Synthesis and Lewis Acidity of Fluorophosphonium Cations

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Supporting Information

DFT calculations

DFT calculations were performed using Gaussian 09.2 Geometry optimization of all the molecules was carried out using the wB97XD/def2-TZV basis sets. Conductor-like polarizable continuum solvation model (CPCM) implemented in the Gaussian 09 software was used for energy calculations in which solvent effect was required. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis of all calculated molecules contained no imaginary frequency showing that these are energy minima. NMR spectra of all the molecules were calculated using gauge-including atomic orbital method (GIAO) and referenced to chemical shift of $[Me_3PF]^+$ (experimental + calculated).

$[Me_3PF]^+$:

P	0.00009300	-0.00018300	-0.03497200
F	-0.00064900	-0.00066300	1.64386700
C	1.53374800	-0.87139600	-0.49837500
H	1.51066200	-1.87926100	-0.09063600
H	1.61571900	-0.91823400	-1.58332500
H	2.38776000	-0.33524600	-0.09115000
C	-0.01138400	1.76364800	-0.49793300
H	-0.01136900	1.85795500	-1.58289400
H	-0.90298200	2.23524100	-0.09130100
H	0.87268600	2.24794400	-0.08983600
C	-1.52170700	-0.89147900	-0.49915200
H	-1.60272400	-0.93860300	-1.58416200

H	-1.48654400	-1.89927200	-0.09201400
H	-2.38271100	-0.36645500	-0.09213500

Sum of electronic and zero-point Energies= -560.519913

Sum of electronic and thermal Energies= -560.511791

Sum of electronic and thermal Enthalpies= -560.510846

Sum of electronic and thermal Free Energies= -560.551949

P Isotropic = 165.4324

Me_3PF_2:

P	0.00766600	0.00001100	-0.00130400
F	1.84787600	0.02908300	-0.21723700
F	-1.83809400	-0.02531500	0.21161000
C	-0.14119900	1.67799600	-0.74502800
H	-0.55483800	2.34111300	0.01022300
H	0.83220600	2.01720300	-1.07711800
H	-0.84970400	1.61839300	-1.56612000
C	0.25743500	-0.18307100	1.81340700
H	-0.70319100	-0.19554500	2.31337900
H	0.80440100	-1.10662400	1.98293700
H	0.87664500	0.64307200	2.15110400
C	-0.12939600	-1.49904700	-1.06166800
H	-0.69989800	-1.22963300	-1.94665600
H	0.86110600	-1.84847900	-1.32586400
H	-0.69079600	-2.24884600	-0.51195000

Sum of electronic and zero-point Energies= -660.634620

Sum of electronic and thermal Energies= -660.624921

Sum of electronic and thermal Enthalpies= -660.623977

Sum of electronic and thermal Free Energies= -660.671495

[*t*Bu$_3$PF]$^+$:

P	-0.00026700	-0.00026300	-0.26699800
C	1.58119300	-1.02256200	0.13541200
C	0.09500200	1.88042000	0.13566200
C	-1.67652800	-0.85851100	0.13583500
C	1.64955900	-2.22943700	-0.81821400
H	2.61416000	-2.71293800	-0.65552500
H	0.88210900	-2.97191300	-0.63162100
H	1.60477400	-1.92632300	-1.86307900
C	2.83313200	-0.16459800	-0.10130200
H	2.91098300	0.67592900	0.58350700
H	3.69969800	-0.80330100	0.07614200
H	2.89761700	0.19165700	-1.12838100
C	1.51190500	-1.46576300	1.60578600
H	0.68858600	-2.14986100	1.80105600
H	2.43543500	-1.99998300	1.83401000
H	1.44490300	-0.62593900	2.29758700
C	-1.27273000	2.53716800	-0.10390500
H	-2.04154000	2.18340700	0.57833700
H	-1.15206400	3.60653400	0.07571800
H	-1.61085400	2.41748900	-1.13215800
C	0.51139000	2.04089000	1.60646500
H	1.51248700	1.66322900	1.80418100
H	0.51847400	3.10794700	1.83400300
H	-0.18712600	1.56757300	2.29668400

C	1.10839400	2.54210500	-0.81607800
H	2.13467400	2.25062300	-0.62475500
H	0.87218700	2.34838100	-1.86126500
H	1.04203900	3.61942300	-0.65619800
C	-2.02408100	-0.57623500	1.60603800
H	-2.19717800	0.48008000	1.80162700
H	-2.95231800	-1.10250900	1.83355200
H	-1.26563200	-0.94387200	2.29735000
C	-2.75652300	-0.31275600	-0.81600200
H	-3.65835200	-0.90445500	-0.65059100
H	-3.01308900	0.72387600	-0.63008300
H	-2.47380200	-0.42762800	-1.86119900
C	-1.56015300	-2.37124200	-0.10263600
H	-1.28703700	-2.60409900	-1.13081700
H	-0.86849900	-2.85879900	0.57952200
H	-2.54573600	-2.80314400	0.07717100
F	-0.00047200	0.00063200	-1.97135200

Gas Phase:

Sum of electronic and zero-point Energies= -914.003862

Sum of electronic and thermal Energies= -913.985142

Sum of electronic and thermal Enthalpies= -913.984198

Sum of electronic and thermal Free Energies= -914.046312

CPCM:

