Supporting Information
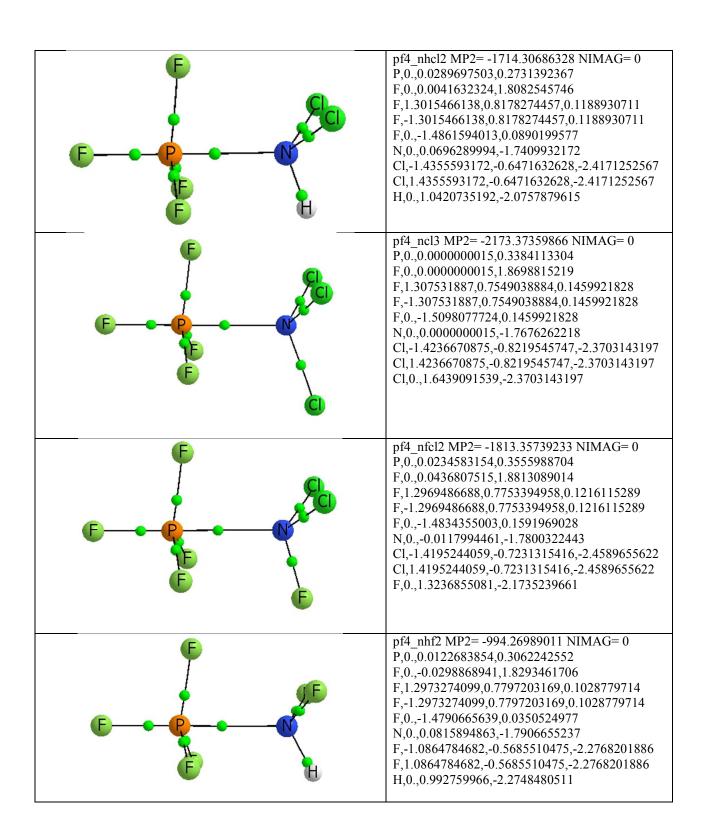

Properties of Cationic Pnicogen-bonded Complexes $F_{4-n}H_nP^+$:N-base

with F-P···N linear and n = 0 - 3

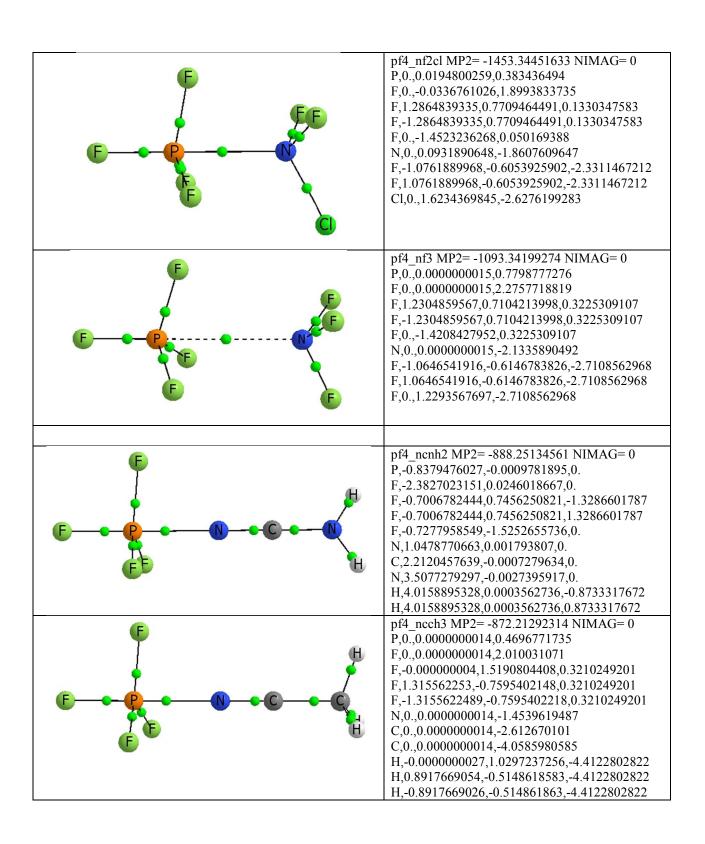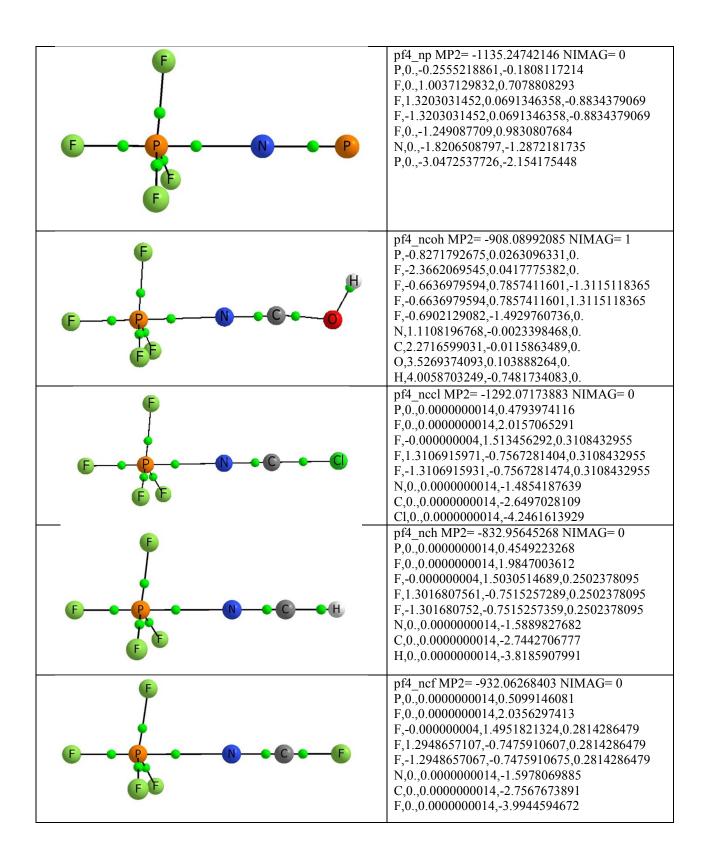Janet E. Del Bene,[*,‡] Ibon Alkorta,[*,§] and José Elguero[§]

Table S1. Geometries, molecular graphs, and total energies of complexes $F_{4-n}H_nP^+$:N-base

	pf4_aug_td MP2= -739.65954193 NIMAG= 0 P F,1,r1 F,1,r1,2,109.47122063 F,1,r1,2,109.47122063,3,120.,0 F,1,r1,2,109.47122063,3,-120.,0 r1=1.49191987
	pf4_nh3 MP2= -796.18769188 NIMAG= 0 P,0.,0.0000000015,0.1507571317 F,0.,0.0000000015,1.6919471686 F,1.3267734873,0.7660130315,0.0255438038 F,-1.3267734873,0.7660130315,0.0255438038 F,0.,-1.5320260586,0.0255438038 N,0.,0.0000000015,-1.7627659508 H,-0.8245442564,-0.4760508469,-2.133161749 H,0.8245442564,-0.4760508469,-2.133161749 H,0.,0.9521016982,-2.133161749
	pf4_nh2cl MP2= -1255.24378714 NIMAG= 0 P,0.,-0.0409523966,0.2115716282 F,0.,-0.0484892386,1.7503432262 F,1.3279542321,0.7094131776,0.0705794606 F,-1.3279542321,0.7094131776,0.0705794606 F,0.,-1.5726601408,0.0635319009 N,0.,-0.0811559416,-1.7383864531 H,-0.8261229229,-0.5787200923,-2.0863223624 H,0.8261229229,-0.5787200923,-2.0863223624 Cl,0.,1.4818687,-2.4975058907
	pf4_nh2f MP2= -895.21899278 NIMAG= 0 P,0.,-0.0104238134,0.2102950796 F,0.,-0.0038143992,1.7434675594 F,1.3146113775,0.7464847078,0.0356094023 F,-1.3146113775,0.7464847078,0.0356094023 F,0.,-1.5400608014,0.0606633903 N,0.,-0.0800111835,-1.7588469262 H,-0.8355750628,-0.5295559163,-2.1500923335 H,0.8355750628,-0.5295559163,-2.1500923335 F,0.,1.2004526277,-2.2695287267

