Supplementary Information – Computational Details

Arylation of *gem*-Difluoroalkenes Using a Pd/Cu Co-Catalytic System that Avoids β-Fluoride Elimination

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1. Complete Authorship of Gaussian 16

Gaussian 16, Revision **A.03**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

GaussView, Version 6.1, Roy Dennington, Todd A. Keith, and John M. Millam, Semichem Inc., Shawnee Mission, KS, 2016.

2. General Computational Procedure

Trimethylamine was used in place of triethylamine in all relevant computational models. Manual conformation search was performed to locate all relevant structures. All conformers were optimized using Gaussian 16 computational package (see above reference). We used B3LYP[i] with the LanL2DZ[ii] basis set for palladium, and 6-31G(d)[iii] for all other atoms at 1 atm and 393.15 K (120 ºC) in 1,4-dioxane using PCM (Polarizable Continuum Model)[iv] in order to match experimental reaction conditions as close as possible. D3BJ corrections were applied using D3BJ software.[v] All reported computed barriers are derived from differences in the final free energies and reported in kcal/mol as converted from hartrees (1 Ha = 627.5095 kcal/mol) and all distances are in Ångströms (Å). All images were generated with CYLview.[vi]

3. Exploration of the Aryl Addition Step

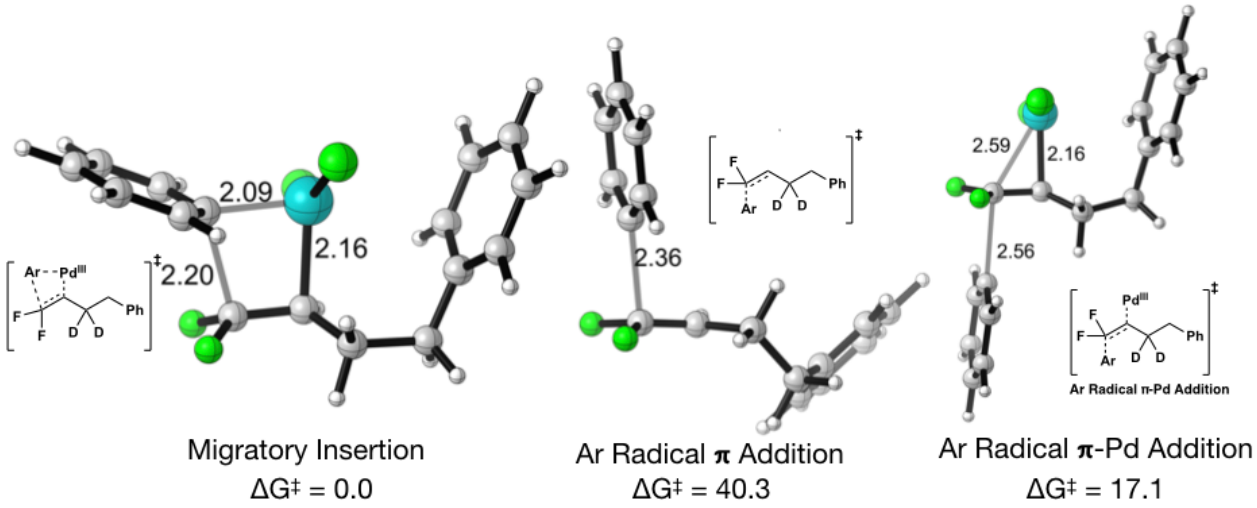
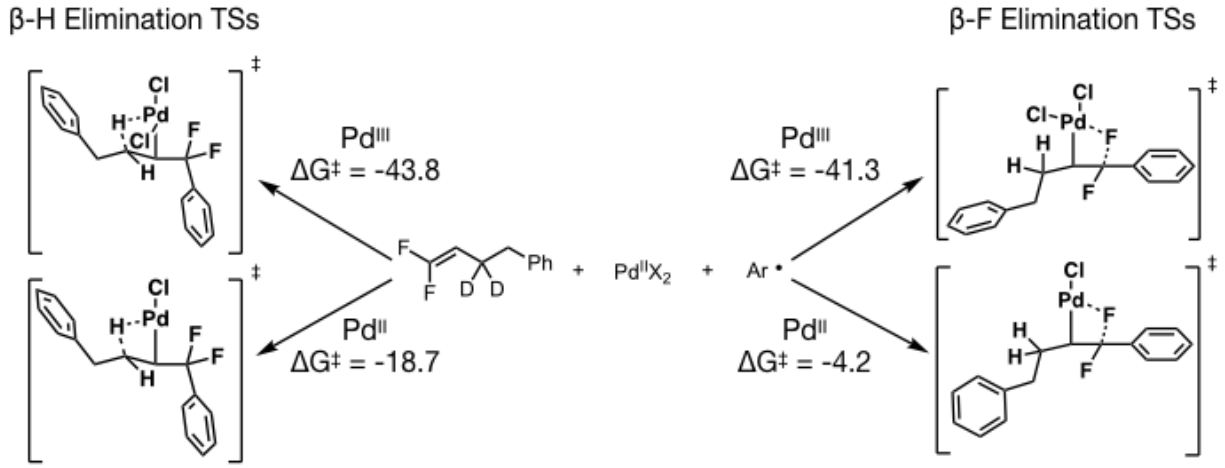


Figure S1. CYLview image of the three TSs for the three possible pathways for the aryl addition step.

We computed TSs for three different arylation mechanisms (Figure S1). Migratory insertion is the most favorable mechanism with aryl radical π-Pd addition being 17.1 kcal/mol higher in Energy. Aryl radical π addition without Pd is the least favorable pathway at 40.3 kcal/mol.

4. Exploration of the Pd Sphere and Conjugation Effect



For the β-H/F elimination process we considered both Pd^{III} and Pd^{II} mechanisms (Figure S2). Pd^{III} TSs were significantly lower in energy than Pd^{II} TSs for both β-H/F eliminations, therefore we concluded that Pd^{III} is the operative mechanism.

Figure S2. Pd^{III} vs Pd^{II}.

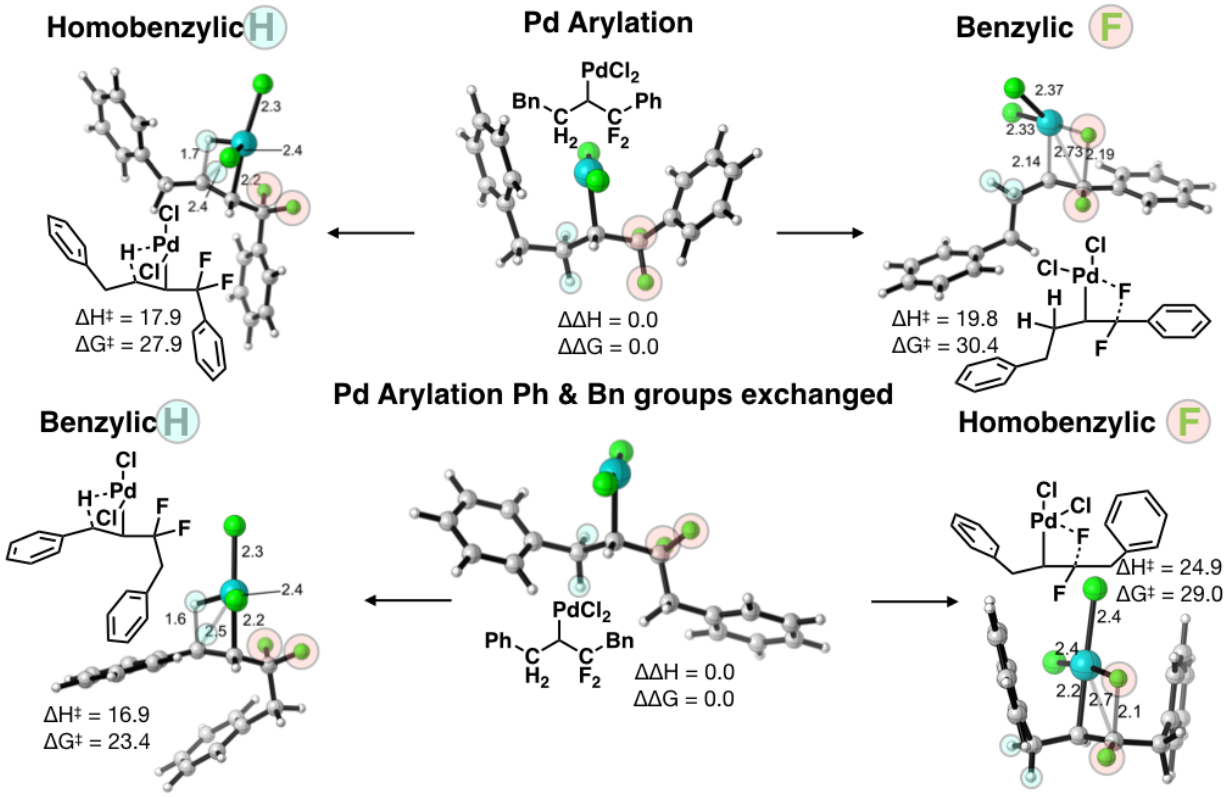


Figure S3. Pd^{III} β-H/F elimination TSs. Top row has TSs for the original substrate, bottom row has TSs for a model substrate in which phenyl and benzyl substituents are exchanged.