Sum of electronic and zero-point Energies= -914.061750

Sum of electronic and thermal Energies= -914.042853

Sum of electronic and thermal Enthalpies= -914.041909

Sum of electronic and thermal Free Energies= -914.104682

P Isotropic = 127.6665

***t*Bu$_3$PF$_2$:**

P	-0.00003100	-0.04831800	0.02365100
F	-0.00016000	0.07442900	1.87801500
F	0.00000800	-0.32175400	-1.82839300
C	0.00035700	1.88719300	-0.07818100
C	1.76119100	-0.91650500	0.03995800
C	2.62147500	-0.31654700	-1.08659800
H	3.60017900	-0.80138800	-1.04494300
H	2.17961500	-0.49617200	-2.06091300
H	2.78386500	0.75255300	-0.97103000
C	1.59609600	-2.41588100	-0.24282300
H	2.59525600	-2.85417900	-0.30641000
H	1.06551300	-2.92702600	0.55830600
H	1.09156900	-2.59357200	-1.18920200
C	2.46807300	-0.74106900	1.38898600
H	1.90147100	-1.17971600	2.20454800
H	3.43554200	-1.24613500	1.31842800
H	2.64959300	0.30278000	1.63045100
C	-2.46857400	-0.73982900	1.38870300
H	-2.64986300	0.30416300	1.62971400
H	-3.43618200	-1.24463400	1.31816700
H	-1.90223900	-1.17835100	2.20450900
C	-1.76152700	-0.91601600	0.03984500
C	-1.59667000	-2.41552200	-0.24219900

H	-2.59588100	-2.85375000	-0.30543100
H	-1.09228000	-2.59375100	-1.18855100
H	-1.06598400	-2.92630300	0.55909600
C	-2.62146700	-0.31624600	-1.08705600
H	-2.17944600	-0.49615500	-2.06124300
H	-3.60023900	-0.80097700	-1.04551500
H	-2.78380700	0.75289500	-0.97172600
C	-1.23247900	2.42997300	0.66482000
H	-1.24290800	2.09426600	1.69915400
H	-1.17007600	3.52087100	0.65912500
H	-2.17073300	2.15713800	0.18850200
C	0.00057700	2.36351000	-1.53300700
H	0.00071100	3.45681800	-1.53026300
H	0.87796700	2.01674300	-2.07440700
H	-0.87674100	2.01693700	-2.07463400
C	1.23314300	2.42966000	0.66507200
H	2.17148300	2.15654200	0.18910400
H	1.17106600	3.52058300	0.65920600
H	1.24321300	2.09419300	1.69948200

Gas Phase:

Sum of electronic and zero-point Energies= -1014.084995

Sum of electronic and thermal Energies= -1014.066066

Sum of electronic and thermal Enthalpies= -1014.065121

Sum of electronic and thermal Free Energies= -1014.127820

CPCM:

Sum of electronic and zero-point Energies= -1014.092562

Sum of electronic and thermal Energies= -1014.073552

Sum of electronic and thermal Enthalpies= -1014.072608

Sum of electronic and thermal Free Energies= -1014.135757

$[Ph_3PF]^+$:

P	-0.00271700	-0.00051500	0.59861000
C	0.98455800	-1.44076000	0.13854100
C	0.49098200	-2.34687300	-0.80032900
C	2.24523500	-1.60480000	0.71835600
C	1.27767600	-3.43338300	-1.16290800
H	-0.48655900	-2.21537900	-1.24411900
C	3.01446500	-2.69967100	0.35316700
H	2.61521200	-0.90178200	1.45268700
C	2.53204900	-3.60867300	-0.58676900
H	0.90995200	-4.14181600	-1.89035800
H	3.98619600	-2.84524000	0.80127100
H	3.13653400	-4.45893200	-0.86842700
C	-1.74234900	-0.13464900	0.13511000
C	-2.51158300	-1.15744800	0.69616400
C	-2.28441900	0.76465800	-0.78306400
C	-3.84506300	-1.27123400	0.33163500
H	-2.08489900	-1.84419100	1.41515100
C	-3.61981700	0.63287300	-1.14382400
H	-1.68406300	1.55607300	-1.21093800
C	-4.39546400	-0.37943100	-0.58733700
H	-4.45459900	-2.05015700	0.76525900
H	-4.05298900	1.32147500	-1.85411400

H	-5.43487300	-0.47327500	-0.86758400
C	0.75458400	1.57254500	0.13659600
C	1.77476000	1.59258100	-0.81446700
C	0.28357500	2.74832200	0.72668900
C	2.32839100	2.81350300	-1.17956900
H	2.13841200	0.67813900	-1.26346900
C	0.85199500	3.95856300	0.35717600
H	-0.50041400	2.72180300	1.47169500
C	1.86942600	3.98977800	-0.59485700
H	3.11820900	2.84439100	-1.91543100
H	0.50551800	4.87452300	0.81241300
H	2.30814900	4.93565900	-0.87858600
F	-0.00367000	0.00344700	2.29483900

Gas Phase:

Sum of electronic and zero-point Energies= -1135.389226

Sum of electronic and thermal Energies= -1135.372478

Sum of electronic and thermal Enthalpies= -1135.371534

Sum of electronic and thermal Free Energies= -1135.435835

CPCM:

Sum of electronic and zero-point Energies= -1135.444994

Sum of electronic and thermal Energies= -1135.428155

Sum of electronic and thermal Enthalpies= -1135.427211

Sum of electronic and thermal Free Energies= -1135.492001

P Isotropic = 201.2278

Ph_3PF_2:

P	0.00162700	-0.00334100	0.00066200

F	-0.00034700	-0.00431700	1.86914100
F	0.00079400	-0.00007800	-1.86846800
C	-1.44814700	-1.12821900	-0.00048900
C	-1.46712500	-2.22589400	0.85463600
C	-2.51507500	-0.86894700	-0.85530000
C	-2.56571800	-3.07883000	0.84478500
H	-0.64381100	-2.40728900	1.52941000
C	-3.61758500	-1.71653600	-0.84691500
H	-2.48321600	-0.02556300	-1.52881300
C	-3.64111900	-2.82243000	-0.00152400
H	-2.58218200	-3.93715000	1.50120000
H	-4.45223100	-1.51475500	-1.50298900
H	-4.49617100	-3.48398800	-0.00205900
C	-0.25245700	1.81331100	0.00122700
C	-1.22661700	2.36917100	0.82466100
C	0.53129500	2.61500100	-0.82280900
C	-1.42276700	3.74600800	0.81452800
H	-1.81894700	1.74095900	1.47344200
C	0.34117200	3.99267500	-0.81423100
H	1.27171700	2.17284100	-1.47301000
C	-0.63694200	4.55689300	0.00013100
H	-2.18368300	4.18243200	1.44565600
H	0.95307400	4.62097500	-1.44550300
H	-0.78713300	5.62752500	-0.00039800
C	1.70367200	-0.68996000	-0.00045600
C	2.02335200	-1.73264400	-0.86487200

C	2.65693100	-0.15992900	0.86389000
C	3.31206400	-2.25551100	-0.85542500
H	1.28292500	-2.12403900	-1.54636200
C	3.94813600	-0.67673600	0.85531300
H	2.39432300	0.63530500	1.54550900
C	4.27410300	-1.72610000	0.00055000
H	3.56351900	-3.07044100	-1.51912000
H	4.69383500	-0.26397300	1.51966600
H	5.27649800	-2.13109400	0.00117100

Gas Phase:

Sum of electronic and zero-point Energies= -1235.477653

Sum of electronic and thermal Energies= -1235.460016

Sum of electronic and thermal Enthalpies= -1235.459072

Sum of electronic and thermal Free Energies= -1235.525028

CPCM:

Sum of electronic and zero-point Energies= -1235.491349

Sum of electronic and thermal Energies= -1235.473232

Sum of electronic and thermal Enthalpies= -1235.472288

Sum of electronic and thermal Free Energies= -1235.540048

[(*p*-FC6H4)$_3$PF]$^+$:

P	-0.00074800	-0.00312400	0.73003000
C	0.11779200	1.73586200	0.27037000
C	1.12460700	2.52018100	0.84420600
C	-0.77464100	2.26831500	-0.66288300
C	1.23469200	3.85204500	0.48396100
C	-0.66017500	3.60074800	-1.02808700

C	0.34181700	4.35858900	-0.44764700
C	-1.56652700	-0.76862200	0.27039600
C	-2.74725700	-0.29863300	0.85607600
C	-1.58412000	-1.79612900	-0.67546800
C	-3.95641800	-0.86683000	0.49448200
C	-2.79610300	-2.36035300	-1.04235000
C	-3.95165500	-1.88122000	-0.45023500
C	1.44604400	-0.97371100	0.26760100
C	1.62887400	-2.23485200	0.84547700
C	2.34960500	-0.46637600	-0.66895700
C	2.73000800	-2.99237000	0.48571100
C	3.44855700	-1.22831700	-1.03417600
C	3.61158100	-2.47175400	-0.44881700
F	-0.00021800	-0.00465900	2.42633400
F	-5.14745400	-2.43767500	-0.81195100
F	4.69646500	-3.22319800	-0.80766900
F	0.45501500	5.67324100	-0.80753700
H	1.80556600	2.10665100	1.57595000
H	1.99050700	4.49360400	0.91000000
H	-1.55479500	1.66170000	-1.10176400
H	-1.32852300	4.05041500	-1.74599700
H	-2.72724600	0.48800400	1.59830600
H	-4.88798000	-0.54013500	0.93013300
H	-0.67028900	-2.16088800	-1.12400500
H	-2.85325600	-3.15398400	-1.77114300
H	0.93280300	-2.61827200	1.57936300

H	2.91277100	-3.96491900	0.91588900
H	4.16873400	-0.87370700	-1.75516400
H	2.20857100	0.50958000	-1.11256000

Gas phase:

Sum of electronic and zero-point Energies= -1433.096915

Sum of electronic and thermal Energies= -1433.077488

Sum of electronic and thermal Enthalpies= -1433.076544

Sum of electronic and thermal Free Energies= -1433.147326

CPCM:

Sum of electronic and zero-point Energies= -1433.164126

Sum of electronic and thermal Energies= -1433.144649

Sum of electronic and thermal Enthalpies= -1433.143705

Sum of electronic and thermal Free Energies= -1433.214706

P Isotropic = 205.6323

(*p*-FC6H4)$_3$PF$_2$:

P	-0.00058600	-0.00096700	0.00043900
F	0.00015200	-0.00112400	-1.86036400
F	-0.00180800	-0.00188700	1.86152300
C	1.45717900	-1.11603400	0.00077300
C	1.52242200	-2.16206700	-0.91587100
C	2.48368900	-0.90325900	0.91709400
C	2.62105100	-3.01222300	-0.91380700
H	0.73295700	-2.31175200	-1.63581100
C	3.59395400	-1.73816600	0.91416000
H	2.41943300	-0.10245000	1.63722300
C	3.62767600	-2.77187200	-0.00022900

