.58951	-0.35151
C	-1.75084	0.91508	0.02786
C	-4.35986	-1.18790	-0.13963
C	-3.21401	-1.64363	-2.20955
C	0.57533	-0.44592	0.80733
H	-2.35278	-2.11999	-2.67957
H	-4.13476	-2.07381	-2.63097
H	-3.17423	-0.57847	-2.43657
H	-5.28685	-1.65278	-0.50593
H	-4.31684	-1.27969	0.94716
H	-4.36573	-0.12907	-0.40041
H	0.75223	-4.67817	-0.30990
H	0.68542	-3.25414	-1.38657
H	1.37997	-3.09786	0.23473
H	-1.76056	-3.37916	2.03959
H	-0.63454	-4.72221	1.70459
H	-0.01747	-3.11133	2.17010
C	1.70715	-0.19298	-0.01145
C	0.73782	-0.36135	2.20156
C	2.98157	0.09168	0.58464
C	1.63854	-0.21875	-1.45063
C	1.97049	-0.07913	2.79117
C	3.11149	0.14527	2.00633
C	4.13088	0.32338	-0.23544
C	2.73130	0.00394	-2.23407
C	4.01944	0.27808	-1.65987
H	-0.12175	-0.51150	2.84818
H	0.66970	-0.40582	-1.90227
H	2.05417	-0.02771	3.87478
H	2.64297	-0.01563	-3.31765
C	-1.72613	1.69525	-1.12313
C	-2.22910	1.56214	1.16376
C	-2.64668	2.89087	1.17830
C	-2.13217	3.02797	-1.16362
C	-2.59414	3.63241	0.00131
F	-2.32531	0.88887	2.34289
F	-3.10599	3.46491	2.30583
F	-1.30358	1.16163	-2.30358
F	-2.08939	3.73425	-2.30857
F	-2.99458	4.91484	-0.01147
C	4.39762	0.42987	2.58066
C	5.49184	0.64681	1.79906

H	4.47963	0.46913	3.66419
H	6.45818	0.86051	2.24862
C	5.16195	0.50641	-2.44612
C	6.39409	0.77415	-1.85125
H	5.07357	0.47311	-3.52900
H	7.26700	0.94835	-2.47420
C	6.51490	0.82181	-0.46276
C	5.40034	0.60143	0.36461
H	7.47834	1.03255	-0.00577

TS_1-pyr

Parameters:

Zero-point correction = 0.466993

Thermal correction to Energy = 0.499423

Thermal correction to Enthalpy = 0.500367

Thermal correction to Gibbs Free Energy = 0.404618

Sum of electronic and zero-point Energies = -1818.639634

Sum of electronic and thermal Energies= -1818.607203

Sum of electronic and thermal Enthalpies = -1818.606259

Sum of electronic and thermal Free Energies = -1818.702009

Imaginary frequency = 128.4311*i*

Coordinates:

C	1.27257	4.10332	-0.26709
H	1.27969	5.14786	0.08520
C	2.71453	3.61013	-0.37357
N	0.44161	3.25500	0.61649
N	2.81113	2.23549	-0.91886
Pd	1.07448	1.02819	0.09507
H	0.80650	4.10599	-1.25613
C	0.73970	3.50966	2.03902
H	3.18057	3.60697	0.61530
H	3.28826	4.31710	-0.99430
C	-0.98853	3.51086	0.36918
C	1.21005	-1.06229	0.12209
C	4.13310	1.65931	-0.60621
C	2.61689	2.23024	-2.38297
C	-0.26420	-0.47012	0.73304
H	1.63622	2.63339	-2.64020
H	3.38995	2.82927	-2.89113
H	2.67000	1.20301	-2.74981
H	4.94839	2.24199	-1.06436
H	4.27930	1.63876	0.47571
H	4.18061	0.63536	-0.98347
H	-1.25876	4.55671	0.58804
H	-1.22758	3.29390	-0.67371
H	-1.58811	2.85493	1.00418
H	1.78842	3.30013	2.25529
H	0.52423	4.55535	2.31360
H	0.12724	2.85050	2.65817
C	-1.48019	-0.33864	-0.04799
C	-0.43395	-0.79084	2.11560
C	-2.75746	-0.59654	0.55489
C	-1.48755	0.13631	-1.40576
C	-1.66601	-1.03129	2.68784
C	-2.85238	-0.96863	1.93148
C	-3.96588	-0.45523	-0.20507
C	-2.63598	0.28931	-2.12675
C	-3.91754	-0.01720	-1.56390
H	0.44440	-0.88623	2.73958
H	-0.53832	0.39014	-1.86208
H	-1.72547	-1.28554	3.74344
H	-2.59106	0.64981	-3.15124
C	1.20313	-1.93315	-1.00291
C	2.27962	-1.37663	1.01870
C	3.19671	-2.39534	0.83531
C	2.10543	-2.96956	-1.20657
C	3.11434	-3.21989	-0.28529
F	2.48411	-0.62290	2.13662
F	4.19581	-2.57732	1.71772
F	0.27223	-1.79795	-1.97303