While investigating why β-H elimination is more favorable than β-F elimination, we considered the effects of chemoselectivity (Figure S3). β-H elimination was shown to be favored over β-F elimination regardless of whether it was in benzylic or homobenzylic position.

Additionally, we considered Pd^{II} as active catalyst (Figure S4). While β-H elimination was shown to be favored over β-F elimination for Pd^{II} regardless of whether H was in benzylic or homobenzylic position, overall energies for this mechanism were higher than for the Pd^{III} mechanism.

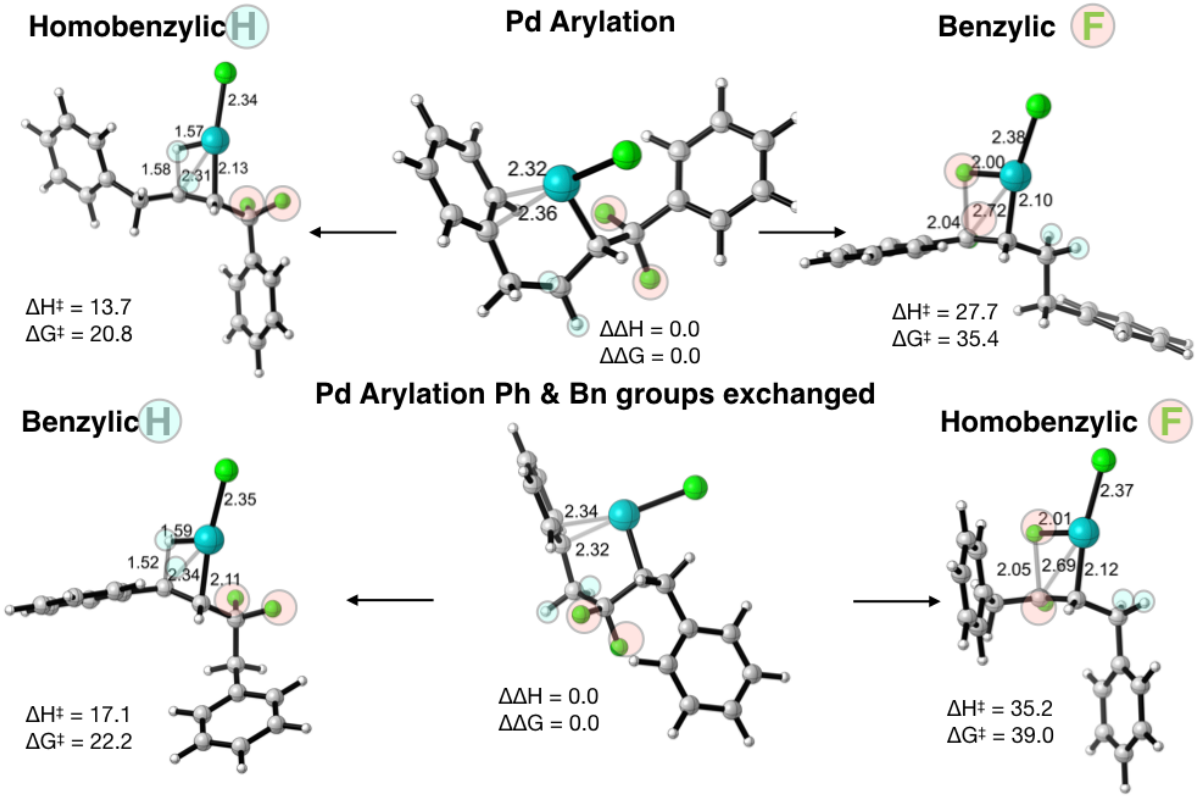


Figure S4. Pd^{II} β-H/F elimination TSs. Top row has TSs for the original substrate, bottom row has TSs for a model substrate in which phenyl and benzyl substituents are exchanged.

5. Model System

While investigating this reaction we computed energies for ground state model transformations (Figure S5). This model reveals that Pd-F bond is much weaker than Pd-H bond, as well as that C-F bond is much weaker than C-H bond.

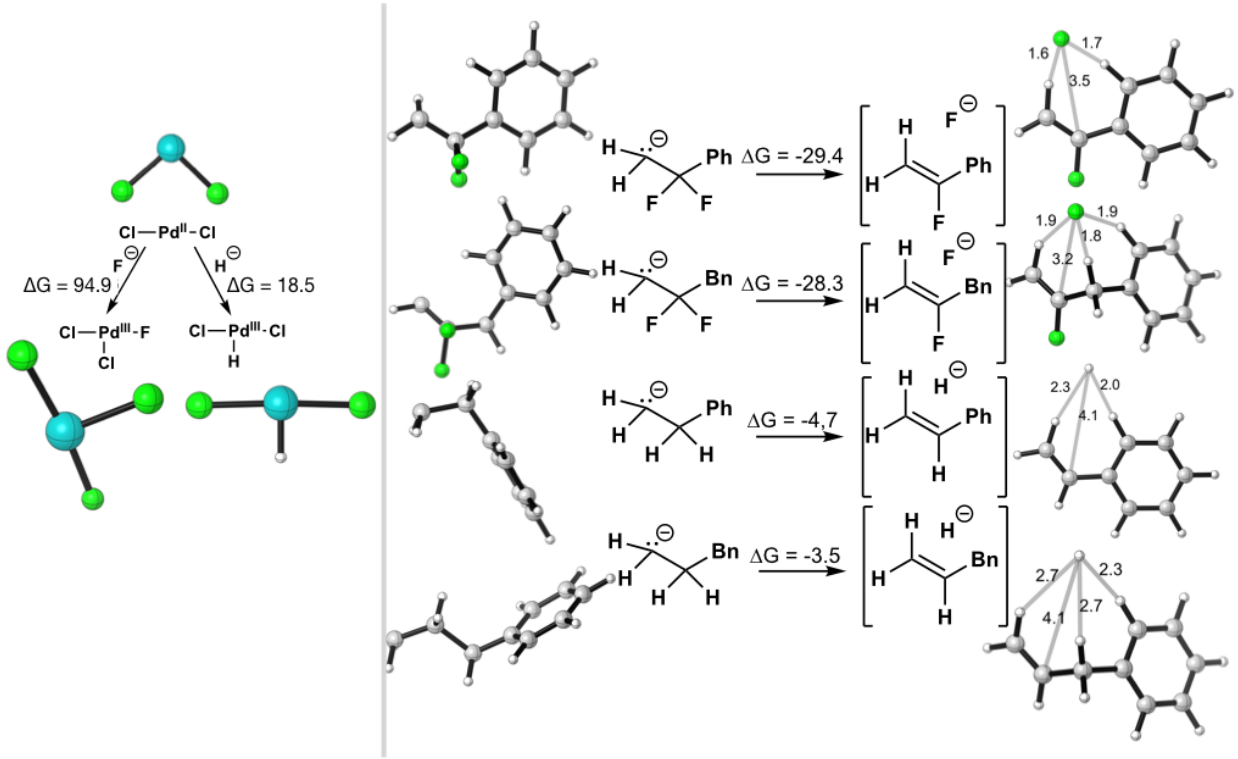


Figure S5. Model system. B3LYP/6-31G(d) & LANL2DZ/PCM(1,4-dioxane)//B3LYP/6-31G(d)++ & LANL2DZ/PCM(1,4-dioxane) at 393 K w/D3BJ corrections.

6. Computed Geometries, Dispersion & Solvation Corrections, and Energies

Manuscript TS Structures

β-H Elimination-TS

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.56473387 Predicted Change= -6.171845D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00030	0.00180	[YES]	0.00030	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-2.088519	-0.448670	-0.550960
C	-3.327019	0.358180	-0.237620
F	-2.359250	-1.791780	-0.413620
F	-1.705159	-0.248930	-1.858180
C	-0.922279	-0.116821	0.360240
H	-1.086839	-0.341860	1.410770
C	0.055071	0.833629	0.010780
H	-0.023359	1.284149	-0.978980
H	1.327031	-0.050551	-0.584160
C	0.828151	1.619229	1.055420
H	0.179082	2.468199	1.316750
H	0.937811	1.008089	1.955890
Pd	0.734271	-1.472201	-0.218410
Cl	2.276460	-2.887681	-1.255610
C	-3.609579	1.525970	-0.955560
H	-2.962738	1.832390	-1.770890
C	-4.738548	2.278911	-0.635160
H	-4.962968	3.178451	-1.200850
C	-5.580228	1.874211	0.403450
H	-6.458678	2.463211	0.651000
C	-5.295109	0.710071	1.120930
H	-5.951749	0.388831	1.923980
H	-3.954859	-0.961520	1.352010
C	2.172072	2.125879	0.571060
C	-4.169149	-0.048840	0.804890
C	3.337591	1.391598	0.831570
H	3.277391	0.474638	1.412550
C	4.573502	1.834828	0.355920
H	5.468691	1.256858	0.566920
C	4.657632	3.016448	-0.382350
H	5.619542	3.362028	-0.750620
C	3.501592	3.756768	-0.641380
H	3.561652	4.681528	-1.208700
C	2.266742	3.313609	-0.166100
H	1.371352	3.900339	-0.362140
Cl	1.046500	-1.995091	2.143180