pf4_nhcl2 MP2= -1714.30686328 NIMAG= 0
P,0.,0.0289697503,0.2731392367
F,0.,0.0041632324,1.8082545746
F,1.3015466138,0.8178274457,0.1188930711
F,-1.3015466138,0.8178274457,0.1188930711
F,0.,-1.4861594013,0.0890199577
N,0.,0.0696289994,-1.7409932172
Cl,-1.4355593172,-0.6471632628,-2.4171252567
Cl,1.4355593172,-0.6471632628,-2.4171252567
H,0.,1.0420735192,-2.0757879615

pf4_ncl3 MP2= -2173.37359866 NIMAG= 0
P,0.,0.0000000015,0.3384113304
F,0.,0.0000000015,1.8698815219
F,1.307531887,0.7549038884,0.1459921828
F,-1.307531887,0.7549038884,0.1459921828
F,0.,-1.5098077724,0.1459921828
N,0.,0.0000000015,-1.7676262218
Cl,-1.4236670875,-0.8219545747,-2.3703143197
Cl,1.4236670875,-0.8219545747,-2.3703143197
Cl,0.,1.6439091539,-2.3703143197

pf4_nfcl2 MP2= -1813.35739233 NIMAG= 0
P,0.,0.0234583154,0.3555988704
F,0.,0.0436807515,1.8813089014
F,1.2969486688,0.7753394958,0.1216115289
F,-1.2969486688,0.7753394958,0.1216115289
F,0.,-1.4834355003,0.1591969028
N,0.,-0.0117994461,-1.7800322443
Cl,-1.4195244059,-0.7231315416,-2.4589655622
Cl,1.4195244059,-0.7231315416,-2.4589655622
F,0.,1.3236855081,-2.1735239661

pf4_nhf2 MP2= -994.26989011 NIMAG= 0
P,0.,0.0122683854,0.3062242552
F,0.,-0.0298868941,1.8293461706
F,1.2973274099,0.7797203169,0.1028779714
F,-1.2973274099,0.7797203169,0.1028779714
F,0.,-1.4790665639,0.0350524977
N,0.,0.0815894863,-1.7906655237
F,-1.0864784682,-0.5685510475,-2.2768201886
F,1.0864784682,-0.5685510475,-2.2768201886
H,0.,0.992759966,-2.2748480511

pf4_nf2cl MP2= -1453.34451633 NIMAG= 0
P,0.,0.0194800259,0.383436494
F,0.,-0.0336761026,1.8993833735
F,1.2864839335,0.7709464491,0.1330347583
F,-1.2864839335,0.7709464491,0.1330347583
F,0.,-1.4523236268,0.050169388
N,0.,0.0931890648,-1.8607609647
F,-1.0761889968,-0.6053925902,-2.3311467212
F,1.0761889968,-0.6053925902,-2.3311467212
Cl,0.,1.6234369845,-2.6276199283

pf4_nf3 MP2= -1093.34199274 NIMAG= 0
P,0.,0.0000000015,0.7798777276
F,0.,0.0000000015,2.2757718819
F,1.2304859567,0.7104213998,0.3225309107
F,-1.2304859567,0.7104213998,0.3225309107
F,0.,-1.4208427952,0.3225309107
N,0.,0.0000000015,-2.1335890492
F,-1.0646541916,-0.6146783826,-2.7108562968
F,1.0646541916,-0.6146783826,-2.7108562968
F,0.,1.2293567697,-2.7108562968

pf4_ncnh2 MP2= -888.25134561 NIMAG= 0
P,-0.8379476027,-0.0009781895,0.
F,-2.3827023151,0.0246018667,0.
F,-0.7006782444,0.7456250821,-1.3286601787
F,-0.7006782444,0.7456250821,1.3286601787
F,-0.7277958549,-1.5252655736,0.
N,1.0478770663,0.001793807,0.
C,2.2120457639,-0.0007279634,0.
N,3.5077279297,-0.0027395917,0.
H,4.0158895328,0.0003562736,-0.8733317672
H,4.0158895328,0.0003562736,0.8733317672

pf4_ncch3 MP2= -872.21292314 NIMAG= 0
P,0.,0.0000000014,0.4696771735
F,0.,0.0000000014,2.010031071
F,-0.000000004,1.5190804408,0.3210249201
F,1.315562253,-0.7595402148,0.3210249201
F,-1.3155622489,-0.7595402218,0.3210249201
N,0.,0.0000000014,-1.4539619487
C,0.,0.0000000014,-2.612670101
C,0.,0.0000000014,-4.0585980585
H,-0.0000000027,1.0297237256,-4.4122802822
H,0.8917669054,-0.5148618583,-4.4122802822
H,-0.8917669026,-0.514861863,-4.4122802822

pf4_np MP2= -1135.24742146 NIMAG= 0
P,0.,-0.2555218861,-0.1808117214
F,0.,1.0037129832,0.7078808293
F,1.3203031452,0.0691346358,-0.8834379069
F,-1.3203031452,0.0691346358,-0.8834379069
F,0.,-1.249087709,0.9830807684
N,0.,-1.8206508797,-1.2872181735
P,0.,-3.0472537726,-2.154175448

pf4_ncoh MP2= -908.08992085 NIMAG= 1
P,-0.8271792675,0.0263096331,0.
F,-2.3662069545,0.0417775382,0.
F,-0.6636979594,0.7857411601,-1.3115118365
F,-0.6636979594,0.7857411601,1.3115118365
F,-0.6902129082,-1.4929760736,0.
N,1.1108196768,-0.0023398468,0.
C,2.2716599031,-0.0115863489,0.
O,3.5269374093,0.103888264,0.
H,4.0058703249,-0.7481734083,0.

pf4_nccl MP2= -1292.07173883 NIMAG= 0
P,0.,0.0000000014,0.4793974116
F,0.,0.0000000014,2.0157065291
F,-0.000000004,1.513456292,0.3108432955
F,1.3106915971,-0.7567281404,0.3108432955
F,-1.3106915931,-0.7567281474,0.3108432955
N,0.,0.0000000014,-1.4854187639
C,0.,0.0000000014,-2.6497028109
Cl,0.,0.0000000014,-4.2461613929

pf4_nch MP2= -832.95645268 NIMAG= 0
P,0.,0.0000000014,0.4549223268
F,0.,0.0000000014,1.9847003612
F,-0.000000004,1.5030514689,0.2502378095
F,1.3016807561,-0.7515257289,0.2502378095
F,-1.301680752,-0.7515257359,0.2502378095
N,0.,0.0000000014,-1.5889827682
C,0.,0.0000000014,-2.7442706777
H,0.,0.0000000014,-3.8185907991