H	2.69595400	-3.83521200	-1.60753200
H	4.40807600	-1.59304900	1.60719700
C	0.23660500	1.81909600	0.00071800
C	1.11006600	2.39729500	-0.91654700
C	-0.45893500	2.60292100	0.91755800
C	1.30012700	3.77338000	-0.91429600
H	1.63256400	1.78691400	-1.63648800
C	-0.28861600	3.98160000	0.91420900
H	-1.12106400	2.14834400	1.63781800
C	0.59057400	4.52616900	-0.00023500
H	1.97635200	4.24837200	-1.60797100
H	-0.81976800	4.61513200	1.60747000
C	-1.69516000	-0.70572100	-0.00046900
C	-2.02329200	-1.70681100	0.90985900
C	-2.63541600	-0.23126600	-0.91116900
C	-3.30264000	-2.24811100	0.90706200
H	-1.29606800	-2.05871900	1.62491100
C	-3.92239900	-0.75433400	-0.90830900
H	-2.37072300	0.53187800	-1.62641800
C	-4.21689700	-1.75174300	-0.00043400
H	-3.58347000	-3.02998000	1.59548900
H	-4.67441600	-0.40067200	-1.59643500
F	4.73309000	-3.61490600	-0.00118300
F	0.77063200	5.90469100	-0.00059600
F	-5.50106200	-2.28426500	-0.00009400

Gas phase:

Sum of electronic and zero-point Energies= -1533.204041

Sum of electronic and thermal Energies= -1533.183593

Sum of electronic and thermal Enthalpies= -1533.182648

Sum of electronic and thermal Free Energies= -1533.256757

CPCM:

Sum of electronic and zero-point Energies= -1533.217937

Sum of electronic and thermal Energies= -1533.197242

Sum of electronic and thermal Enthalpies= -1533.196298

Sum of electronic and thermal Free Energies= -1533.270389

$[(C_6F_5)Ph_2PF]^+$:

P	0.82002000	0.13766900	0.60811600
C	1.82096300	-1.34192500	0.35281900
C	1.69318600	-2.40801900	1.24497300
C	2.67444400	-1.40010100	-0.74926600
C	2.44597100	-3.55198000	1.02455100
C	3.41560900	-2.55538000	-0.95641600
C	3.29985000	-3.62557600	-0.07392800
C	1.52322200	1.63756500	-0.09338300
C	2.85223000	1.94208700	0.21911100
C	0.76307800	2.45786400	-0.92777800
C	3.41746500	3.09107300	-0.31254900
C	1.34691000	3.59903200	-1.45905000
C	2.66721800	3.91423700	-1.15025300
C	-0.94741600	-0.05465000	0.21263800
C	-1.86703800	0.84620700	0.74370100
C	-1.43097000	-1.07516800	-0.59918000

C	-3.22064000	0.71730100	0.51459700
C	-2.78307600	-1.21570000	-0.84320400
C	-3.67743500	-0.31874800	-0.28431900
F	0.78319400	0.30231400	2.28875000
F	-1.42529700	1.88618800	1.50681700
F	-4.09578300	1.60231300	1.04751300
F	-4.99781800	-0.44915300	-0.52510300
F	-3.23222500	-2.21801500	-1.63628800
F	-0.57519300	-1.95612900	-1.19162700
H	1.03811600	-2.34685700	2.10327300
H	2.36761100	-4.38335800	1.70925700
H	3.87923600	-4.52217700	-0.24124500
H	4.08154000	-2.61930200	-1.80414000
H	2.76477600	-0.57022500	-1.43704400
H	3.43415000	1.30422800	0.87133100
H	4.43978100	3.34437600	-0.07441100
H	3.11417000	4.80724700	-1.56293600
H	0.77123200	4.24267000	-2.10729400
H	-0.26422600	2.22198900	-1.16749000

Gas phase:

Sum of electronic and zero-point Energies= -1631.517293

Sum of electronic and thermal Energies= -1631.495959

Sum of electronic and thermal Enthalpies= -1631.495015

Sum of electronic and thermal Free Energies= -1631.569542

CPCM:

Sum of electronic and zero-point Energies= -1631.582855

Sum of electronic and thermal Energies= -1631.561418

Sum of electronic and thermal Enthalpies= -1631.560473

Sum of electronic and thermal Free Energies= -1631.635762

P Isotropic = 218.4500

$(C_6F_5)Ph_2PF_2$:

P	0.78003200	0.00285000	-0.00204500
F	0.66512900	-0.17124000	-1.83631000
F	0.67660400	0.18645900	1.83232900
C	-1.06639900	-0.00497100	0.00323200
C	-1.78797700	1.09102200	0.44300700
C	-1.77992700	-1.10681100	-0.43520200
C	-3.16873300	1.09633300	0.44371500
C	-3.16048000	-1.12324700	-0.43442400
C	-3.85664000	-0.01615300	0.00506700
C	1.71706100	-1.57184900	0.15739700
C	2.59204900	-1.93278500	-0.86429000
C	1.56415000	-2.37190000	1.28614100
C	3.32643600	-3.10702800	-0.74722700
H	2.69415000	-1.31627600	-1.74343800
C	2.29160500	-3.55280200	1.38521800
H	0.89518500	-2.07765500	2.07893600
C	3.17375600	-3.91873300	0.37314500
H	4.01314900	-3.38713800	-1.53293200
H	2.16930500	-4.18204200	2.25499200
H	3.74002700	-4.83570300	0.45696400
C	1.70289100	1.58411600	-0.16510700