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1865.56473387 Predicted Change= -6.171845D-10
Zero-point correction (ZPE)= -1865.2996 0.26506
Internal Energy (U)= -1865.2651 0.29960
Enthalpy (H)= -1865.2638 0.30084
Gibbs Free Energy (G)= -1865.3826 0.18208
Entropy (S)= 0.00030208

Frequencies -- -700.0611 18.3528 29.5620

β-F Elimination-TS

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

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# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.56569559 Predicted Change= -2.251110D-08

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.04810	0.00180	[NO]	0.04810	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.334468	-0.126434	0.134446
C	2.118331	-1.381850	0.612447
H	1.735566	-2.266592	0.089983
H	1.929804	-1.532029	1.682652
C	3.605387	-1.244918	0.365079
H	1.721714	0.755916	0.650194
H	1.497723	0.024243	-0.936325
C	-0.148487	-0.236941	0.434239
H	-0.397744	-0.261625	1.494509
C	-0.952429	-1.129492	-0.361964
F	-0.374759	-1.611545	-1.443149
F	-1.806166	0.469579	-1.596911
C	-2.202478	-1.751231	-0.002288
Pd	-1.122258	1.586716	-0.104605
Cl	-0.537438	2.638576	1.890646
Cl	-0.285049	3.272868	-1.549766
C	4.437083	-0.643236	1.319220
H	4.011195	-0.295869	2.258200
C	5.803314	-0.488809	1.080385
H	6.433242	-0.022591	1.833273
C	6.359406	-0.935079	-0.120369
H	7.423349	-0.817132	-0.306909
C	5.540869	-1.535990	-1.078773
H	5.965415	-1.888971	-2.014878
C	4.174915	-1.688411	-0.836054

H	3.543529	-2.160167	-1.586130
C	-2.770036	-2.707168	-0.873370
H	-2.266151	-2.954641	-1.800004
C	-3.970422	-3.320658	-0.542389
H	-4.404612	-4.054467	-1.213665
C	-4.620468	-2.987495	0.650717
H	-5.560925	-3.467192	0.905327
C	-4.068613	-2.036960	1.518727
H	-4.578867	-1.779227	2.441046
C	-2.867892	-1.419799	1.200445
H	-2.456432	-0.678628	1.877132

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1865.56569559 Predicted Change= -2.251110D-08
Zero-point correction (ZPE)= -1865.2957 0.26998
Internal Energy (U)= -1865.2615 0.30413
Enthalpy (H)= -1865.2603 0.30538
Gibbs Free Energy (G)= -1865.3796 0.18600
Entropy (S)= 0.00030364

Frequencies -- -144.7880 4.0036 25.1144

Arylation Step TS Structures

Migratory Insertion TS

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

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# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.53392473 Predicted Change= -1.451323D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00138	0.00180	[YES]	0.00138	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z

C	-1.483912	1.646939	-0.775880
C	-1.980081	-0.359731	-0.030070
F	-1.938962	1.549719	-2.012360
F	-2.307093	2.350149	-0.024820
C	-0.086142	1.670670	-0.536340
H	0.164178	2.287720	0.324440
C	0.864218	1.688291	-1.723060
H	0.543337	2.515101	-2.376320
H	0.769138	0.770801	-2.311860
C	2.338968	1.915932	-1.323920
H	2.403777	2.828282	-0.717180
H	2.899078	2.112432	-2.244700
C	2.970118	0.753232	-0.588310
C	3.749469	-0.186867	-1.269000
H	3.923019	-0.067647	-2.335860
C	4.303350	-1.278077	-0.597240
H	4.907120	-1.995587	-1.146140
C	4.081680	-1.455467	0.770600
H	4.510980	-2.308537	1.287890
C	3.313469	-0.524958	1.466970
H	3.145619	-0.632908	2.534590
C	2.764789	0.577852	0.794510
H	2.249238	1.338562	1.372760
C	-2.856911	-0.220591	1.060590
H	-2.559201	0.346649	1.933980
C	-4.108111	-0.832442	1.001390
H	-4.785731	-0.736143	1.844840
C	-4.488890	-1.555812	-0.132700
H	-5.467610	-2.025543	-0.171860
C	-3.619910	-1.665992	-1.222450
H	-3.916250	-2.221372	-2.107560
C	-2.361580	-1.069661	-1.182020
H	-1.689770	-1.158411	-2.025740
Pd	0.045679	-0.240630	0.465200
Cl	-0.141852	0.945600	2.661370
Cl	0.648510	-2.104609	-0.967510

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1865.53392473 Predicted Change= -1.451323D-08
Zero-point correction (ZPE)= -1865.2649 0.26894
Internal Energy (U)= -1865.2308 0.30306
Enthalpy (H)= -1865.2296 0.30430
Gibbs Free Energy (G)= -1865.3423 0.19156
Entropy (S)= 0.00028677

Frequencies -- -460.8400 32.9938 43.5314

Ar Radical Π Addition

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

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# b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C16H15F2(2) C1[X(C16H15F2)] #Atoms= 33
Charge = 0 Multiplicity = 2

SCF Energy= -818.299953351 Predicted Change= -1.113207D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00208	0.00180	[NO]	0.00208	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.015134	-1.653396	0.501874
C	2.640008	0.024779	0.187395
F	1.633689	-2.513191	-0.313342
F	1.372818	-1.875242	1.768530
C	-0.097661	-0.974461	0.161882
H	-0.574233	-0.404419	0.952299
C	-0.598906	-0.846574	-1.245162
H	-0.034345	-1.515772	-1.902765
H	-0.421295	0.176950	-1.607041
C	-2.111194	-1.162792	-1.387591
H	-2.291988	-2.191515	-1.054934
H	-2.358003	-1.125889	-2.456258
C	-3.011582	-0.211077	-0.627328
C	-3.276238	1.072752	-1.127757
H	-2.847073	1.373198	-2.081641
C	-4.086297	1.964839	-0.425045
H	-4.281913	2.953130	-0.833151
C	-4.649940	1.587442	0.796531
H	-5.283727	2.280132	1.343714
C	-4.397510	0.312841	1.305671
H	-4.834835	0.007112	2.252669
C	-3.585657	-0.576739	0.597773
H	-3.398302	-1.570593	0.998369
C	3.297261	0.069585	-1.026795
H	3.091278	-0.649682	-1.815649
C	4.262885	1.072598	-1.203769
H	4.807685	1.137849	-2.143063

C	4.525463	1.982861	-0.175970
H	5.273222	2.758200	-0.319588
C	3.832732	1.902001	1.035835
H	4.043257	2.611442	1.833097
C	2.863406	0.906018	1.227564
H	2.320281	0.831684	2.166610

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -818.299953351 Predicted Change= -1.113207D-09
Zero-point correction (ZPE)= -818.0368 0.26307
Internal Energy (U)= -818.0096 0.29028
Enthalpy (H)= -818.0084 0.29152
Gibbs Free Energy (G)= -818.1100 0.18994
Entropy (S)= 0.00025839

Frequencies -- -392.4678 10.9980 14.9899

Ar Radical P-Pd Addition

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016
==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---
Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.50819624 Predicted Change= -1.571888D-09
==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00121	0.00180	[YES]	0.00121	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	1.307771	-0.625664	0.843348
F	1.794241	-1.840880	0.809498
C	0.617164	-0.029564	-0.222486
H	0.814525	-0.533422	-1.166599
C	0.409294	1.473082	-0.287909
H	1.387549	1.915737	-0.521035
H	0.094383	1.857693	0.685273
C	-0.584131	1.918687	-1.390953
H	-0.306499	1.435602	-2.335995
H	-0.434356	2.994817	-1.535043
C	-2.042350	1.657287	-1.080414
C	-2.777204	2.561138	-0.303211
H	-2.295842	3.463857	0.066243
C	-4.115664	2.318966	0.004845
H	-4.666916	3.035229	0.607982
C	-4.749202	1.161854	-0.458152
H	-5.792052	0.976403	-0.216932
C	-4.037350	0.255341	-1.241310
H	-4.521390	-0.637019	-1.628606
C	-2.692230	0.501523	-1.554668
H	-2.167690	-0.177611	-2.220655

Pd	-1.195184	-1.061419	0.348455
Cl	-1.674917	0.152131	2.298031
Cl	-0.859562	-2.608044	-1.401641
C	3.576096	0.232337	0.036223
C	4.184446	-0.508611	-0.949607
C	4.086517	1.331845	0.685783
C	5.467774	-0.079569	-1.330024
H	3.720230	-1.376096	-1.409543
C	5.371758	1.735587	0.283578
H	3.547438	1.859269	1.467226
C	6.049448	1.033354	-0.716519
H	6.002986	-0.622930	-2.104464
H	5.833073	2.596619	0.760367
H	7.041786	1.354843	-1.018921
F	1.469599	-0.069424	2.011833