pf4_ncf MP2= -932.06268403 NIMAG= 0
P,0.,0.0000000014,0.5099146081
F,0.,0.0000000014,2.0356297413
F,-0.000000004,1.4951821324,0.2814286479
F,1.2948657107,-0.7475910607,0.2814286479
F,-1.2948657067,-0.7475910675,0.2814286479
N,0.,0.0000000014,-1.5978069885
C,0.,0.0000000014,-2.7567673891
F,0.,0.0000000014,-3.9944594672

pf4_nccn MP2= -925.01640149 NIMAG= 0
P,0.,0.0000000014,0.8337969281
F,0.,0.0000000014,2.3371894777
F,-0.0000000038,1.4390463186,0.4335005258
F,1.2462506699,-0.7195231539,0.4335005258
F,-1.246250666,-0.7195231605,0.4335005258
N,0.,0.0000000014,-1.803213713
C,0.,0.0000000014,-2.9741091004
C,0.,0.0000000014,-4.3501998451
N,0.,0.0000000014,-5.5278268347

pf4_n2 MP2= -849.03357885 NIMAG= 0
P,0.,0.1098696292,0.0776431973
F,0.,1.331146192,0.9404048488
F,1.226273447,0.1353653303,-0.7710752362
F,-1.226273447,0.1353653303,-0.7710752362
F,0.,-1.090184164,0.9633973746
N,0.,-2.3466633675,-1.6592040548
N,0.,-3.2555968926,-2.3025785697

MP2=-640.4853667 NIMAG=0
P
H,1,r0
F,1,r1,2,a1
F,1,r1,2,a1,3,120.,0
F,1,r1,2,a1,3,-120.,0

r0=1.38272554
r1=1.50203637
a1=110.51974411

phf3_B_nh3 MP2= -697.00415879 NIMAG= 0
P,0.,-0.0370060333,0.1810198104
F,0.,-0.0331950827,1.7339400616
F,1.3135121137,0.7533739946,0.0380219867
F,-1.3135121137,0.7533739946,0.0380219867
H,0.,-1.4162900212,0.0658894141
N,0.,-0.0126298368,-1.7926580017
H,-0.8242973716,-0.4758672274,-2.1782345715
H,0.8242973716,-0.4758672274,-2.1782345715
H,0.,0.944110306,-2.1505488522

phf3_B_nh2cl MP2= -1156.06132705 NIMAG= 0
P,0.,-0.0768266963,0.249232616
F,0.,-0.0919025257,1.7971965803
F,1.3080690032,0.7055515255,0.0878321087
F,-1.3080690032,0.7055515255,0.0878321087
H,0.,-1.4545710997,0.0965686056
N,0.,-0.0949209615,-1.7720062004
H,-0.8254077896,-0.5833305983,-2.1334307479
H,0.8254077896,-0.5833305983,-2.1334307479
Cl,0.,1.473777635,-2.5216883104

phf3_B_nh2f MP2= -796.03667802 NIMAG= 0
P,0.,-0.0597347311,0.2600497939
F,0.,-0.0539642938,1.8024123908
F,1.2977595769,0.7220967275,0.0592506317
F,-1.2977595769,0.7220967275,0.0592506317
H,0.,-1.4349583905,0.1018577543
N,0.,-0.0863364978,-1.8030978885
H,-0.832249736,-0.5124947736,-2.2246840564
H,0.832249736,-0.5124947736,-2.2246840564
F,0.,1.2157980604,-2.2716010442

phf3_B_nhcl2 MP2= -1615.13247167 NIMAG= 0
P,0.,0.0179191201,0.301343523
F,0.,-0.1216348183,1.8365239014
F,1.2727618051,0.8567442582,0.167117823
F,-1.2727618051,0.8567442582,0.167117823
H,0.,-1.3359560642,0.0012558877
N,0.,0.0893854109,-1.7813983588
Cl,-1.4327819193,-0.6972387023,-2.3714412336
Cl,1.4327819193,-0.6972387023,-2.3714412336
H,0.,1.0312900363,-2.1925752589

phf3_B_ncl3 MP2= -2074.20147042 NIMAG= 0
P,0.,-0.0159756418,0.3683727483
F,0.,-0.148966066,1.8990688804
F,1.2700026506,0.8082805171,0.198363019
F,-1.2700026506,0.8082805171,0.198363019
H,0.,-1.3609048065,0.0359432985
N,0.,0.0156514516,-1.7978764031
Cl,-1.4216745663,-0.8598015375,-2.3250889108
Cl,1.4216745663,-0.8598015375,-2.3250889108
Cl,0.,1.6132294445,-2.4853850056

phf3_B_nfcl2 MP2= -1714.18355434 NIMAG= 0
P,0.,0.0076594662,0.4087438674
F,0.,-0.0713284305,1.9371473372
F,1.26521183,0.8146205683,0.1758382284
F,-1.26521183,0.8146205683,0.1758382284
H,0.,-1.3374424084,0.0879079393
N,0.,-0.0059258637,-1.8218930771
Cl,-1.419994474,-0.7622532368,-2.4557934525
Cl,1.419994474,-0.7622532368,-2.4557934525
F,0.,1.3022831084,-2.2848270429

phf3_nfcl2_FP MP2= -1714.18355434 NIMAG= 0
P,0.,0.0076594662,0.4087438674
F,0.,-0.0713284305,1.9371473372
F,1.26521183,0.8146205683,0.1758382284
F,-1.26521183,0.8146205683,0.1758382284
H,0.,-1.3374424084,0.0879079393
N,0.,-0.0059258637,-1.8218930771
Cl,-1.419994474,-0.7622532368,-2.4557934525
Cl,1.419994474,-0.7622532368,-2.4557934525
F,0.,1.3022831084,-2.2848270429

phf3_B_nhf2 MP2= -895.09614651 NIMAG= 0
P,0.,0.0079647051,0.3985113355
F,0.,-0.1734502413,1.9132892303
F,1.2625604206,0.8258858952,0.2000421047
F,-1.2625604206,0.8258858952,0.2000421047
H,0.,-1.300380267,-0.0429114207
N,0.,0.1085916367,-1.8688710164
F,-1.088122825,-0.6129160012,-2.2777691135
F,1.088122825,-0.6129160012,-2.2777691135
H,0.,0.9313322142,-2.4879871239

phf3_B_nf2cl MP2= -1354.17235851 NIMAG= 0
P,0.,0.0035885038,0.493765561
F,0.,-0.1903277206,1.9993897531
F,1.2483832648,0.8166434583,0.2452598186
F,-1.2483832648,0.8166434583,0.2452598186
H,0.,-1.2753630296,-0.0227839709
N,0.,0.1129282462,-1.9394694787
F,-1.0776776733,-0.6334509135,-2.3661336858
F,1.0776776733,-0.6334509135,-2.3661336858
Cl,0.,1.5640029296,-2.8415140498

phf3_B_nf3 MP2= -994.16851739 NIMAG= 0
P,0.,-0.0098031541,0.7339549965
F,0.,-0.0775947619,2.2395371153
F,1.2273290468,0.7619692998,0.3349642118
F,-1.2273290468,0.7619692998,0.3349642118
H,0.,-1.2937592654,0.2312565609
N,0.,-0.0553783839,-2.0990120549
F,-1.0651663664,-0.643120479,-2.7023326833
F,1.0651663664,-0.643120479,-2.7023326833
F,0.,1.1987926317,-2.6143533647