C	2.63438100	1.91197400	0.81642300
C	1.48067700	2.42237000	-1.25321900
C	3.35688500	3.09366200	0.69955000
C	2.19613700	3.61064700	-1.35115600
C	3.13475500	3.94459600	-0.37935800
F	-1.14904200	2.21990800	0.88142000
F	-3.85534500	2.19587300	0.87286600
F	-5.21912900	-0.02152000	0.00570800
F	-3.83877100	-2.22817000	-0.86293700
F	-1.13190800	-2.23021900	-0.87453400
H	2.78968600	1.26368100	1.66491500
H	4.08744500	3.34930300	1.45334700
H	3.69123000	4.86760800	-0.46245100
H	2.02017000	4.27134300	-2.18778600
H	0.76755700	2.15365200	-2.01623800

Gas phase:

Sum of electronic and zero-point Energies= -1731.629191

Sum of electronic and thermal Energies= -1731.606981

Sum of electronic and thermal Enthalpies= -1731.606037

Sum of electronic and thermal Free Energies= -1731.682133

CPCM:

Sum of electronic and zero-point Energies= -1731.643150

Sum of electronic and thermal Energies= -1731.620629

Sum of electronic and thermal Enthalpies= -1731.619685

Sum of electronic and thermal Free Energies= -1731.696946

$[(C_6F_5)_2PhPF]^+$:

P	-0.05495300	0.71186000	0.63433800
C	-0.21108400	2.42509700	0.11261000
C	0.47520200	3.40830300	0.82734500
C	-0.99399400	2.72458900	-1.00212000
C	0.36465300	4.72501500	0.40773700
C	-1.08445400	4.04737100	-1.41075500
C	-0.40741400	5.04097700	-0.70863800
C	-1.46548500	-0.30980300	0.12804600
C	-2.72197600	0.00961800	0.63780400
C	-1.36588800	-1.39548200	-0.73596400
C	-3.83619800	-0.74092800	0.32722000
C	-2.47142300	-2.15269900	-1.06241200
C	-3.70719600	-1.82525700	-0.52657700
C	1.53889900	-0.09051100	0.31655200
C	1.80004800	-1.31687600	0.92215700
C	2.51646700	0.45584800	-0.50799100
C	3.00272200	-1.96383400	0.75481200
C	3.72696600	-0.18335200	-0.69198600
C	3.96863200	-1.39188300	-0.06060600
F	-0.10338500	0.73122600	2.31468300
F	-2.85282600	1.08509400	1.46264400
F	-5.04551300	-0.41756100	0.83863500
F	-4.78972700	-2.55975700	-0.84488300
F	-2.35384100	-3.20268700	-1.90785800
F	-0.16507900	-1.72311400	-1.29801300
F	0.82753200	-1.89801300	1.68330100

F	3.23618400	-3.15185700	1.35767500
F	5.14641500	-2.01881400	-0.24270400
F	4.66964900	0.36412500	-1.49460500
F	2.29768800	1.62801300	-1.16669700
H	1.06601800	3.16408000	1.69980500
H	0.87843700	5.50385100	0.95112100
H	-0.48608600	6.06950200	-1.03012400
H	-1.68362200	4.30232100	-2.27208800
H	-1.52518400	1.95529100	-1.54676600

Gas phase:

Sum of electronic and zero-point Energies= -2127.644301

Sum of electronic and thermal Energies= -2127.618334

Sum of electronic and thermal Enthalpies= -2127.617389

Sum of electronic and thermal Free Energies= -2127.702367

CPCM:

Sum of electronic and zero-point Energies= -2127.717446

Sum of electronic and thermal Energies= -2127.691474

Sum of electronic and thermal Enthalpies= -2127.690530

Sum of electronic and thermal Free Energies= -2127.775256

P Isotropic = 237.6989

$(C_6F_5)_2PhPF_2$:

P	-0.00000300	0.67500800	0.00001200
F	-0.11601600	0.55961300	1.80896000
F	0.11602600	0.55963500	-1.80894100
C	-1.58265200	-0.26509700	-0.11230200
C	-1.65929600	-1.48841400	-0.75721700

C	-2.73991600	0.23893800	0.45609300
C	-2.84672900	-2.18958500	-0.83415900
C	-3.93827500	-0.44465400	0.38250100
C	-3.98935000	-1.66443700	-0.26264300
C	-0.00001100	2.51902600	0.00001200
C	-0.07243200	3.20509400	1.21064200
C	0.07240500	3.20508600	-1.21062200
C	-0.07146000	4.59420300	1.20240600
H	-0.13921600	2.66597600	2.14047000
C	0.07142000	4.59419600	-1.20239600
H	0.13919300	2.66596200	-2.14044700
C	-0.00002300	5.28889200	0.00000200
H	-0.12921200	5.12938200	2.13928000
H	0.12916700	5.12936800	-2.13927400
H	-0.00002800	6.37026600	0.00000000
C	1.58265400	-0.26508200	0.11231200
C	2.73990200	0.23895400	-0.45611000
C	1.65931800	-1.48839100	0.75724000
C	3.93826700	-0.44463100	-0.38253700
C	2.84675700	-2.18955100	0.83417100
C	3.98936400	-1.66440300	0.26262400
F	2.73469700	1.45114100	-1.08631200
F	5.06692800	0.08106200	-0.93644800
F	5.16358800	-2.34617400	0.33751600
F	2.89528900	-3.39696700	1.46330300
F	0.55085800	-2.05789000	1.31630500