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1865.50819624 Predicted Change= -1.571888D-09
Zero-point correction (ZPE)= -1865.2410 0.26714
Internal Energy (U)= -1865.2057 0.30242
Enthalpy (H)= -1865.2045 0.30367
Gibbs Free Energy (G)= -1865.3246 0.18357
Entropy (S)= 0.00030547

Frequencies -- -268.7850 23.8438 27.5871

Pd^{III} TS Structures Ph & Bn Groups Exchanged

β-H Elimination-TS Ph & Bn Groups Exchanged

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.56896035 Predicted Change= -5.202034D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00137	0.00180	[YES]	0.00137	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.883051	-1.250110	-1.252840
F	-0.950022	-2.412500	-0.520790
F	-0.081932	-1.527020	-2.345910
C	-0.211541	-0.189880	-0.404650
H	-0.718001	0.016820	0.531860
C	0.559049	0.832670	-1.027080
H	0.712709	0.713100	-2.099910
H	2.039249	0.291719	-0.766640
Pd	1.737649	-1.014981	0.103830
Cl	3.878638	-1.977602	0.088770
Cl	1.162009	-0.753131	2.438160
C	-2.281441	-0.896309	-1.766480
H	-2.170371	-0.060549	-2.464860
H	-2.608392	-1.766589	-2.348250
C	-3.280741	-0.555459	-0.679890
C	-3.818682	-1.558908	0.138710
C	-3.679011	0.771441	-0.471810
C	-4.731501	-1.239408	1.143810
H	-3.519152	-2.592029	-0.010760
C	-4.593310	1.092592	0.533520
H	-3.276230	1.559431	-1.104400
C	-5.120831	0.087052	1.344690
H	-5.139792	-2.028018	1.769670
H	-4.893650	2.126602	0.679310
H	-5.833231	0.334042	2.126880
C	0.743240	2.206060	-0.518680
C	1.164230	3.189539	-1.431920
C	0.495270	2.565920	0.818310
C	1.308401	4.513629	-1.025410
H	1.371070	2.913739	-2.463010
C	0.649201	3.888120	1.220250
H	0.215940	1.810320	1.545470
C	1.051261	4.864549	0.301460
H	1.626381	5.266669	-1.740000
H	0.463131	4.158290	2.255210
H	1.171822	5.894709	0.623830

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1865.56896035 Predicted Change= -5.202034D-09

Zero-point correction (ZPE)=	-1865.3036	0.26530	
Internal Energy (U)=	-1865.2692	0.29968	
Enthalpy (H)=	-1865.2680	0.30093	
Gibbs Free Energy (G)=	-1865.3856	0.18332	
Entropy (S)=	0.00029913		
Frequencies --	-718.0311	17.9589	24.2017

β-F Elimination-TS Ph & Bn Groups Exchanged

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016
==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---
Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.56246633 Predicted Change= -1.141609D-09
==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.669120	-1.173379	0.242131
C	-0.589649	-0.147291	-0.074869
H	-0.419849	0.624759	0.675551
C	-0.415149	0.320419	-1.402069
Pd	1.388940	-1.079293	0.075641
Cl	1.301270	-1.148312	2.394441
Cl	1.617787	-3.411503	-0.177909
F	1.498680	-0.745053	-1.874909
F	-1.016509	-0.345130	-2.360509
H	-1.429631	-1.631460	1.204421
H	-1.667641	-1.967289	-0.508919
C	-3.028740	-0.488808	0.307081
C	-3.874770	-0.457197	-0.810209
C	-3.441649	0.146302	1.487231
C	-5.110269	0.189674	-0.746659
H	-3.571140	-0.951728	-1.729209
C	-4.674738	0.795754	1.550571
H	-2.798599	0.119732	2.364111
C	-5.512218	0.819994	0.432671
H	-5.760559	0.195495	-1.617239
H	-4.984418	1.276034	2.474771

H	-6.474668	1.321645	0.482731
C	0.144833	1.626769	-1.852089
H	-0.737897	2.242230	-2.090889
H	0.652822	1.439518	-2.803429
C	1.038423	2.342638	-0.861699
C	0.515074	3.314288	-0.000079
C	2.409463	2.044376	-0.806709
C	1.344755	3.971807	0.910301
H	-0.542526	3.564379	-0.044739
C	3.237814	2.705596	0.102731
H	2.816312	1.295366	-1.479309
C	2.706925	3.667516	0.964011
H	0.927446	4.724748	1.572721
H	4.297743	2.470215	0.133001
H	3.351965	4.181565	1.670651

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1865.56246633 Predicted Change= -1.141609D-09
Zero-point correction (ZPE)= -1865.2926 0.26984
Internal Energy (U)= -1865.2586 0.30378
Enthalpy (H)= -1865.2574 0.30503
Gibbs Free Energy (G)= -1865.3727 0.18968
Entropy (S)= 0.00029339

Frequencies -- -123.8083 22.6551 28.6133

Pd^{II} TS Structures

β-H Elimination-TS Pd^{II}

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15ClF2Pd C1[X(C16H15ClF2Pd)] #Atoms= 35
Charge = 0 Multiplicity = 1

SCF Energy= -1405.37821739 Predicted Change= -8.434242D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00790	0.00180	[NO]	0.00790	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.008629	-0.564094	0.441287
C	3.185396	0.347826	0.172136
F	2.386449	-1.874164	0.225191
F	1.629424	-0.469259	1.759261
C	0.813042	-0.280152	-0.446232
H	1.036810	-0.354976	-1.510595
C	-0.248395	0.563932	-0.038177
H	-0.195402	0.953743	0.978221
H	-1.448092	-0.370434	0.391304
C	-0.989435	1.449315	-1.036954
H	-0.333213	2.314043	-1.209555
H	-1.079329	0.922394	-1.992183
Pd	-0.726342	-1.693152	-0.071872
Cl	-2.147881	-3.539851	0.171867
C	3.352314	1.522258	0.914478
H	2.665868	1.754721	1.722121
C	4.414459	2.379495	0.627686
H	4.547193	3.285555	1.211887
C	5.307184	2.071247	-0.401328
H	6.133490	2.740769	-0.622820
C	5.139507	0.899136	-1.142163
H	5.836581	0.651322	-1.937413
H	3.957431	-0.880761	-1.424320
C	-2.343275	1.928858	-0.554980
C	4.080038	0.037804	-0.859220
C	-3.505630	1.203725	-0.850671
H	-3.439615	0.302943	-1.456302
C	-4.748096	1.629690	-0.377614
H	-5.639720	1.056764	-0.616175
C	-4.843925	2.788878	0.394611
H	-5.811087	3.122163	0.760582
C	-3.692269	3.521307	0.690242
H	-3.759872	4.428486	1.284569
C	-2.451143	3.093043	0.217149
H	-1.558587	3.672929	0.443476

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1405.37821739 Predicted Change= -8.434242D-09
Zero-point correction (ZPE)= -1405.1140 0.26421

Internal Energy (U)=	-1405.0823	0.29586	
Enthalpy (H)=	-1405.0811	0.29710	
Gibbs Free Energy (G)=	-1405.1922	0.18601	
Entropy (S)=	0.00028257		
Frequencies --	-736.2549	17.3274	21.7784

β-F Elimination-TS Pd^{II}

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15ClF2Pd C1[X(C16H15ClF2Pd)] #Atoms= 35
Charge = 0 Multiplicity = 1

SCF Energy= -1405.35860125 Predicted Change= -4.449727D-09

==========

Optimization completed on the basis of negligible forces. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00288	0.00180	[NO]	0.00288	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.375264	0.126852	0.192449
C	2.244731	-1.090952	0.613442
H	1.906870	-1.973644	0.057321
H	2.077760	-1.297869	1.677719
C	3.716790	-0.852308	0.357457
H	1.726744	1.010105	0.739564
H	1.530749	0.330849	-0.871403
C	-0.105470	-0.061675	0.482564
H	-0.345355	-0.194063	1.540086
C	-0.861459	-0.943971	-0.365124
F	-0.244045	-1.373365	-1.454444
F	-1.804976	0.525312	-1.404002
C	-2.051513	-1.699318	-0.010487
Pd	-1.087647	1.733275	0.024159
Cl	-1.900818	3.965211	-0.090658
C	4.548936	-0.343842	1.363760
H	4.136812	-0.151885	2.352361
C	5.898516	-0.087094	1.115575
H	6.528708	0.303481	1.910257
C	6.437595	-0.335185	-0.148206
H	7.488134	-0.137329	-0.342946

C	5.619070	-0.842813	-1.159696
H	6.030776	-1.042661	-2.145477
C	4.270894	-1.098697	-0.906740
H	3.640337	-1.497623	-1.698732
C	-2.464262	-2.762096	-0.837529
H	-1.899873	-2.999031	-1.731671
C	-3.589468	-3.507027	-0.502732
H	-3.901785	-4.327655	-1.140924
C	-4.316958	-3.196175	0.649110
H	-5.197405	-3.777631	0.906736
C	-3.919150	-2.135002	1.470326
H	-4.491768	-1.888639	2.358844
C	-2.793414	-1.388941	1.147177
H	-2.504452	-0.553712	1.776043