F	2.00503	-3.73837	-2.30582
F	3.98909	-4.22006	-0.47042
C	-4.13307	-1.24647	2.50555
C	-5.27798	-1.14856	1.76939
H	-4.17510	-1.53867	3.55179
H	-6.24404	-1.36554	2.21725
C	-5.11309	0.10893	-2.29464
C	-6.34110	-0.18820	-1.70556
H	-5.06775	0.44370	-3.32757
H	-7.25527	-0.08822	-2.28388
C	-6.40518	-0.60582	-0.37702
C	-5.23569	-0.74088	0.39390
H	-7.36571	-0.82812	0.08011

Int2_1-pyr

Prameters:

Zero-point correction = 0.469235 (Hartree/Particle)

Thermal correction to Energy = 0.501890

Thermal correction to Enthalpy = 0.502834

Thermal correction to Gibbs Free Energy = 0.406646

Sum of electronic and zero-point Energies = -1818.665795

Sum of electronic and thermal Energies = -1818.633140

Sum of electronic and thermal Enthalpies = -1818.632196

Sum of electronic and thermal Free Energies = -1818.728384

Corrdinates:

C	-0.50985	4.30828	-0.10351
H	-0.18573	5.35220	-0.25160
C	-1.27784	3.84795	-1.33932
N	0.64750	3.44180	0.21075
N	-1.83220	2.48686	-1.18625
Pd	-0.16427	1.21128	-0.05998
H	-1.17269	4.30345	0.76625
C	1.76945	3.70468	-0.71149
H	-0.61399	3.84129	-2.20830
H	-2.07705	4.57655	-1.55599
C	1.08775	3.69708	1.59551
C	2.06122	-0.93185	0.36821
C	-2.15923	1.92123	-2.50689
C	-3.04612	2.49428	-0.34800
C	0.69287	-0.54448	0.85029
H	-2.82667	2.90453	0.63898
H	-3.84845	3.09408	-0.80992
H	-3.39889	1.46973	-0.21674
H	-2.91830	2.52591	-3.03073
H	-1.25720	1.87763	-3.12142
H	-2.54077	0.90611	-2.38424
H	1.38378	4.74994	1.73793
H	0.27535	3.46306	2.28719
H	1.93926	3.05886	1.82979
H	1.47218	3.50335	-1.74189
H	2.10927	4.75197	-0.64108
H	2.59910	3.04419	-0.46021
C	-0.50990	-0.89927	0.08685
C	0.54868	-0.40999	2.28363
C	-1.74898	-1.17622	0.80814
C	-0.45742	-1.28710	-1.31348
C	-0.64667	-0.60228	2.92532
C	-1.81952	-0.99688	2.21340
C	-2.89431	-1.65196	0.09843
C	-1.55197	-1.75086	-1.97529
C	-2.81675	-1.93092	-1.30687
H	1.43930	-0.18161	2.86307
H	0.48455	-1.18123	-1.84196
H	-0.70669	-0.48189	4.00411
H	-1.48827	-1.99580	-3.03240
C	2.34188	-2.22630	-0.09707
C	3.16805	-0.07796	0.45023
C	4.44600	-0.44474	0.04183
C	3.60892	-2.62017	-0.52094
C	4.67128	-1.72593	-0.45139

F	3.02637	1.17320	0.93508
F	5.46060	0.42840	0.12591
F	1.37582	-3.16073	-0.13325
F	3.81474	-3.86716	-0.96794
F	5.89567	-2.09385	-0.84741
C	-3.05832	-1.23223	2.88185
C	-4.17395	-1.64205	2.20215
H	-3.10007	-1.08092	3.95807
H	-5.10942	-1.81224	2.72887
C	-3.95725	-2.38900	-1.97756
C	-5.16437	-2.58311	-1.29366
H	-3.89503	-2.60165	-3.04181
H	-6.03679	-2.93833	-1.83537
C	-5.25105	-2.33647	0.06940
C	-4.12755	-1.87824	0.79303
H	-6.18616	-2.50003	0.59877

Int1_2-pyr

Parameters:

Zero-point correction = 0.469431

Thermal correction to Energy = 0.502058

Thermal correction to Enthalpy = 0.503002

Thermal correction to Gibbs Free Energy = 0.405977

Sum of electronic and zero-point Energies = -1818.684934

Sum of electronic and thermal Energies = -1818.652307

Sum of electronic and thermal Enthalpies = -1818.651362

Sum of electronic and thermal Free Energies = -1818.748387

Coordinates:

C	2.52895	-3.77438	0.53703
H	2.56145	-4.85331	0.32556
C	3.66791	-3.07514	-0.19252
N	1.19910	-3.21400	0.16523
N	3.69411	-1.61672	0.09463
Pd	1.51571	-1.00034	0.04142
H	2.64541	-3.65657	1.61708
C	0.76139	-3.73335	-1.15213
H	3.55413	-3.19624	-1.27290
H	4.62449	-3.54260	0.08638
C	0.19976	-3.60537	1.18685
C	1.86413	0.99046	-0.07331
C	4.52771	-0.92668	-0.91448
C	4.25173	-1.34896	1.44036
C	-0.44401	-0.54664	0.01956
H	3.65200	-1.84033	2.20725
H	5.28972	-1.70668	1.51197
H	4.22774	-0.27540	1.62958
H	5.55829	-1.31096	-0.90331
H	4.09903	-1.07346	-1.90735
H	4.54451	0.14171	-0.69608
H	0.12330	-4.69995	1.25780
H	0.49226	-3.20128	2.15774
H	-0.77189	-3.19256	0.91634
H	1.47916	-3.46066	-1.92687
H	0.66162	-4.82841	-1.12409
H	-0.20313	-3.29185	-1.40449
C	2.04284	1.78115	1.05646
C	1.96703	1.66293	-1.28640
C	2.23239	3.02662	-1.39128
C	2.30996	3.14787	1.00762
C	2.40502	3.77607	-0.23077
F	1.81276	0.98481	-2.45618
F	2.32872	3.62835	-2.59154
F	1.96259	1.22461	2.29784
F	2.47966	3.86642	2.13332
F	2.66543	5.09225	-0.30577
C	-1.11183	-0.14031	1.18723
C	-1.20205	-0.69114	-1.15442
C	-2.59345	-0.47657	-1.18048
C	-3.37741	-0.63519	-2.37701
C	-3.26047	-0.08882	0.01975

C	-4.72478	-0.42916	-2.37694
C	-4.66962	0.13168	0.02227
C	-5.42280	-0.03905	-1.18053
C	-2.50091	0.08328	1.21588
H	-0.71541	-0.97273	-2.08588
H	-0.55014	0.01848	2.10476
H	-2.86756	-0.92604	-3.29240
H	-5.29979	-0.55490	-3.29100
C	-3.19317	0.48603	2.41208
C	-4.53993	0.69491	2.41829
H	-2.61307	0.62162	3.32170
H	-5.04454	0.99815	3.33225
C	-6.81034	0.18148	-1.15261
C	-7.44777	0.56304	0.02806
H	-7.38560	0.05265	-2.06585
H	-8.52122	0.72976	0.03039
C	-6.71927	0.73463	1.20547
C	-5.33001	0.52555	1.22727
H	-7.22421	1.03454	2.12014

TS_2-pyr

Parameters:

Zero-point correction = 0.467171

Thermal correction to Energy = 0.499741

Thermal correction to Enthalpy = 0.500686

Thermal correction to Gibbs Free Energy = 0.403851

Sum of electronic and zero-point Energies = -1818.644433

Sum of electronic and thermal Energies= -1818.611863

Sum of electronic and thermal Enthalpies = -1818.610919

Sum of electronic and thermal Free Energies = -1818.707753

Imaginary frequency = 237.8934*i*

Coordinates:

C	-1.97942	-4.05131	-0.35958
H	-1.87820	-5.11954	-0.10520
C	-3.20766	-3.48715	0.35362
N	-0.74318	-3.30888	-0.03294
N	-3.46857	-2.07144	0.00548
Pd	-1.38027	-1.01938	-0.01298
H	-2.12245	-3.99692	-1.44234
C	-0.23117	-3.67551	1.30009
H	-3.06444	-3.53972	1.43626
H	-4.08138	-4.11590	0.11567
C	0.29702	-3.57249	-1.04237
C	-1.38366	1.03975	0.00399
C	-4.36235	-1.45787	1.00622
C	-4.08798	-1.95514	-1.32973
C	0.22618	0.31858	-0.00544
H	-3.43528	-2.38029	-2.09344
H	-5.06084	-2.47259	-1.36562
H	-4.24055	-0.89986	-1.56442
H	-5.34293	-1.96028	1.03712
H	-3.90306	-1.51568	1.99512
H	-4.51556	-0.40573	0.75664
H	0.57620	-4.63869	-1.07282
H	-0.06314	-3.27338	-2.02922
H	1.18597	-2.98356	-0.80701
H	-0.97786	-3.46691	2.06816
H	0.03758	-4.74402	1.34867
H	0.65585	-3.07797	1.52052
C	-1.83879	1.69568	-1.17028
C	-1.83070	1.68466	1.18708
C	-2.55954	2.86352	1.21283
C	-2.56743	2.87483	-1.18006
C	-2.92624	3.48363	0.02052
F	-1.56798	1.12674	2.39879
F	-2.94348	3.40132	2.38491
F	-1.58391	1.14946	-2.38952
F	-2.95936	3.42371	-2.34438
F	-3.62792	4.62861	0.02824
C	0.97018	0.36536	-1.21408