S8

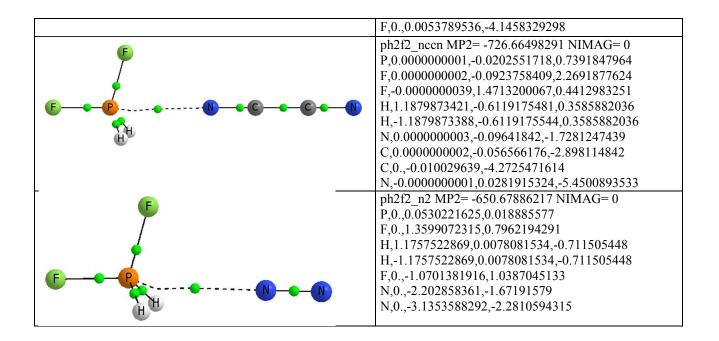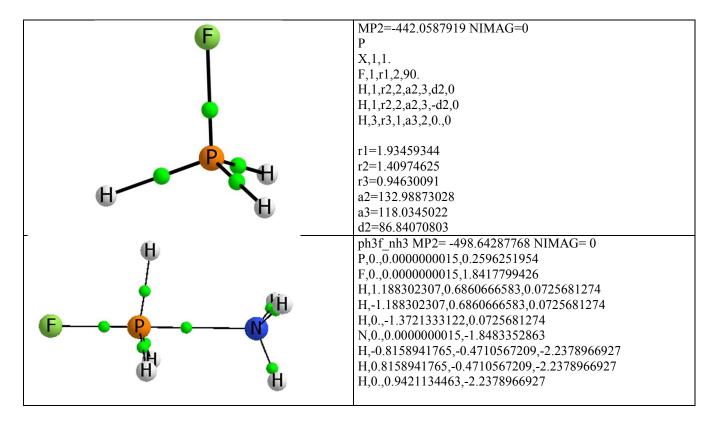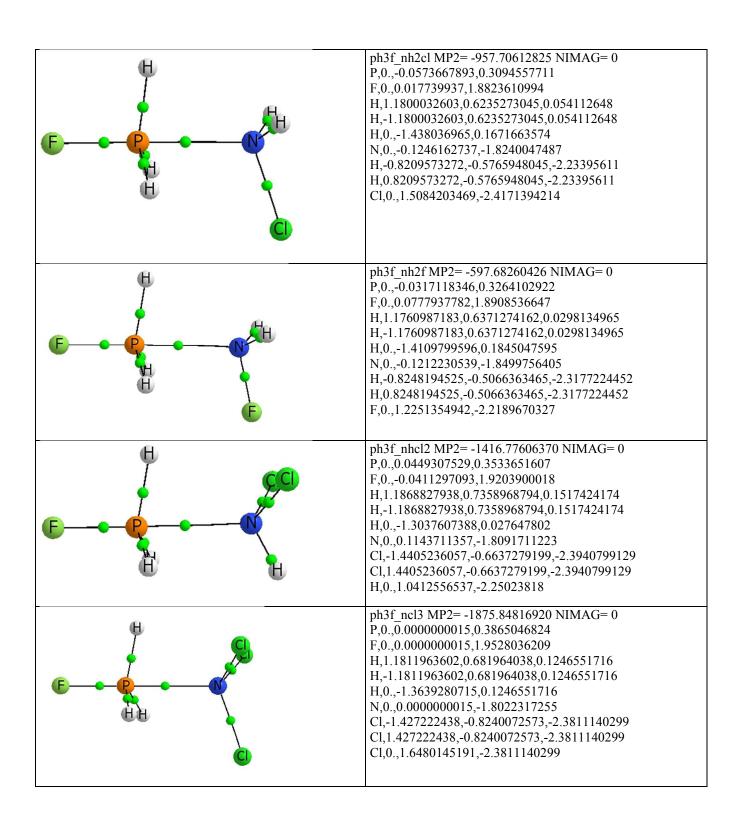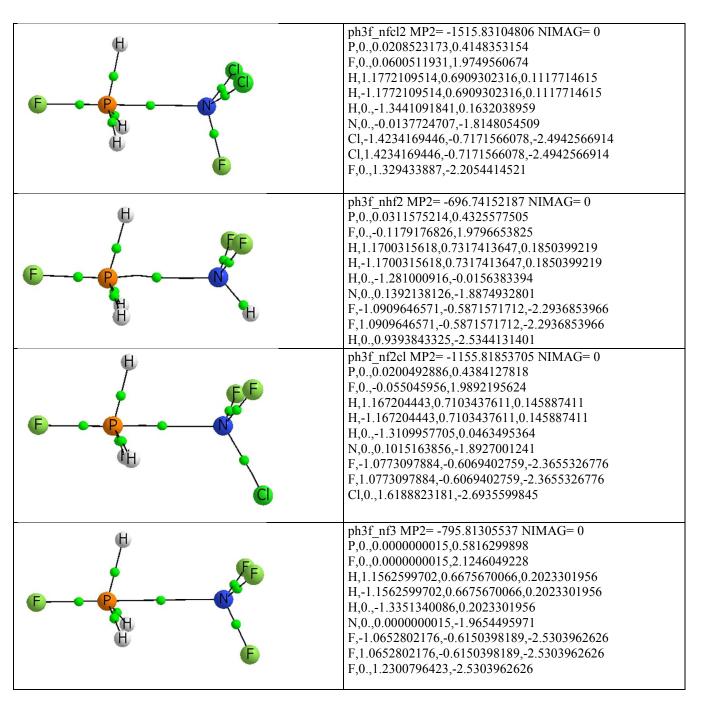|	
	phf3_B_ncnh2 MP2= -789.07195798 NIMAG= 0 P,-0.9074562443,-0.0328207044,0. F,-2.4576214879,0.0059004841,0. F,-0.7143967094,0.7518126888,-1.2974757657 F,-0.7143967094,0.7518126888,1.2974757657 H,-0.7804534158,-1.4035694917,0. N,1.0936008071,-0.0978364986,0. C,2.2600098433,-0.0550987135,0. N,3.5610274091,-0.0461727962,0. H,4.062103987,0.0573319839,-0.8703800213 H,4.062103987,0.0573319839,0.8703800213
	phf3_B_ncch3 MP2= -773.03446909 NIMAG= 0 P,-0.0000000028,0.0279676889,0.5628989684 F,-0.000000007,0.0579278212,2.106662368 H,-0.0000000057,1.3876985625,0.3502018688 F,1.2844945953,-0.769130086,0.373017749 F,-1.2844945959,-0.7691300925,0.3730177422 N,0.0000000026,0.0366452503,-1.5024772919 C,0.0000000057,0.0243536214,-2.6644054607 C,0.0000000095,0.005014355,-4.112570918 H,0.0000000079,1.0279487747,-4.4841821982 H,0.8907430218,-0.5146479369,-4.4607253907 H,-0.8907429983,-0.5146479414,-4.4607253954
	phf3_B_np MP2= -1036.06791940 NIMAG= 0 P,0.,-0.2357317988,-0.1275895161 F,0.,1.0159965037,0.7830845528 F,1.2925685504,0.0841063346,-0.8788490082 F,-1.2925685504,0.0841063346,-0.8788490082 H,0.,-1.1727499085,0.8850883695 N,0.,-1.8932777766,-1.2974808355 P,0.,-3.1128164776,-2.183360849
	phf3_B_ncoh MP2= -808.91277322 NIMAG= 0 P,0.9483421439,0.0177298902,0. F,2.4866872592,0.0811534226,0. H,0.6802607036,1.3665426302,0. F,0.7510743545,-0.7854651856,-1.2751790153 F,0.7510743545,-0.7854651856,1.2751790153 N,-1.1715987182,0.0162671884,0. C,-2.3369105509,0.0162270755,0. O,-3.5985775176,0.1394716263,0. H,-4.069834036,-0.7147447572,0.
	phf3_B_nccl MP2= -1192.89553520 NIMAG= 0 P,-0.0000000041,0.0225507816,0.6190057569 F,-0.0000000083,0.0647072462,2.1502953658 H,-0.0000000068,1.3629928656,0.3171353488 F,1.2654261712,-0.7708362467,0.3672477809 F,-1.2654261741,-0.7708362532,0.3672477742 N,0.0000000017,0.0635894751,-1.610877057 C,0.0000000049,0.0332088755,-2.7796458687 Cl,0.0000000093,-0.0064022556,-4.3842995187