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1405.35860125 Predicted Change= -4.449727D-09
Zero-point correction (ZPE)= -1405.0905 0.26808
Internal Energy (U)= -1405.0588 0.29974
Enthalpy (H)= -1405.0576 0.30098
Gibbs Free Energy (G)= -1405.1698 0.18875
Entropy (S)= 0.00028548

Frequencies -- -250.2093 19.9208 22.2690

β-H Elimination-TS Pd^{II} Ph & Bn Groups Exchanged

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15ClF2Pd C1[X(C16H15ClF2Pd)] #Atoms= 35
Charge = 0 Multiplicity = 1

SCF Energy= -1405.38203890 Predicted Change= -8.702636D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]

Displ 0.00084 || 0.00180 [YES] 0.00084 || 0.00180 [YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.884420	-1.221348	1.172011
F	1.049944	-2.385314	0.447067
F	0.167253	-1.564240	2.298352
C	0.078086	-0.255735	0.333311
H	0.589853	0.063165	-0.572433
C	-0.856755	0.635923	0.940236
H	-0.964399	0.529818	2.019845
H	-2.214443	-0.024047	0.744605
Pd	-1.732018	-1.162536	-0.253860
Cl	-3.528974	-2.422906	-1.086818
C	2.259696	-0.722602	1.627023
H	2.092484	0.127062	2.297298
H	2.683602	-1.534901	2.229544
C	3.194787	-0.335921	0.499997
C	3.804705	-1.318488	-0.293675
C	3.465412	1.011846	0.229594
C	4.662383	-0.959149	-1.333364
H	3.605333	-2.367430	-0.095265
C	4.324150	1.373457	-0.810602
H	3.006123	1.784839	0.841753
C	4.924255	0.387907	-1.595491
H	5.128996	-1.732556	-1.937333
H	4.525509	2.423727	-1.003185
H	5.595117	0.666387	-2.403503
C	-1.133752	2.007870	0.422182
C	-1.346737	3.035828	1.350930
C	-1.155034	2.308279	-0.948120
C	-1.549216	4.347605	0.919739
H	-1.346550	2.810964	2.414669
C	-1.360111	3.616873	-1.376562
H	-1.034706	1.512833	-1.679145
C	-1.554337	4.640960	-0.443939
H	-1.708254	5.135596	1.650093
H	-1.379575	3.836949	-2.439893
H	-1.720186	5.659808	-0.781946

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1405.38203890 Predicted Change= -8.702636D-10
Zero-point correction (ZPE)= -1405.1172 0.26474
Internal Energy (U)= -1405.0859 0.29609
Enthalpy (H)= -1405.0846 0.29734
Gibbs Free Energy (G)= -1405.1935 0.18847

Entropy (S)= 0.00027692

Frequencies -- -704.7131 18.2903 30.1971

β-F Elimination-TS Pd^{II} Ph & Bn Groups Exchanged

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250,ts,calcfc,noeigentest) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15ClF2Pd C1[X(C16H15ClF2Pd)] #Atoms= 35
Charge = 0 Multiplicity = 1

SCF Energy= -1405.35728925 Predicted Change= -1.849721D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00037	0.00180	[YES]	0.00037	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.621887	-1.415110	-0.194212
C	0.528033	-0.375517	0.047346
H	0.469484	0.426623	-0.691657
C	0.274390	0.095138	1.364571
Pd	-1.344805	-1.324007	-0.244029
Cl	-3.266906	-2.527463	-0.923267
F	-1.535453	-0.777737	1.683219
F	0.827386	-0.566577	2.364782
H	1.383265	-1.960220	-1.116138
H	1.622804	-2.148835	0.616995
C	2.997633	-0.777200	-0.340111
C	3.777214	-0.486291	0.788352
C	3.496285	-0.446865	-1.606513
C	5.027817	0.118004	0.651704
H	3.406959	-0.741626	1.778013
C	4.745873	0.160024	-1.745417
H	2.906152	-0.674520	-2.491689
C	5.515333	0.444439	-0.615800
H	5.623905	0.328076	1.535778
H	5.119714	0.403831	-2.736218
H	6.490241	0.912038	-0.722344
C	-0.182967	1.460172	1.765630

H	0.744435	1.991459	2.031644
H	-0.748297	1.342003	2.696049
C	-0.956356	2.243599	0.727142
C	-0.324751	3.242454	-0.023858
C	-2.318855	1.987052	0.515229
C	-1.039271	3.971236	-0.977332
H	0.728803	3.457465	0.140797
C	-3.032468	2.717452	-0.435697
H	-2.810115	1.212835	1.095582
C	-2.394516	3.709245	-1.185009
H	-0.537620	4.745209	-1.551557
H	-4.087768	2.510694	-0.589045
H	-2.952639	4.277998	-1.923511

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1405.35728925 Predicted Change= -1.849721D-10
Zero-point correction (ZPE)= -1405.0888 0.26844
Internal Energy (U)= -1405.0576 0.29964
Enthalpy (H)= -1405.0564 0.30088
Gibbs Free Energy (G)= -1405.1646 0.19261
Entropy (S)= 0.00027539

Frequencies -- -275.8297 22.4393 24.4458

Model System Structures

H anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

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# b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18)
Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= OH Stoichiometry= H(1-) OH[O(H)] #Atoms= 1
Charge = -1 Multiplicity = 1

SCF Energy= -0.549083240314 Predicted Change= -0.000000D+00

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00000	0.00180	[YES]	0.00000	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z

```
---------------------------------------------------------------------
      H         0.000000       0.000000       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 393.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -0.549083240314    Predicted Change= -0.000000D+00
 Zero-point correction (ZPE)=           -0.5490     0.00000
 Internal Energy (U)=                -0.5472     0.00186
 Enthalpy (H)=                   -0.5459     0.00311
 Gibbs Free Energy (G)=              -0.5631    -0.01404
 Entropy (S)=                         4.365e-05
---------------------------------------------------------------------
```

F anion

```
---------------------------------------------------------------------
 Using  Gaussian 16:  ES64L-G16RevA.03 25-Dec-2016
=====================================================================
 # b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18)
 Temperature=393.15
 #N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq
---------------------------------------------------------------------
 Pointgroup= OH   Stoichiometry= F(1-)   OH[O(F)]  #Atoms= 1
 Charge = -1    Multiplicity = 1
---------------------------------------------------------------------
 SCF Energy= -99.8323175207          Predicted Change= -0.000000D+00
=====================================================================
 Optimization completed.            {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00000 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00000 ||  0.00180   [ YES ]      0.00000 ||  0.00180   [ YES ]
---------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type      X          Y          Z
---------------------------------------------------------------------
      F         0.000000       0.000000       0.000000
---------------------------------------------------------------------
 Statistical Thermodynamic Analysis
 Temperature= 393.150 Kelvin       Pressure= 1.00000 Atm
=====================================================================
 SCF Energy=     -99.8323175207    Predicted Change= -0.000000D+00
 Zero-point correction (ZPE)=           -99.8323     0.00000
 Internal Energy (U)=                -99.8304     0.00186
 Enthalpy (H)=                   -99.8292     0.00311
 Gibbs Free Energy (G)=              -99.8518    -0.01953
 Entropy (S)=                         5.76e-05
---------------------------------------------------------------------
```

$PdCl_2H$

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= Cl2HPd(2) C1[X(Cl2HPd)] #Atoms= 4
Charge = 0 Multiplicity = 2

SCF Energy= -1047.75206429 Predicted Change= -6.017181D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00072	0.00180	[YES]	0.00072	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cl	2.274951	0.014900	0.000271
H	0.000017	1.469357	-0.000353
Pd	-0.000001	-0.042956	-0.000193
Cl	-2.274950	0.014901	0.000271

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1047.75206429 Predicted Change= -6.017181D-09
Zero-point correction (ZPE)= -1047.7436 0.00842
Internal Energy (U)= -1047.7362 0.01578
Enthalpy (H)= -1047.7350 0.01703
Gibbs Free Energy (G)= -1047.7858 -0.03382
Entropy (S)= 0.00012935

Frequencies -- 79.5882 132.8921 308.6133

$PdCl_2F$

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250,gdiis,maxstep=10)
freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= Cl2FPd(2) C1[X(Cl2FPd)] #Atoms= 4

Charge = 0 Multiplicity = 2

SCF Energy= -1146.95252501 Predicted Change= -6.151696D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00001	0.00030	[YES]
Displ	0.00029	0.00180	[YES]	0.00029	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cl	2.259942	-0.303887	0.133528
Pd	0.000021	-0.118750	-0.108442
Cl	-2.259988	-0.303892	0.133518
F	-0.000021	1.754970	0.049838

Statistical Thermodynamic Analysis

Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1146.95252501 Predicted Change= -6.151696D-09

Zero-point correction (ZPE)= -1146.9486 0.00391

Internal Energy (U)= -1146.9404 0.01209

Enthalpy (H)= -1146.9391 0.01334

Gibbs Free Energy (G)= -1146.9938 -0.04133

Entropy (S)= 0.00013907

Frequencies -- 95.4056 149.7922 170.0046

CH_2CF_2Bn anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15

#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H9F2(1-) C1[X(C9H9F2)] #Atoms= 20