F	-0.55082000	-2.05792100	-1.31624200
F	-2.89523900	-3.39701100	-1.46327300
F	-5.16356900	-2.34621600	-0.33754900
F	-5.06695100	0.08104000	0.93637900
F	-2.73473800	1.45113900	1.08626700

Gas phase:

Sum of electronic and zero-point Energies= -2227.776181

Sum of electronic and thermal Energies= -2227.749521

Sum of electronic and thermal Enthalpies= -2227.748577

Sum of electronic and thermal Free Energies= -2227.833255

CPCM:

Sum of electronic and zero-point Energies= -2227.791710

Sum of electronic and thermal Energies= -2227.764980

Sum of electronic and thermal Enthalpies= -2227.764036

Sum of electronic and thermal Free Energies= -2227.849028

$(C_6F_4H)_3PF_2$

P	0.00231700	-0.00108400	0.00070500
F	0.00282000	-0.00095100	1.81917600
F	0.00195800	-0.00405600	-1.81794800
C	-1.05358100	-1.50118800	0.00194700
C	-0.66214500	-2.64872700	-0.66642600
C	-2.26606600	-1.51738800	0.67011200
C	-1.46095800	-3.77502400	-0.66083500
C	-3.05965600	-2.64735100	0.66367900
C	-2.66915300	-3.79032100	0.00100500

C	-0.77156000	1.66223200	-0.00060700
C	-0.18573600	2.72193100	0.67089700
C	-1.95993800	1.89299800	-0.67261100
C	-0.77362600	3.97133300	0.66547700
C	-2.54136500	3.14534400	-0.66683100
C	-1.95758500	4.20042800	-0.00065800
C	1.82957200	-0.16242800	-0.00017000
C	2.62417200	0.75181300	-0.67088200
C	2.45341800	-1.20103000	0.66972700
C	3.99932800	0.62758200	-0.66606600
C	3.82916500	-1.31869800	0.66267600
C	4.62023600	-0.40772000	-0.00237300
F	2.05865800	1.81257400	-1.32851500
F	4.75057900	1.56097700	-1.33266700
F	4.40672800	-2.36909000	1.32836200
F	1.71232100	-2.14626400	1.32906700
F	0.53950200	-2.69424300	-1.32324000
F	-1.03049100	-4.89442800	-1.32543100
F	-4.25896300	-2.61723700	1.32763600
F	-2.71161400	-0.40065000	1.32723500
F	1.00369100	2.55403900	1.33013600
F	-0.15491300	4.99648700	1.33345600
F	-3.72468800	3.32844300	-1.33487900
F	-2.59457000	0.87322900	-1.33191400
H	-3.29136400	-4.67126000	0.00036600
H	5.69461200	-0.50212300	-0.00329900

H	-2.41430200	5.17747000	-0.00026900

Gas phase:

Sum of electronic and zero-point Energies= -2426.257938

Sum of electronic and thermal Energies= -2426.229556

Sum of electronic and thermal Enthalpies= -2426.228612

Sum of electronic and thermal Free Energies= -2426.316364

CPCM:

Sum of electronic and zero-point Energies= -2426.278279

Sum of electronic and thermal Energies= -2426.249809

Sum of electronic and thermal Enthalpies= -2426.248865

Sum of electronic and thermal Free Energies= -2426.336786

$[(C_6F_4H)_3PF]^+$:

P	-0.00285000	-0.00112100	-0.60377300
C	1.20633800	-1.27289900	-0.16325000
C	2.47016000	-1.19771200	-0.74044700
C	0.93403500	-2.31706700	0.71252700
C	3.42211400	-2.16021800	-0.47862800
C	1.89786800	-3.27256100	0.97434000
C	3.14265000	-3.20511400	0.38136400
C	-1.70848800	-0.41011600	-0.16035500
C	-2.27598300	-1.54596600	-0.72957500
C	-2.47791000	0.35678200	0.70666000
C	-3.58677100	-1.88460500	-0.46805200
C	-3.78867700	0.00449400	0.96783200

C	-4.35311900	-1.11131900	0.38306200
C	0.49788500	1.68002800	-0.15990000
C	-0.19328000	2.74138000	-0.73578200
C	1.53942600	1.95972500	0.71687700
C	0.17164400	4.04485700	-0.47251400
C	1.89230400	3.26983900	0.98011900
C	1.21761100	4.31860400	0.38798200
F	-0.00464900	-0.00015800	-2.27859500
F	-1.50636400	-2.33299300	-1.53761500
F	-4.11378100	-2.99632000	-1.04292500
F	-4.51900000	0.77331300	1.81810600
F	-1.94259100	1.45319100	1.32104900
F	-1.25459900	2.47164200	-1.55133900
F	-0.51870100	5.05918000	-1.05451700
F	2.91578600	3.51486300	1.84023100
F	2.21104300	0.94592600	1.33962900
F	2.76084500	-0.14105600	-1.55515800
F	4.64487200	-2.06214900	-1.06129000
F	1.60452400	-4.28392500	1.83364600
F	-0.27911100	-2.39894100	1.33540000
H	3.89001100	-3.95577800	0.59225000
H	-5.37841400	-1.37884800	0.59203100
H	1.49986700	5.33949700	0.59915700

Gas phase:

Sum of electronic and zero-point Energies= -2326.123511

Sum of electronic and thermal Energies= -2326.095835

Sum of electronic and thermal Enthalpies= -2326.094891

Sum of electronic and thermal Free Energies= -2326.183012

CPCM:

Sum of electronic and zero-point Energies= -2326.195946

Sum of electronic and thermal Energies= -2326.168155

Sum of electronic and thermal Enthalpies= -2326.167211

Sum of electronic and thermal Free Energies= -2326.256304

$[(C_6F_5)_3PF]^+$:

P	0.00280300	-0.00265300	0.66462700
C	-1.23488900	-1.24249200	0.22237600
C	-2.50161800	-1.13299100	0.79016100
C	-0.99037900	-2.30012000	-0.64694500
C	-3.48528500	-2.06179900	0.53877000
C	-1.96718800	-3.23599100	-0.91618300
C	-3.21357400	-3.11667000	-0.32100700
C	1.69565700	-0.45090100	0.22053400
C	2.23978400	-1.60159200	0.78535800
C	2.48526600	0.29549400	-0.64757100
C	3.53795800	-1.98171100	0.53235100
C	3.78587100	-0.07507100	-0.91820100
C	4.31155900	-1.21287100	-0.32566000
C	-0.45570900	1.68796500	0.22158700
C	0.26300400	2.73485300	0.79321000

C	-1.49048900	1.99816200	-0.65413200
C	-0.05703900	4.04909900	0.53998500
C	-1.81971600	3.30972600	-0.92536200
C	-1.10341500	4.33430700	-0.32576100
F	0.00278900	-0.00306200	2.33993800
F	1.45638600	-2.37125600	1.59357500
F	4.04933300	-3.09846200	1.09477400
F	5.57840900	-1.57796500	-0.58989800
F	4.54173200	0.66293600	-1.76206200
F	1.98039900	1.40476700	-1.26081900
F	1.31675500	2.44159700	1.60742900
F	0.64862200	5.05053600	1.10936400
F	-1.42043200	5.61385100	-0.59085300
F	-2.82990500	3.59500500	-1.77752500
F	-2.19186600	1.00596000	-1.27484000
F	-2.76989900	-0.06841800	1.59909100
F	-4.70618400	-1.94047000	1.10415500
F	-4.16836000	-4.02608300	-0.58422200
F	-1.71298600	-4.25999800	-1.76170400
F	0.22066800	-2.42278000	-1.26312200

Gas phase:

Sum of electronic and zero-point Energies= -2623.770037

Sum of electronic and thermal Energies= -2623.739499

Sum of electronic and thermal Enthalpies= -2623.738555

Sum of electronic and thermal Free Energies= -2623.833135

CPCM:

Sum of electronic and zero-point Energies= -2623.848803

Sum of electronic and thermal Energies= -2623.818069

Sum of electronic and thermal Enthalpies= -2623.817125

Sum of electronic and thermal Free Energies= -2623.914619

P Isotropic = 256.0543

$(C_6F_5)_3PF_2$:

P	-0.00015000	-0.00522600	0.00015600
F	-0.00132000	-0.00717700	1.80423500
F	0.00112900	-0.00668400	-1.80396800
C	0.03087000	1.82915200	0.00018900
C	-0.93645600	2.55625100	-0.67185300
C	1.02238500	2.52304800	0.67206400
C	-0.92265100	3.93671700	-0.67475100
C	1.05573700	3.90322400	0.67452200
C	0.07832900	4.60974200	-0.00023300
C	1.57537900	-0.94565400	-0.00047000
C	1.68456400	-2.15336100	0.66696800
C	2.68806200	-0.46488100	-0.66905500
C	2.86605700	-2.86755000	0.66875900
C	3.87938800	-1.16226200	-0.67251500
C	3.96577700	-2.36778100	-0.00243000
C	-1.60666000	-0.89171600	0.00060800
C	-1.75674800	-2.09463800	-0.66756400
C	-2.70229600	-0.37420000	0.66994200
C	-2.96170300	-2.76849400	-0.66955400
C	-3.91650900	-1.03095900	0.67323500

C	-4.04375100	-2.23236800	0.00227400
F	-0.69976400	-2.66447800	-1.31771200
F	-3.08488200	-3.95787800	-1.31900400
F	-5.23341800	-2.88692200	0.00340800
F	-4.98612300	-0.49790000	1.32387000
F	-2.61653700	0.82349300	1.32019000
F	-1.95413500	1.92117400	-1.32433600
F	-1.89153300	4.63401800	-1.32787600
F	0.10152400	5.96738100	-0.00050100
F	2.04788300	4.56725000	1.32739200
F	2.01784800	1.85373100	1.32459000
F	0.60871000	-2.68746800	1.31652600
F	2.94881600	-4.06088100	1.31737200
F	5.13264100	-3.06217600	-0.00375600
F	4.96661700	-0.66516800	-1.32242700
F	2.64294500	0.73554900	-1.31835200

Gas phase:

Sum of electronic and zero-point Energies= -2723.918407

Sum of electronic and thermal Energies= -2723.886967

Sum of electronic and thermal Enthalpies= -2723.886023

Sum of electronic and thermal Free Energies= -2723.981254

CPCM:

Sum of electronic and zero-point Energies= -2723.936750

Sum of electronic and thermal Energies= -2723.905255

Sum of electronic and thermal Enthalpies= -2723.904310

Sum of electronic and thermal Free Energies= -2723.999542

$(C_6F_5)_3B$:

B	-0.00109300	-0.00133900	-0.00046700
C	0.57878900	1.45231100	-0.00020200
C	1.67997900	1.80844500	0.77291200
C	0.02601300	2.46946500	-0.77286200
C	2.19820300	3.08685200	0.79263900
C	0.53126600	3.75310700	-0.79214000
C	1.62135900	4.06210700	0.00029100
C	0.96873200	-1.22948600	-0.00105000
C	2.13024500	-1.25387300	-0.76780000
C	0.72470000	-2.36512000	0.76582700
C	2.99146800	-2.33152000	-0.78709500
C	1.57463900	-3.45166200	0.78513000
C	2.71196200	-3.43397300	-0.00090300
C	-1.54985700	-0.22534400	-0.00005600
C	-2.40915600	0.55475100	0.76848500
C	-2.15454300	-1.21641000	-0.76786900
C	-3.77555300	0.36504800	0.78836800
C	-3.51889800	-1.42033300	-0.78656400
C	-4.33169300	-0.62615900	0.00109600
F	-1.05191800	2.20089000	-1.58058400
F	-0.03092300	4.71347100	-1.57857300
F	2.27592100	0.87107600	1.58077700
F	3.26748000	3.39519400	1.57905900
F	1.30494800	-4.53579700	1.56535900
F	-0.38923300	-2.41845000	1.56740900

F	2.43936900	-0.18241000	-1.56953600
F	4.10873900	-2.31897000	-1.56710600
F	-1.89604700	1.54359400	1.57172200
F	-4.57727800	1.14161400	1.57006400
F	-4.06940800	-2.39182100	-1.56756600
F	-1.38322600	-2.02050100	-1.57078400
F	-5.67648300	-0.81999300	0.00157600
F	2.12558000	5.32381400	0.00033100
F	3.55464800	-4.49976900	-0.00069300

Gas phase:

Sum of electronic and zero-point Energies= -2207.824793

Sum of electronic and thermal Energies= -2207.795596

Sum of electronic and thermal Enthalpies= -2207.794652

Sum of electronic and thermal Free Energies= -2207.887876

$[(C_6F_5)_3BF]^-$:

C	-0.44596200	1.51057500	0.30398100
C	0.16497300	2.61206000	0.89384400
C	-1.41288100	1.82402300	-0.63726000
C	-0.18471700	3.91911900	0.61655800
C	-1.79133600	3.12000400	-0.94404700
C	-1.17180800	4.17604100	-0.31316400
C	-1.08518300	-1.14180600	0.30472900
C	-2.34145500	-1.16991600	0.90050400
C	-0.87614200	-2.12907900	-0.64473500
C	-3.29782000	-2.12610900	0.62112700
C	-1.80897800	-3.10425500	-0.95426500

C	-3.02986200	-3.10284200	-0.31646400
C	1.53111500	-0.37057900	0.30369500
C	2.27993700	0.30203100	-0.64832600
C	2.18521200	-1.44218000	0.90244700
C	3.59103200	-0.01721600	-0.95724300
C	3.49239400	-1.79051700	0.62385600
C	4.20243200	-1.07206700	-0.31660700
F	-2.70856500	-0.18799500	1.79315300
F	-4.52158800	-2.10723200	1.24496600
F	-1.53689400	-4.06572200	-1.89723600
F	0.30474900	-2.18669300	-1.36324600
F	-2.06380500	0.83146100	-1.34807100
F	1.20463000	2.43753900	1.77968000
F	0.45100800	4.96878400	1.23394200
F	-2.76797900	3.36630400	-1.87843500
F	1.52116100	-2.24851800	1.79948400
F	4.08995800	-2.85687300	1.25082200
F	4.28629600	0.69701300	-1.90280400
F	1.73808800	1.35103300	-1.36930300
B	0.00009400	-0.00023800	0.77166300
F	5.50082900	-1.40616300	-0.61135200
F	-1.53035200	5.46827500	-0.60634600
F	-3.96956700	-4.05909200	-0.61119100
F	0.00134500	-0.00018000	2.23148300

Gas phase:

Sum of electronic and zero-point Energies= -2307.893519

Sum of electronic and thermal Energies= -2307.863343

Sum of electronic and thermal Enthalpies= -2307.862399

Sum of electronic and thermal Free Energies= -2307.956266

$[F]^-$:

CPCM:

Sum of electronic and zero-point Energies= -99.971129

Sum of electronic and thermal Energies= -99.969713

Sum of electronic and thermal Enthalpies= -99.968769

Sum of electronic and thermal Free Energies= -99.985288

COF_2:

C	0.00000000	0.14912700	0.00000000
O	-0.00005900	1.33290700	0.00000000
F	-1.08963900	-0.64217800	0.00000000
F	1.08969200	-0.64204600	0.00000000

Gas phase:

Sum of electronic and zero-point Energies= -312.942577

Sum of electronic and thermal Energies= -312.939232

Sum of electronic and thermal Enthalpies= -312.938288

Sum of electronic and thermal Free Energies= -312.968464

$[COF_3]^-$:

C	0.00036200	-0.00187100	0.20582200
O	0.00348200	-0.01209600	1.43385300
F	-0.46646200	1.22325900	-0.45930500
F	-0.82464800	-1.00854400	-0.47708300
F	1.28777400	-0.20271500	-0.47536400

Gas phase:

Sum of electronic and zero-point Energies= -412.888447

Sum of electronic and thermal Energies= -412.884114

Sum of electronic and thermal Enthalpies= -412.883170

Sum of electronic and thermal Free Energies= -412.915895