phf3_B_nch MP2= -733.78242109 NIMAG= 0
P,-0.0000000018,0.016292037,0.6381196491
F,-0.000000006,0.0803660284,2.1593671081
H,-0.0000000042,1.332680536,0.2468261687
F,1.2498888219,-0.7734345023,0.338190558
F,-1.2498888198,-0.7734345088,0.3381905513
N,0.0000000045,0.0673405691,-1.7633225792
C,0.0000000077,0.0383815181,-2.9237140153
H,0.0000000106,0.0101736236,-3.9952056683

phf3_B_ncf MP2= -832.89044477 NIMAG= 0
P,-0.0000000031,0.0119426896,0.7002354952
F,-0.0000000072,0.0841952343,2.2174400185
H,-0.0000000052,1.3162702164,0.2697349543
F,1.2426900798,-0.7764821376,0.3785349018
F,-1.2426900804,-0.7764821438,0.3785348953
N,0.0000000031,0.0911947107,-1.7768030539
C,0.0000000063,0.0470911897,-2.9414762194
F,0.0000000096,0.0013858205,-4.1864153218

phf3_B_nccn MP2= -825.84445957 NIMAG= 0
P,-0.0000000041,0.0108480146,0.8011777499
F,-0.0000000083,0.0897736783,2.3137446952
H,-0.0000000062,1.3039066358,0.334732664
F,1.2366344171,-0.7744484345,0.4561055573
F,-1.2366344196,-0.7744484407,0.4561055508
N,0.0000000024,0.0967946521,-1.7770617181
C,0.0000000056,0.0587719352,-2.9474831059
C,0.0000000093,0.0133507606,-4.3224524975
N,0.0000000125,-0.023671784,-5.4997527005

phf3_B_n2 MP2= -749.86017760 NIMAG= 0
P,0.,0.0792385996,0.0641405361
F,0.,1.2424669527,1.0205546408
F,1.2228816341,0.2103020181,-0.7989683278
F,-1.2228816341,0.2103020181,-0.7989683278
H,0.,-1.1023522534,0.7748715113
N,0.,-2.3733820359,-1.5478863698
N,0.,-3.2484539586,-2.2369001709

MP2=-541.3030215 NIMAG=0
P
X,1,1.
F,1,r1,2,a1
F,1,r1,2,a1,3,180.,0
H,1,r2,2,a2,3,90.,0
H,1,r2,2,a2,3,-90.,0

r1=1.51576987
r2=1.38832146
a1=54.28363185
a2=122.42874339

	ph2f2_nh3 MP2= -597.82004848 NIMAG= 0 P,0.,0.0385440648,0.2152629671 F,0.,0.0380082289,1.7816634808 H,1.2117377934,0.6922781534,0.066693235 H,-1.2117377934,0.6922781534,0.066693235 F,0.,-1.5002884043,0.0543433737 N,0.,0.0185531414,-1.8200385623 H,-0.816941519,-0.467456538,-2.1912416322 H,0.816941519,-0.467456538,-2.1912416322 H,0.,0.9555409753,-2.225011429
	ph2f2_nh2cl MP2= -1056.88421556 NIMAG= 0 P,0.,-0.0191443026,0.264638668 F,0.,0.0615431245,1.8212901552 H,1.2036692974,0.6294247933,0.0414505009 H,-1.2036692974,0.6294247933,0.0414505009 F,0.,-1.5630770969,0.1608032314 N,0.,-0.1135690988,-1.8012587958 H,-0.8237956139,-0.5737377034,-2.1976321508 H,0.8237956139,-0.5737377034,-2.1976321508 Cl,0.,1.5228662948,-2.3750821755
	ph2f2_nh2f MP2= -696.85925516 NIMAG= 0 P,0.,0.0075185223,0.279014376 F,0.,0.1045180422,1.8292437128 H,1.2006258403,0.6474755046,0.0253553857 H,-1.2006258403,0.6474755046,0.0253553857 F,0.,-1.5320564566,0.1678634106 N,0.,-0.102419533,-1.8229687894 H,-0.8286572419,-0.5041523634,-2.271238986 H,0.8286572419,-0.5041523634,-2.271238986 F,0.,1.2357750301,-2.2044614207
	ph2f2_nhcl2 MP2= -1515.94871411 NIMAG= 0 P,0.,0.0613668607,0.343918081 F,0.,0.089707148,1.8964603915 H,1.2232027608,0.6759289089,0.1227662088 H,-1.2232027608,0.6759289089,0.1227662088 F,0.,-1.4571867047,0.1263472661 N,0.,0.1182739856,-1.8012011258 Cl,-1.4452093719,-0.6160944543,-2.4310284526 Cl,1.4452093719,-0.6160944543,-2.4310284526 H,0.,1.0681585864,-2.1924197642
	ph2f2_ncl3 MP2= -1975.02311931 NIMAG= 0 P,0.,0.0216334359,0.3710380247 F,0.,0.1506654713,1.9146104499 H,1.2168203056,0.6215879409,0.0824449834 H,-1.2168203056,0.6215879409,0.0824449834 F,0.,-1.5076669053,0.2375153553 N,0.,-0.0109955818,-1.8013440111 Cl,-1.4294814788,-0.7870761845,-2.42664417 Cl,1.4294814788,-0.7870761845,-2.42664417 Cl,0.,1.6772860813,-2.2665645763

ph2f2_nfcl2 MP2= -1615.00573337 NIMAG= 0
P,0.,0.0421826196,0.4017656362
F,0.,0.1830025072,1.9388782931
H,1.2092321891,0.6377805077,0.0799824898
H,-1.2092321891,0.6377805077,0.0799824898
F,0.,-1.4837234722,0.2577585267
N,0.,-0.0181319694,-1.8153731338
Cl,-1.4238122101,-0.6759301054,-2.5255896653
Cl,1.4238122101,-0.6759301054,-2.5255896653
F,0.,1.3529022518,-2.1249022421

ph2f2_nhf2 MP2= -795.91382829 NIMAG= 0
P,0.,0.0410525557,0.4937532916
F,0.,-0.0041890196,2.0262264373
H,1.1969501467,0.6595315232,0.1846401175
H,-1.1969501467,0.6595315232,0.1846401175
F,0.,-1.4270329144,0.0937267767
N,0.,0.183558735,-1.9387778829
F,-1.0928547931,-0.5430798628,-2.3453495691
F,1.0928547931,-0.5430798628,-2.3453495691
H,0.,0.9736949418,-2.5969373136

ph2f2_nf2cl MP2= -1254.99206919 NIMAG= 0
P,0.,0.0385748784,0.457918531
F,0.,0.0873910435,1.9910111658
H,1.1958433905,0.6464791699,0.1164409973
H,-1.1958433905,0.6464791699,0.1164409973
F,0.,-1.4570034594,0.1621991311
N,0.,0.0992103751,-1.9163339479
F,-1.0765476829,-0.5742998591,-2.4286449076
F,1.0765476829,-0.5742998591,-2.4286449076
Cl,0.,1.6686630914,-2.6227018954