Charge = -1 Multiplicity = 1

SCF Energy= -548.064923671 Predicted Change= -2.146595D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00122	0.00180	[YES]	0.00122	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	-1.951840	0.139935	0.038159
F	-1.733888	-0.068845	1.412495
F	-3.139440	-0.868832	-0.133675
C	-2.200270	1.495972	-0.285091
H	-2.326131	1.667337	-1.358685
H	-2.997025	1.958232	0.307561
C	-0.863994	-0.606221	-0.743698
H	-1.027333	-1.680275	-0.609584
C	0.574026	-0.279058	-0.378406
H	-1.033447	-0.390802	-1.807472
C	1.498390	-1.309378	-0.158915
H	1.165276	-2.344009	-0.225356
C	2.834665	-1.034946	0.146927
H	3.530679	-1.854194	0.317097
C	3.271089	0.287339	0.242694
H	4.309530	0.507472	0.482219
C	2.357622	1.324750	0.030352
H	2.686343	2.359599	0.109492
C	1.026013	1.046106	-0.278845
H	0.277854	1.828741	-0.403707

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -548.064923671 Predicted Change= -2.146595D-08
Zero-point correction (ZPE)= -547.9107 0.15413
Internal Energy (U)= -547.8943 0.17062
Enthalpy (H)= -547.8930 0.17186
Gibbs Free Energy (G)= -547.9613 0.10354
Entropy (S)= 0.00017379

Frequencies -- 71.0056 107.4349 133.5342

CH_2CF_2Ph anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18)
Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H7F2(1-) C1[X(C8H7F2)] #Atoms= 17
Charge = -1 Multiplicity = 1

SCF Energy= -508.751848058 Predicted Change= -4.063829D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00011	0.00180	[YES]	0.00011	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-2.088982	1.321993	-0.536456
H	-3.182199	1.317123	-0.554260
H	-1.637070	1.704391	-1.453313
C	-1.497646	0.153477	-0.021536
F	-1.943973	-0.167566	1.296716
C	0.015330	0.074825	-0.046140
F	-1.926887	-1.211570	-0.651502
C	0.786583	1.244248	0.034948
H	0.257485	2.190511	0.089568
C	2.181375	1.190407	0.048076
H	2.756585	2.113388	0.098943
C	2.839092	-0.041938	0.012601
H	3.926212	-0.087383	0.035494
C	2.082240	-1.215787	-0.046413
H	2.582401	-2.182553	-0.074448
C	0.688455	-1.157487	-0.078725
H	0.095649	-2.061671	-0.147039

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -508.751848058 Predicted Change= -4.063829D-10
Zero-point correction (ZPE)= -508.6264 0.12541
Internal Energy (U)= -508.6118 0.13997
Enthalpy (H)= -508.6106 0.14121
Gibbs Free Energy (G)= -508.6743 0.07745
Entropy (S)= 0.00016219

Frequencies -- 83.9154 129.6057 214.6674

CH_2CH_2Bn anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq

Pointgroup= C1 Stoichiometry= C9H11(1-) C1[X(C9H11)] #Atoms= 20
Charge = -1 Multiplicity = 1

SCF Energy= -349.546064021 Predicted Change= -1.141720D-08
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00139	0.00180	[YES]	0.00139	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.329136	-0.000489	-0.597379
H	1.972196	0.876880	-1.168973
H	1.972794	-0.879017	-1.167598
C	3.819359	0.000159	-0.448987
H	4.135407	-0.884710	0.145572
H	4.134912	0.886547	0.143572
C	1.409341	0.000103	0.741329
H	1.697253	-0.884810	1.322937
C	-0.055838	0.000063	0.459687
H	1.697249	0.885433	1.322291
C	-0.763520	1.202849	0.241509
H	-0.247262	2.149265	0.395660
C	-2.099960	1.205160	-0.152867
H	-2.615753	2.152779	-0.300902
C	-2.784433	-0.000026	-0.353512
H	-3.828071	-0.000017	-0.659418
C	-2.099933	-1.205138	-0.152779
H	-2.615643	-2.152806	-0.300769
C	-0.763465	-1.202748	0.241622
H	-0.247200	-2.149139	0.395893

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -349.546064021 Predicted Change= -1.141720D-08
Zero-point correction (ZPE)= -349.3775 0.16850
Internal Energy (U)= -349.3630 0.18296
Enthalpy (H)= -349.3618 0.18421
Gibbs Free Energy (G)= -349.4257 0.12033
Entropy (S)= 0.00016247

Frequencies -- 70.7824 96.2996 111.5091

CH_2CH_2Ph anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016
==========
b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)

opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C8H9(1-) C1[X(C8H9)] #Atoms= 17
Charge = -1 Multiplicity = 1

SCF Energy= -310.234819954 Predicted Change= -3.591343D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00037	0.00180	[YES]	0.00037	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.831249	-0.000017	0.769099
H	2.489471	0.877191	1.363376
H	2.489143	-0.877009	1.363512
C	2.025551	-0.000021	-0.545419
H	2.286839	0.882044	-1.158846
C	0.525554	-0.000013	-0.337058
H	2.286755	-0.882110	-1.158864
C	-0.206934	-1.200866	-0.198034
H	0.319972	-2.147799	-0.317811
C	-1.570202	-1.204407	0.087164
H	-2.098726	-2.153367	0.178282
C	-2.271174	-0.000005	0.237062
H	-3.336287	0.000027	0.458381
C	-1.570179	1.204431	0.087128
H	-2.098741	2.153374	0.178175
C	-0.206934	1.200872	-0.198017
H	0.319995	2.147799	-0.317754

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -310.234819954 Predicted Change= -3.591343D-09
Zero-point correction (ZPE)= -310.0946 0.14013
Internal Energy (U)= -310.0824 0.15236
Enthalpy (H)= -310.0812 0.15361
Gibbs Free Energy (G)= -310.1394 0.09540
Entropy (S)= 0.00014806

Frequencies -- 93.9152 140.4683 275.9692

CH_2CFBn + F anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

---

b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H9F C1[X(C9H9F)] #Atoms= 19
Charge = 0 Multiplicity = 1

SCF Energy= -448.195540829 Predicted Change= -2.368700D-09

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00095	0.00180	[YES]	0.00095	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
C	2.187466	0.000191	-0.049878
F	2.098783	-1.288515	-0.476275
C	3.109964	0.800403	-0.572632
H	3.191802	1.829266	-0.243220
H	3.795210	0.444027	-1.333784
C	1.165457	0.311920	1.005430
H	1.326761	-0.371899	1.850141
C	-0.265466	0.174701	0.507125
H	1.345343	1.326970	1.372166
C	-0.868758	-1.085700	0.406100
H	-0.309355	-1.970760	0.696933
C	-2.175462	-1.213113	-0.066444
H	-2.629608	-2.198078	-0.136502
C	-2.898531	-0.079857	-0.445495
H	-3.917500	-0.178306	-0.810088
C	-2.305636	1.180341	-0.349720
H	-2.860988	2.068428	-0.639893
C	-0.997338	1.304134	0.121660
H	-0.540897	2.288874	0.193856

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -448.195540829 Predicted Change= -2.368700D-09
Zero-point correction (ZPE)= -448.0410 0.15445
Internal Energy (U)= -448.0265 0.16904
Enthalpy (H)= -448.0252 0.17028
Gibbs Free Energy (G)= -448.0914 0.10412
Entropy (S)= 0.00016829

Frequencies -- 27.6676 69.9360 96.6620

CH_2CFPh + F anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016
==========
# b3lyp/6-31G(d) gfprint gfinput scf=(direct,verytight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18)
Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq
---
Pointgroup= C1 Stoichiometry= C8H7F C1[X(C8H7F)] #Atoms= 16
Charge = 0 Multiplicity = 1

SCF Energy= -408.885223133 Predicted Change= -1.196023D-10
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00016	0.00180	[YES]	0.00016	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-1.694183	0.058297	0.000574
C	-0.221781	0.050513	-0.001300
F	-2.226472	-1.194962	-0.037851
C	-2.539506	1.089560	0.036994
H	-2.184581	2.111198	0.075387
H	-3.609429	0.918371	0.030965
C	0.520333	1.245080	-0.020179
H	0.010617	2.203384	-0.041096
C	1.911450	1.213511	-0.016975
H	2.468630	2.146185	-0.032297
C	2.590263	-0.008884	0.003467
H	3.676501	-0.030264	0.005210
C	1.862924	-1.199037	0.019887
H	2.380206	-2.154466	0.034830
C	0.468482	-1.172334	0.017129
H	-0.091593	-2.099989	0.030082

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -408.885223133 Predicted Change= -1.196023D-10
Zero-point correction (ZPE)= -408.7593 0.12588
Internal Energy (U)= -408.7469 0.13830
Enthalpy (H)= -408.7456 0.13954

Gibbs Free Energy (G)= -408.8064 0.07880
Entropy (S)= 0.00015449

Frequencies -- 21.0567 159.7853 225.8619

CH_2CHBn + H anion

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18)
Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C9H10 C1[X(C9H10)] #Atoms= 19
Charge = 0 Multiplicity = 1