C	0.96539	0.31235	1.20733
C	2.36600	0.31828	1.22954
C	3.11156	0.29287	2.46262
C	3.09306	0.34891	0.00117
C	4.47389	0.29592	2.46815
C	4.51663	0.35486	0.00406
C	5.22953	0.32735	1.24318
C	2.37055	0.37558	-1.23025
H	0.43964	0.31598	2.15324
H	0.44802	0.40758	-2.16111
H	2.55882	0.27223	3.39853
H	5.01852	0.27728	3.40874
C	3.12108	0.40992	-2.46021
C	4.48335	0.41494	-2.46019
H	2.57203	0.43334	-3.39820
H	5.03164	0.44214	-3.39845
C	6.63389	0.33263	1.22031
C	7.32710	0.36491	0.00977
H	7.17932	0.31224	2.16021
H	8.41329	0.36943	0.01196
C	6.63851	0.39207	-1.20360
C	5.23432	0.38755	-1.23216
H	7.18760	0.41770	-2.14125

Int2_2-pyr

Parameters:

Zero-point correction = 0.469380

Thermal correction to Energy = 0.502032

Thermal correction to Enthalpy = 0.502976

Thermal correction to Gibbs Free Energy = 0.406124

Sum of electronic and zero-point Energies = -1818.673542

Sum of electronic and thermal Energies= -1818.640890

Sum of electronic and thermal Enthalpies = -1818.639946

Sum of electronic and thermal Free Energies = -1818.736798

Coordinates:

C	-1.22795	4.14247	0.41045
H	-1.45177	4.99614	1.07192
C	0.20728	4.26944	-0.09290
N	-1.48431	2.86093	1.10443
N	0.56381	3.21564	-1.06759
Pd	-0.31838	1.21846	-0.17548
H	-1.92179	4.20691	-0.43238
C	-0.92983	2.87540	2.47185
H	0.90286	4.19126	0.74699
H	0.34562	5.27215	-0.53129
C	-2.93814	2.62115	1.17372
C	-1.86931	-1.34064	-0.06147
C	2.02937	3.12937	-1.20426
C	-0.03229	3.48315	-2.38976
C	-0.43989	-0.92736	0.07432
H	-1.12068	3.51334	-2.32065
H	0.32385	4.44076	-2.80549
H	0.24129	2.67923	-3.07602
H	2.45696	4.07147	-1.58585
H	2.47623	2.90559	-0.23341
H	2.28449	2.32113	-1.89208
H	-3.45777	3.43090	1.71276
H	-3.34726	2.55362	0.16296
H	-3.12510	1.68084	1.69197
H	0.15175	3.01746	2.44364
H	-1.37833	3.67946	3.07962
H	-1.13238	1.91569	2.95067
C	-2.80161	-1.13982	0.97082
C	-2.38212	-1.99348	-1.19508
C	-3.71949	-2.36521	-1.31578
C	-4.13872	-1.50273	0.87822
C	-4.60830	-2.12469	-0.27502
F	-1.58303	-2.30391	-2.23501
F	-4.14662	-2.98180	-2.42740
F	-2.42380	-0.51934	2.11171

F	-4.97868	-1.24948	1.89299
F	-5.89447	-2.48353	-0.37907
C	0.26259	-1.29705	1.27455
C	0.36859	-0.55830	-1.08019
C	1.80284	-0.73783	-1.04278
C	2.60285	-0.55309	-2.21045
C	2.44062	-1.11705	0.16092
C	3.96669	-0.69428	-2.17671
C	3.85832	-1.26602	0.20923
C	4.64202	-1.04512	-0.96683
C	1.64529	-1.37630	1.33940
H	-0.08181	-0.58177	-2.06830
H	-0.31173	-1.56097	2.15655
H	2.10624	-0.29321	-3.14268
H	4.55601	-0.54507	-3.07799
C	2.33044	-1.75056	2.55266
C	3.68376	-1.87171	2.60033
H	1.73206	-1.93998	3.44089
H	4.17808	-2.15582	3.52587
C	6.04592	-1.19418	-0.89359
C	6.65828	-1.55067	0.29934
H	6.64096	-1.02762	-1.78789
H	7.73834	-1.66128	0.34053
C	5.89554	-1.77378	1.45497
C	4.50327	-1.64049	1.43276
H	6.38630	-2.05645	2.38284

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