ph2f2_nf3 MP2= -894.98753838 NIMAG= 0
P,0.,0.018850921,0.6474857864
F,0.,0.1269482443,2.1666943769
H,1.1812814495,0.5975257999,0.2146685844
H,-1.1812814495,0.5975257999,0.2146685844
F,0.,-1.4676930036,0.3340624825
N,0.,0.0254363297,-2.0282762126
F,-1.0644012322,-0.5815000951,-2.6032340484
F,1.0644012322,-0.5815000951,-2.6032340484
F,0.,1.2647611397,-2.5859054303

ph2f2_ncnh2 MP2= -689.89144710 NIMAG= 0
P,-0.9668754415,0.0301979687,0.
F,-2.5254813873,0.0355613125,0.
H,-0.7570152939,0.6566892308,-1.2108232197
H,-0.7570152939,0.6566892308,1.2108232197
F,-0.752785093,-1.4894752777,0.
N,1.1220777888,0.1161257061,0.
C,2.290188972,0.0679087909,0.
N,3.5950553845,0.0624517287,0.
H,4.0912503963,-0.0744226396,-0.8680747459
H,4.0912503963,-0.0744226396,0.8680747459

	ph2f2_ncch3 MP2= -673.85460217 NIMAG= 0 P,0.0000000001,-0.0288253848,0.6284146757 F,0.0000000002,-0.0612313551,2.1799731931 F,-0.0000000039,1.4866241497,0.4099250252 H,1.2053148537,-0.6494582504,0.3756949721 H,-1.2053148503,-0.6494582568,0.3756949721 N,0.0000000002,-0.0657190848,-1.5335755223 C,0.0000000001,-0.039731666,-2.6970302185 C,0.,-0.005079357,-4.1464021579 H,-0.0000000027,1.0315548176,-4.4775377551 H,0.8900359621,-0.5093377969,-4.5172225712 H,-0.8900359594,-0.5093378016,-4.5172225712
	ph2f2_np MP2= -936.88738443 NIMAG= 0 P,0.,-0.1625496902,-0.1574776135 F,0.,1.1226029936,0.7203928432 H,1.2089503707,0.0177288551,-0.8006239466 H,-1.2089503707,0.0177288551,-0.8006239466 F,0.,-1.2036659766,0.9714013848 N,0.,-1.8818112675,-1.3951215417 P,0.,-3.1380850971,-2.2343795819
	ph2f2_ncoh MP2= -709.73346184 NIMAG= 0 P,-0.9847753027,0.0568496763,0. F,-2.5305793836,0.1357434732,0. H,-0.6891222227,0.6631169141,-1.2023699937 H,-0.6891222227,0.6631169141,1.2023699937 F,-0.7882792045,-1.4593124478,0. N,1.2303121604,0.0493816278,0. C,2.3971389922,0.0207646262,0. O,3.6649089898,0.1116356708,0. H,4.1087423058,-0.7562090158,0.
	ph2f2_nccl MP2= -1093.71663333 NIMAG= 0 P,0.0000000001,-0.0264194293,0.6424968807 F,0.0000000002,-0.0740566715,2.1847432182 F,-0.0000000039,1.4787178268,0.3896248697 H,1.1992258192,-0.6340575241,0.3349414595 H,-1.1992258158,-0.6340575305,0.3349414595 N,0.0000000002,-0.0827956215,-1.6316076931 C,0.0000000001,-0.041415477,-2.801091386 Cl,0.,0.0135434071,-4.4067797836
	ph2f2_nch MP2= -634.60350271 NIMAG= 0 P,0.0000000001,-0.0240643141,0.61391474 F,0.0000000002,-0.0887477286,2.1505422728 F,-0.0000000039,1.4763232928,0.3483195528 H,1.1943670749,-0.6236787711,0.2720666866 H,-1.1943670716,-0.6236787774,0.2720666866 N,0.0000000002,-0.0730835362,-1.7417872817 C,0.0000000001,-0.0384813455,-2.9020074506 H,0.,-0.0055784342,-3.9736311591
	ph2f2_ncf MP2= -733.71135622 NIMAG= 0 P,0.0000000001,-0.0216617329,0.6588016065 F,0.0000000002,-0.0900358824,2.1924618613 F,-0.000000004,1.4746997398,0.3789080872 H,1.1916229214,-0.616628342,0.2989016682 H,-1.1916229181,-0.6166283485,0.2989016682 N,0.0000000003,-0.0925375238,-1.7380486981 C,0.0000000001,-0.04372522,-2.9022091127

	F,0.,0.0053789536,-4.1458329298
	ph2f2_nccn MP2= -726.66498291 NIMAG= 0 P,0.0000000001,-0.0202551718,0.7391847964 F,0.0000000002,-0.0923758409,2.2691877624 F,-0.0000000039,1.4713200067,0.4412983251 H,1.1879873421,-0.6119175481,0.3585882036 H,-1.1879873388,-0.6119175544,0.3585882036 N,0.0000000003,-0.09641842,-1.7281247439 C,0.0000000002,-0.056566176,-2.898114842 C,0.,-0.010029639,-4.2725471614 N,-0.0000000001,0.0281915324,-5.4500893533
	ph2f2_n2 MP2= -650.67886217 NIMAG= 0 P,0.,0.0530221625,0.018885577 F,0.,1.3599072315,0.7962194291 H,1.1757522869,0.0078081534,-0.711505448 H,-1.1757522869,0.0078081534,-0.711505448 F,0.,-1.0701381916,1.0387045133 N,0.,-2.202858361,-1.67191579 N,0.,-3.1353588292,-2.2810594315
	MP2=-442.0587919 NIMAG=0 P X,1,1. F,1,r1,2,90. H,1,r2,2,a2,3,d2,0 H,1,r2,2,a2,3,-d2,0 H,3,r3,1,a3,2,0.,0 r1=1.93459344 r2=1.40974625 r3=0.94630091 a2=132.98873028 a3=118.0345022 d2=86.84070803
	ph3f_nh3 MP2= -498.64287768 NIMAG= 0 P,0.,0.0000000015,0.2596251954 F,0.,0.0000000015,1.8417799426 H,1.188302307,0.6860666583,0.0725681274 H,-1.188302307,0.6860666583,0.0725681274 H,0.,-1.3721333122,0.0725681274 N,0.,0.0000000015,-1.8483352863 H,-0.8158941765,-0.4710567209,-2.2378966927 H,0.8158941765,-0.4710567209,-2.2378966927 H,0.,0.9421134463,-2.2378966927

ph3f_nh2cl MP2= -957.70612825 NIMAG= 0
P,0.,-0.0573667893,0.3094557711
F,0.,0.017739937,1.8823610994
H,1.1800032603,0.6235273045,0.054112648
H,-1.1800032603,0.6235273045,0.054112648
H,0.,-1.438036965,0.1671663574
N,0.,-0.1246162737,-1.8240047487
H,-0.8209573272,-0.5765948045,-2.23395611
H,0.8209573272,-0.5765948045,-2.23395611
Cl,0.,1.5084203469,-2.4171394214

ph3f_nh2f MP2= -597.68260426 NIMAG= 0
P,0.,-0.0317118346,0.3264102922
F,0.,0.0777937782,1.8908536647
H,1.1760987183,0.6371274162,0.0298134965
H,-1.1760987183,0.6371274162,0.0298134965
H,0.,-1.4109799596,0.1845047595
N,0.,-0.1212230539,-1.8499756405
H,-0.8248194525,-0.5066363465,-2.3177224452
H,0.8248194525,-0.5066363465,-2.3177224452
F,0.,1.2251354942,-2.2189670327