SCF Energy= -348.958215881 Predicted Change= -4.014581D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00023	0.00180	[YES]	0.00023	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	2.415023	-0.182342	-0.499262
C	1.429745	-0.807632	0.457184
H	1.470161	-1.901325	0.358517
C	-0.005016	-0.353307	0.228014
H	1.734695	-0.576772	1.487043
C	-1.027875	-1.281549	0.000299
C	-2.346528	-0.863619	-0.196132
C	-2.661063	0.495493	-0.169279
C	-1.648168	1.432113	0.054221
C	-0.333076	1.010124	0.248490
H	-0.790607	-2.343113	-0.021269
H	-3.125794	-1.600988	-0.371360
H	-3.685722	0.823709	-0.322378
H	-1.883052	2.493325	0.075416
H	0.452800	1.743434	0.412791
H	2.218903	-0.355176	-1.558177
C	3.470368	0.549790	-0.139136
H	3.697925	0.748764	0.906588
H	4.150236	0.973711	-0.873563

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

```
==========================================================================
 SCF Energy=     -348.958215881    Predicted Change= -4.014581D-10
 Zero-point correction (ZPE)=          -348.7961      0.16209
 Internal Energy (U)=              -348.7825      0.17566
 Enthalpy (H)=                 -348.7813      0.17691
 Gibbs Free Energy (G)=            -348.8445      0.11370
 Entropy (S)=                      0.00016078
---------------------------------------------------------------------------
 Frequencies --     29.8010              80.7421              147.4957
```

CH_2CHPh + H anion

```
---------------------------------------------------------------------------
 Using  Gaussian 16:  ES64L-G16RevA.03 25-Dec-2016
==========================================================================
 # b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
 opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18)
 Temperature=393.15
 #N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq
---------------------------------------------------------------------------
 Pointgroup= C1   Stoichiometry= C8H8   C1[X(C8H8)]  #Atoms= 16
 Charge = 0     Multiplicity = 1
---------------------------------------------------------------------------
 SCF Energy= -309.649584146         Predicted Change= -3.076375D-09
==========================================================================
 Optimization completed.           {Found       2       times}
 Item      Max Val.    Criteria    Pass?      RMS Val.    Criteria    Pass?
 Force      0.00001 ||  0.00045   [ YES ]      0.00000 ||  0.00030   [ YES ]
 Displ      0.00052 ||  0.00180   [ YES ]      0.00052 ||  0.00180   [ YES ]
---------------------------------------------------------------------------
     Atomic         Coordinates (Angstroms)
      Type      X          Y          Z
---------------------------------------------------------------------------
      C        1.955182     -0.529814      0.000118
      C        0.515264     -0.220515      0.000068
      H        2.186617     -1.595174      0.000287
      C        2.977659      0.335307     -0.000135
      H        2.840465      1.413419     -0.000401
      H        4.004692     -0.017048     -0.000126
      C       -0.406459     -1.281922     -0.000002
      H       -0.035235     -2.304398     -0.000026
      C       -1.781235     -1.046518     -0.000065
      H       -2.472407     -1.885245     -0.000106
      C       -2.265728      0.261940     -0.000051
      H       -3.335795      0.450711     -0.000107
      C       -1.362420      1.330047      0.000026
      H       -1.730588      2.352721      0.000050
      C        0.009134      1.092956      0.000084
      H        0.693865      1.936124      0.000170
---------------------------------------------------------------------------
```

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm
==========

SCF Energy= -309.649584146 Predicted Change= -3.076375D-09
Zero-point correction (ZPE)= -309.5158 0.13373
Internal Energy (U)= -309.5044 0.14510
Enthalpy (H)= -309.5032 0.14634
Gibbs Free Energy (G)= -309.5604 0.08917
Entropy (S)= 0.00014543

Frequencies -- 45.6840 208.2377 239.8721

Noteworthy Structures

Substrate

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016
==========

# b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18)
Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d) Freq
---

Pointgroup= C1 Stoichiometry= C10H10F2 C1[X(C10H10F2)] #Atoms= 22
Charge = 0 Multiplicity = 1

SCF Energy= -586.742092055 Predicted Change= -2.042220D-08
==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00435	0.00180	[NO]	0.00435	0.00180	[NO]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	3.383795	0.062490	-0.116256
F	3.308296	1.337743	-0.492404
F	4.639876	-0.238664	0.202581
C	2.365741	-0.783758	-0.070826
H	2.590871	-1.792582	0.261403
C	0.949856	-0.421405	-0.423270
H	0.592497	-1.078612	-1.227823
H	0.909183	0.600412	-0.814661
C	-0.016264	-0.548538	0.781417
H	0.327297	0.121187	1.578942
H	0.044659	-1.569644	1.179238
C	-1.448200	-0.225525	0.411863
C	-1.931169	1.088153	0.491520

H	-1.275845	1.876199	0.857059
C	-3.239611	1.396226	0.115475
H	-3.595656	2.420619	0.189288
C	-4.090454	0.390863	-0.348759
H	-5.110557	0.628010	-0.638824
C	-3.623023	-0.922361	-0.432153
H	-4.279218	-1.713121	-0.786743
C	-2.313654	-1.224878	-0.054491
H	-1.958873	-2.251777	-0.116593

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -586.742092055 Predicted Change= -2.042220D-08
Zero-point correction (ZPE)= -586.5663 0.17575
Internal Energy (U)= -586.5484 0.19364
Enthalpy (H)= -586.5471 0.19489
Gibbs Free Energy (G)= -586.6231 0.11895
Entropy (S)= 0.00019317

Frequencies -- 22.6501 40.4633 59.5960

$PdCl_2$

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= CS Stoichiometry= Cl2Pd CS[SG(Cl2Pd)] #Atoms= 3
Charge = 0 Multiplicity = 1

SCF Energy= -1047.16179115 Predicted Change= -1.331833D-08

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00002	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00041	0.00180	[YES]	0.00041	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
Cl	1.650801	-0.880575	-0.000000
Cl	-1.650801	-0.880634	0.000000
Pd	-0.000000	0.650881	-0.000000

Statistical Thermodynamic Analysis

Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1047.16179115 Predicted Change= -1.331833D-08
Zero-point correction (ZPE)= -1047.1598 0.00191
Internal Energy (U)= -1047.1539 0.00783
Enthalpy (H)= -1047.1527 0.00907
Gibbs Free Energy (G)= -1047.2010 -0.03928
Entropy (S)= 0.00012301

Frequencies -- 139.9257 343.8746 357.5210

Ph Radical

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

# b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
guess=(mix,always) opt=(maxcycle=250) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/6-31G(d) Freq

---

Pointgroup= C1 Stoichiometry= C6H5(2) C1[X(C6H5)] #Atoms= 11
Charge = 0 Multiplicity = 2

SCF Energy= -231.562342746 Predicted Change= -4.724579D-08

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00004	0.00045	[YES]	0.00002	0.00030	[YES]
Displ	0.00034	0.00180	[YES]	0.00034	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	0.000003	1.324922	-0.000000
H	0.000026	2.411419	0.000002
C	1.214573	0.632764	-0.000023
H	2.155061	1.179020	-0.000029
C	1.226945	-0.772114	0.000026
C	-0.000010	-1.400119	0.000002
H	2.163715	-1.323126	0.000018
C	-1.226949	-0.772108	-0.000029
H	-2.163732	-1.323097	-0.000014
H	-2.155057	1.179025	0.000036
C	-1.214564	0.632782	0.000022

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -231.562342746 Predicted Change= -4.724579D-08

Zero-point correction (ZPE)= -231.4747 0.08760
Internal Energy (U)= -231.4673 0.09499
Enthalpy (H)= -231.4661 0.09624
Gibbs Free Energy (G)= -231.5138 0.04847
Entropy (S)= 0.0001215

Frequencies -- 402.4224 426.8693 600.1701

Cl Radical

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016
==========
b3lyp/6-31G(d) gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/6-31G(d) Freq
---
Pointgroup= OH Stoichiometry= Cl(2) OH[O(Cl)] #Atoms= 1
Charge = 0 Multiplicity = 2

SCF Energy= -460.136699740 Predicted Change= -0.000000D+00
==========
Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00000	0.00180	[YES]	0.00000	0.00180	[YES]

Atomic Coordinates (Angstroms)

Type	X	Y	Z
Cl	0.000000	0.000000	0.000000

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm
==========
SCF Energy= -460.136699740 Predicted Change= -0.000000D+00
Zero-point correction (ZPE)= -460.1367 0.00000
Internal Energy (U)= -460.1348 0.00186
Enthalpy (H)= -460.1335 0.00311
Gibbs Free Energy (G)= -460.1582 -0.02153
Entropy (S)= 6.269e-05

Arylated Substrate Pd^{III}

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016
==========
b3lyp/gen pseudo=read 6D 10F gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman

SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.60631764 Predicted Change= -6.557508D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00003	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00062	0.00180	[YES]	0.00062	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.607461	1.637814	-0.175524
C	2.614129	0.549335	0.117938
F	1.376216	2.380951	0.950401
F	2.136161	2.518762	-1.110248
C	0.281417	1.171423	-0.783842
H	0.481189	0.799006	-1.789993
C	-0.829939	2.202749	-0.737802
H	-0.416264	3.093484	-1.238935
H	-1.042102	2.488026	0.294501
C	-2.129983	1.795103	-1.461824
H	-1.897376	1.503234	-2.493499
H	-2.776016	2.678229	-1.516358
C	-2.867466	0.675986	-0.763899
C	-3.827568	0.934823	0.218205
H	-4.071790	1.962812	0.471941
C	-4.470494	-0.111745	0.879144
H	-5.213925	0.112683	1.638768
C	-4.167042	-1.449451	0.579103
H	-4.679958	-2.253223	1.098268
C	-3.225339	-1.732741	-0.398579
H	-2.998891	-2.758172	-0.675259
C	-2.567416	-0.676679	-1.072117
H	-1.975331	-0.906800	-1.952810
C	3.490722	0.118804	-0.884479
H	3.468249	0.588856	-1.861685
C	4.393579	-0.908028	-0.620621
H	5.074886	-1.238165	-1.399340
C	4.425286	-1.512497	0.641072
H	5.130188	-2.314822	0.840004
C	3.557388	-1.080002	1.642887
H	3.586942	-1.535995	2.628238
C	2.651658	-0.046507	1.388617
H	1.987698	0.306218	2.169753

Pd	-0.292124	-0.620892	0.116169
Cl	0.485883	-1.934325	-1.713537
Cl	-0.865267	0.318321	2.211865

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1865.60631764 Predicted Change= -6.557508D-09
Zero-point correction (ZPE)= -1865.3342 0.27204
Internal Energy (U)= -1865.3005 0.30580
Enthalpy (H)= -1865.2992 0.30705
Gibbs Free Energy (G)= -1865.4112 0.19508
Entropy (S)= 0.0002848

Frequencies -- 36.1154 40.9199 49.9966

Arylated Substrate Pd^{III} Ph & Bn Groups Exchanged

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.60345838 Predicted Change= -1.253719D-09

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.337176	1.737641	0.087493
C	0.654460	2.256100	-0.951802
H	0.192731	2.150517	-1.938043
C	1.975993	1.519703	-0.895072
H	0.792081	3.324994	-0.761398
F	0.137333	2.022549	1.347457
F	-1.511076	2.442417	-0.043438
C	-0.669674	0.245573	-0.011719
H	-0.846863	-0.040255	-1.049971
C	-1.759201	-0.276614	0.919145
H	-1.710719	0.246591	1.877182

H	-1.564713	-1.331774	1.121635
C	-3.138289	-0.146500	0.281650
Pd	1.161654	-0.708866	0.277088
Cl	0.445159	-2.554228	-1.099866
Cl	0.961574	-1.370589	2.538403
C	-3.558910	-1.089926	-0.667230
H	-2.891149	-1.902112	-0.946354
C	-4.828129	-1.003967	-1.239985
H	-5.142492	-1.747308	-1.967741
C	-5.695556	0.026136	-0.868965
H	-6.686845	0.090480	-1.309490
C	-5.284530	0.969749	0.074865
H	-5.955376	1.771431	0.372241
C	-4.011768	0.887256	0.641558
H	-3.694588	1.627794	1.370372
C	2.235560	0.437761	-1.769350
H	1.506190	0.167577	-2.527402
C	3.479277	-0.222557	-1.739925
H	3.661660	-1.042237	-2.427291
C	4.457719	0.175535	-0.833927
H	5.417520	-0.331163	-0.810252
C	4.202343	1.236502	0.047719
H	4.964596	1.547587	0.755681
C	2.975542	1.897012	0.024396
H	2.785146	2.716483	0.710395

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -1865.60345838 Predicted Change= -1.253719D-09
Zero-point correction (ZPE)= -1865.3318 0.27159
Internal Energy (U)= -1865.2975 0.30589
Enthalpy (H)= -1865.2963 0.30714
Gibbs Free Energy (G)= -1865.4124 0.19096
Entropy (S)= 0.00029552

Frequencies -- 18.1599 30.3332 49.6524

Arylated Substrate Pd^{II}

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

==========

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15ClF2Pd C1[X(C16H15ClF2Pd)] #Atoms= 35
Charge = 0 Multiplicity = 1

SCF Energy= -1405.41278866 Predicted Change= -5.966931D-10

==========

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00005	0.00180	[YES]	0.00005	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	1.352931	1.411271	0.320268
C	2.537271	0.475971	0.344968
F	0.812751	1.510801	1.593488
F	1.822511	2.689961	0.025768
C	0.221831	1.150001	-0.677272
H	0.646871	0.929531	-1.658742
C	-0.776129	2.325181	-0.716312
H	-0.410809	3.071481	-1.432142
H	-0.789499	2.821801	0.258208
C	-2.198149	1.905661	-1.097422
H	-2.233449	1.601811	-2.150032
H	-2.872789	2.768411	-1.000692
C	-2.717729	0.756491	-0.247162
C	-2.288609	0.557651	1.096948
H	-1.611569	1.259011	1.570758
C	-2.891389	-0.447219	1.898398
H	-2.562469	-0.567249	2.926408
C	-3.889559	-1.251369	1.379348
H	-4.344479	-2.025149	1.990388
C	-4.331319	-1.051869	0.052588
H	-5.121999	-1.678679	-0.349882
C	-3.765989	-0.068129	-0.739002
H	-4.115509	0.081251	-1.757082
C	3.481881	0.546561	-0.684762
H	3.357681	1.269791	-1.485212
C	4.586431	-0.302869	-0.678522
H	5.315271	-0.244739	-1.482082
C	4.757181	-1.222169	0.359168
H	5.618191	-1.884979	0.362818
C	3.820251	-1.286119	1.391158
H	3.950221	-1.996089	2.203228
C	2.712881	-0.437589	1.386968
H	1.987671	-0.484559	2.191698
Pd	-0.777089	-0.582419	-0.246572
Cl	0.679101	-2.017999	-1.397342

Statistical Thermodynamic Analysis

Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

SCF Energy= -1405.41278866 Predicted Change= -5.966931D-10
Zero-point correction (ZPE)= -1405.1418 0.27095
Internal Energy (U)= -1405.1110 0.30177
Enthalpy (H)= -1405.1097 0.30302
Gibbs Free Energy (G)= -1405.2139 0.19883
Entropy (S)= 0.00026502

Frequencies -- 28.4308 35.5052 49.4276

Arylated Substrate Pd^{II} Ph & Bn Groups Exchanged

Using Gaussian 16: ES64L-G16RevA.03 25-Dec-2016

# b3lyp/gen pseudo=read 6D 10F gfprint gfinput
scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman
SCRF=(PCM,SOLVENT=1,4-dioxane) iop(1/8=18) Temperature=393.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk UB3LYP/ChkBas Freq

---

Pointgroup= C1 Stoichiometry= C16H15Cl2F2Pd(2) C1[X(C16H15Cl2F2Pd)] #Atoms= 36
Charge = 0 Multiplicity = 2

SCF Energy= -1865.60345838 Predicted Change= -1.253719D-09

Optimization completed. {Found 2 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00000	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00061	0.00180	[YES]	0.00061	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-0.337176	1.737641	0.087493
C	0.654460	2.256100	-0.951802
H	0.192731	2.150517	-1.938043
C	1.975993	1.519703	-0.895072
H	0.792081	3.324994	-0.761398
F	0.137333	2.022549	1.347457
F	-1.511076	2.442417	-0.043438
C	-0.669674	0.245573	-0.011719
H	-0.846863	-0.040255	-1.049971
C	-1.759201	-0.276614	0.919145
H	-1.710719	0.246591	1.877182
H	-1.564713	-1.331774	1.121635
C	-3.138289	-0.146500	0.281650
Pd	1.161654	-0.708866	0.277088
Cl	0.445159	-2.554228	-1.099866
Cl	0.961574	-1.370589	2.538403
C	-3.558910	-1.089926	-0.667230

H	-2.891149	-1.902112	-0.946354
C	-4.828129	-1.003967	-1.239985
H	-5.142492	-1.747308	-1.967741
C	-5.695556	0.026136	-0.868965
H	-6.686845	0.090480	-1.309490
C	-5.284530	0.969749	0.074865
H	-5.955376	1.771431	0.372241
C	-4.011768	0.887256	0.641558
H	-3.694588	1.627794	1.370372
C	2.235560	0.437761	-1.769350
H	1.506190	0.167577	-2.527402
C	3.479277	-0.222557	-1.739925
H	3.661660	-1.042237	-2.427291
C	4.457719	0.175535	-0.833927
H	5.417520	-0.331163	-0.810252
C	4.202343	1.236502	0.047719
H	4.964596	1.547587	0.755681
C	2.975542	1.897012	0.024396
H	2.785146	2.716483	0.710395

Statistical Thermodynamic Analysis
Temperature= 393.150 Kelvin Pressure= 1.00000 Atm

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SCF Energy= -1865.60345838 Predicted Change= -1.253719D-09
Zero-point correction (ZPE)= -1865.3318 0.27159
Internal Energy (U)= -1865.2975 0.30589
Enthalpy (H)= -1865.2963 0.30714
Gibbs Free Energy (G)= -1865.4124 0.19096
Entropy (S)= 0.00029552

Frequencies -- 18.1599 30.3332 49.6524

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