ph3f_nhcl2 MP2= -1416.77606370 NIMAG= 0
P,0.,0.0449307529,0.3533651607
F,0.,-0.0411297093,1.9203900018
H,1.1868827938,0.7358968794,0.1517424174
H,-1.1868827938,0.7358968794,0.1517424174
H,0.,-1.3037607388,0.027647802
N,0.,0.1143711357,-1.8091711223
Cl,-1.4405236057,-0.6637279199,-2.3940799129
Cl,1.4405236057,-0.6637279199,-2.3940799129
H,0.,1.0412556537,-2.25023818

ph3f_ncl3 MP2= -1875.84816920 NIMAG= 0
P,0.,0.0000000015,0.3865046824
F,0.,0.0000000015,1.9528036209
H,1.1811963602,0.681964038,0.1246551716
H,-1.1811963602,0.681964038,0.1246551716
H,0.,-1.3639280715,0.1246551716
N,0.,0.0000000015,-1.8022317255
Cl,-1.427222438,-0.8240072573,-2.3811140299
Cl,1.427222438,-0.8240072573,-2.3811140299
Cl,0.,1.6480145191,-2.3811140299

ph3f_nfcl2 MP2= -1515.83104806 NIMAG= 0
P,0.,0.0208523173,0.4148353154
F,0.,0.0600511931,1.9749560674
H,1.1772109514,0.6909302316,0.1117714615
H,-1.1772109514,0.6909302316,0.1117714615
H,0.,-1.3441091841,0.1632038959
N,0.,-0.0137724707,-1.8148054509
Cl,-1.4234169446,-0.7171566078,-2.4942566914
Cl,1.4234169446,-0.7171566078,-2.4942566914
F,0.,1.329433887,-2.2054414521

ph3f_nhf2 MP2= -696.74152187 NIMAG= 0
P,0.,0.0311575214,0.4325577505
F,0.,-0.1179176826,1.9796653825
H,1.1700315618,0.7317413647,0.1850399219
H,-1.1700315618,0.7317413647,0.1850399219
H,0.,-1.281000916,-0.0156383394
N,0.,0.1392138126,-1.8874932801
F,-1.0909646571,-0.5871571712,-2.2936853966
F,1.0909646571,-0.5871571712,-2.2936853966
H,0.,0.9393843325,-2.5344131401

ph3f_nf2cl MP2= -1155.81853705 NIMAG= 0
P,0.,0.0200492886,0.4384127818
F,0.,-0.055045956,1.9892195624
H,1.167204443,0.7103437611,0.145887411
H,-1.167204443,0.7103437611,0.145887411
H,0.,-1.3109957705,0.0463495364
N,0.,0.1015163856,-1.8927001241
F,-1.0773097884,-0.6069402759,-2.3655326776
F,1.0773097884,-0.6069402759,-2.3655326776
Cl,0.,1.6188823181,-2.6935599845

ph3f_nf3 MP2= -795.81305537 NIMAG= 0
P,0.,0.0000000015,0.5816299898
F,0.,0.0000000015,2.1246049228
H,1.1562599702,0.6675670066,0.2023301956
H,-1.1562599702,0.6675670066,0.2023301956
H,0.,-1.3351340086,0.2023301956
N,0.,0.0000000015,-1.9654495971
F,-1.0652802176,-0.6150398189,-2.5303962626
F,1.0652802176,-0.6150398189,-2.5303962626
F,0.,1.2300796423,-2.5303962626

ph3f_ncnh2 MP2= -590.71685869 NIMAG= 0
P,1.3086107002,-0.008146257,0.
F,2.8813025039,-0.0208554966,0.
H,1.0624904769,0.6733986379,-1.1766664425
H,1.0465629022,-1.3648421219,0.
H,1.0624904769,0.6733986379,1.1766664425
N,-0.8465071044,0.0212953155,0.
C,-2.015811261,0.0154808033,0.
N,-3.3242264405,-0.0392774479,0.
H,-3.8198435238,0.1188501147,-0.8645526029

	H,-3.8198435238,0.1188501147,0.8645526029
	ph3f_ncch3 MP2= -574.68078852 NIMAG= 0 P,0.,0.0000000014,0.655386858 F,0.,0.0000000014,2.223381736 H,-0.0000000036,1.3554238258,0.3844543269 H,1.1738314666,-0.6777119077,0.3844543269 H,-1.173831463,-0.6777119139,0.3844543269 N,0.,0.0000000014,-1.5419430258 C,0.,0.0000000014,-2.706112659 C,0.,0.0000000014,-4.1568552662 H,-0.0000000027,1.0271931572,-4.5155024626 H,0.8895753689,-0.5135965742,-4.5155024626 H,-0.8895753662,-0.5135965788,-4.5155024626
	ph3f_np MP2= -837.71327399 NIMAG= 0 P,0.,-0.1589921934,-0.1128508232 F,0.,1.1240912158,0.7943990932 H,1.1779383201,0.0274342318,-0.8139472543 H,-1.1779383201,0.0274342318,-0.8139472543 H,0.,-1.1502561117,0.8524044659 N,0.,-1.93227015,-1.3655729651 P,0.,-3.1676480507,-2.2383984953
	ph3f_ncoh MP2= -610.55958240 NIMAG= 0 P,1.3237766235,-0.0043864573,0. F,2.8878264081,0.0322570194,0. H,1.0036057853,1.3404538471,0. H,1.0516512229,-0.6868633408,-1.1705692276 H,1.0516512229,-0.6868633408,1.1705692276 N,-0.9107639057,-0.0429984144,0. C,-2.0778417509,-0.0115013762,0. O,-3.340926572,0.1432780881,0. H,-3.8269466639,-0.7011536149,0.
	ph3f_nccl MP2= -994.54312966 NIMAG= 0 P,0.,0.0000000014,0.6439788884 F,0.,0.0000000014,2.2051075788 H,-0.0000000036,1.349218933,0.34108106 H,1.1684578718,-0.6746094612,0.34108106 H,-1.1684578682,-0.6746094675,0.34108106 N,0.,0.0000000014,-1.6255469521 C,0.,0.0000000014,-2.7957387755 Cl,0.,0.0000000014,-4.403179356
	ph3f_nch MP2= -535.43013225 NIMAG= 0 P,0.,0.0000000014,0.600294238 F,0.,0.0000000014,2.1573567154 H,-0.0000000036,1.345477476,0.2794261362 H,1.165217675,-0.6727387328,0.2794261362 H,-1.1652176715,-0.672738739,0.2794261362 N,0.,0.0000000014,-1.7207690096 C,0.,0.0000000014,-2.8813259219 H,0.,0.0000000014,-3.9535423012

	ph3f_ncf MP2= -634.53773402 NIMAG= 0 P,0.,0.0000000014,0.6404816168 F,0.,0.0000000014,2.1953018422 H,-0.0000000036,1.3426560965,0.3068156279 H,1.1627742887,-0.6713280431,0.3068156279 H,-1.1627742851,-0.6713280492,0.3068156279 N,0.,0.0000000014,-1.7131316609 C,0.,0.0000000014,-2.8779338052 F,0.,0.0000000014,-4.1223897859
	ph3f_nccn MP2= -627.49134879 NIMAG= 0 P,0.,0.0000000014,0.7040865525 F,0.,0.0000000014,2.2555229169 H,-0.0000000035,1.3400438332,0.3566987831 H,1.1605120023,-0.6700219114,0.3566987831 H,-1.1605119987,-0.6700219175,0.3566987831 N,0.,0.0000000014,-1.6934563043 C,0.,0.0000000014,-2.8637655668 C,0.,0.0000000014,-4.2387631835 N,0.,0.0000000014,-5.4170486919
	ph3f_n2 MP2= -551.50391259 NIMAG= 0 P,0.,0.0105647817,0.0073352352 F,0.,1.2674690996,0.8957973791 H,1.1493838619,0.0611731415,-0.7695176211 H,-1.1493838619,0.0611731415,-0.7695176211 H,0.,-1.087945328,0.856124878 N,0.,-2.1920095076,-1.5497376158 N,0.,-3.1012946024,-2.1930556229

Table S2. The electron density at the BCP (ρ_{BCP}), the Laplacian of the electron density at the BCP ($\nabla^2\rho_{BCP}$), and the total energy density at the BCP (H_{BCP}) of complexes $F_{4-n}H_nP^+$:N-base

ρ_{BCP}

Base	F_4P^+	F_3HP^+	$F_2H_2P^+$	FH_3P^+
NH3	0.122	0.106	0.091	0.077
NClH2	0.115	0.098	0.087	0.073
NFH2	0.110	0.090	0.080	0.067
NCl2H	0.103	0.088	0.075	0.070
NCl3	0.088	0.076	0.072	0.066
NFCl2	0.082	0.065	0.065	0.060
NF2H	0.086	0.059	0.040	0.049
NF2Cl	0.063	0.042	0.046	0.048
NF3	0.015	0.018	0.024	0.030
NCNH2	0.108	0.085	0.070	0.059
NCCH3	0.101	0.076	0.061	0.055
NP	0.108	0.086	0.070	0.061
NCOH	0.097	0.068	0.054	0.050
NCCl	0.092	0.055	0.048	0.047
NCH	0.080	0.039	0.041	0.043
NCF	0.069	0.033	0.037	0.039
NCCN	0.023	0.027	0.032	0.036
N2	0.010	0.013	0.015	0.019

$\nabla^2\rho_{BCP}$

Base	F_4P^+	F_3HP^+	$F_2H_2P^+$	FH_3P^+
NH3	0.025	-0.015	-0.025	-0.001
NClH2	-0.030	-0.066	-0.037	0.005
NFH2	-0.013	-0.055	-0.019	0.026
NCl2H	-0.096	-0.070	-0.018	0.015
NCl3	-0.097	-0.026	-0.002	0.023
NFCl2	-0.068	0.008	0.020	0.041
NF2H	-0.059	0.030	0.061	0.064
NF2Cl	-0.001	0.059	0.059	0.065
NF3	0.048	0.052	0.062	0.072

$\nabla^2\rho_{BCP}$

NCNH2	0.152	0.030	0.034	0.064
NCCH3	0.107	0.008	0.044	0.068
NP	0.074	-0.013	0.016	0.050
NCOH	0.094	0.022	0.059	0.076
NCCl	0.068	0.051	0.069	0.079
NCH	0.016	0.072	0.075	0.082
NCF	0.012	0.076	0.078	0.084
NCCN	0.065	0.072	0.077	0.084
N2	0.041	0.046	0.054	0.064

H_{BCP}

Base	F_4P^+	F_3HP^+	$F_2H_2P^+$	FH_3P^+
NH3	-0.112	-0.091	-0.070	-0.049
NClH2	-0.106	-0.081	-0.062	-0.043
NFH2	-0.098	-0.069	-0.053	-0.034
NCl2H	-0.091	-0.062	-0.043	-0.036
NCl3	-0.064	-0.041	-0.037	-0.032
NFCl2	-0.055	-0.030	-0.029	-0.025
NF2H	-0.065	-0.024	-0.009	-0.015
NF2Cl	-0.031	-0.009	-0.012	-0.014
NF3	0.001	0.001	-0.001	-0.003
NCNH2	-0.087	-0.061	-0.039	-0.026
NCCH3	-0.08	-0.049	-0.028	-0.021
NP	-0.091	-0.063	-0.039	-0.027
NCOH	-0.075	-0.036	-0.020	-0.016
NCCl	-0.071	-0.020	-0.014	-0.014
NCH	-0.057	-0.007	-0.009	-0.010
NCF	-0.043	-0.004	-0.006	-0.008
NCCN	-0.001	-0.001	-0.004	-0.006
N2	0.002	0.002	0.001	0.001

Figure S1. Plots of ρ_{BCP}, $\nabla^2\rho_{BCP}$, and H_{BCP} (au) versus the P-N distance (Å) for complexes
$F_{4-n}H_nP^+$:N-base
■ sp^3 bases; □ sp N-bases

$$y = 7.3989e^{-2.1398x}$$
$$R^2 = 0.9946$$

$$y = 5.7477e^{-2.0998x}$$
$$R^2 = 0.9969$$

ρ_{BCP}

$\nabla^2\rho_{BCP}$

H_{BCP}

Table S3. Spin-spin coupling constants ^{1p}J(P-N) and their components (Hz) for complexes of F$_4$P$^+$, F$_3$HP$^+$, F$_2$H$_2$P$^+$, and FH$_3$P$^+$ with nitrogen bases

F4P+:N-base

	PSO	DSO	FC	SD	^{1p}J(P-N)
NH3	0.8	-0.2	-25.8	-1.7	-26.9
NFH2	0.5	-0.2	-19.0	-1.7	-20.3
NP	1.1	-0.2	-15.2	-0.8	-15.1
NCH	0.5	-0.2	0.9	-0.5	0.7
NCF	0.4	-0.2	8.6	-0.3	8.4
N2	0.1	-0.1	1.5	0.0	1.5

F3HP+:N-base

	PSO	DSO	FC	SD	^{1p}J(P-N)
NH3	0.2	-0.1	26.7	-1.7	25.1
NClH2	0.3	-0.2	31.0	-1.3	29.9
NFH2	0.5	-0.1	34.2	-1.2	33.4
NF2H	0.2	-0.1	26.9	-0.4	26.6
NCNH2	0.2	-0.2	57.5	-0.6	56.9
NP	0.5	-0.2	50.5	-0.6	50.3
NCOH	0.2	-0.1	55.2	-0.3	54.9
NCH	0.0	-0.1	19.8	-0.1	19.6
NCF	0.0	-0.1	11.8	-0.1	11.6
N2	0.0	-0.1	-4.7	0.0	-4.8

F2H2P+:N-base

	PSO	DSO	FC	SD	^{1p}J(P-N)
NH3	-0.8	-0.1	33.4	-1.6	30.9
NH2Cl	-0.6	-0.1	30.9	-1.4	28.8
NH2F	-0.5	-0.1	32.3	-1.1	30.6
NHF2	0.1	-0.1	-2.5	-0.2	-2.8
NF3	0.1	-0.1	-14.0	0.0	-14.0
NHNH2	0.0	-0.1	52.8	-0.4	52.2
NCCH3	-0.4	-0.1	38.3	-0.4	37.4
NP	0.0	-0.1	40.2	-0.5	39.7
NCOH	-0.4	-0.1	29.4	-0.3	28.5
NCCl	-0.3	-0.1	17.0	-0.2	16.4
NCH	-0.3	-0.1	4.5	-0.2	3.9
NCF	-0.3	-0.1	-3.1	-0.1	-3.6
NCCN	-0.2	-0.1	-9.6	-0.1	-10.0
N2	0.0	-0.1	-15.9	0.0	-16.0

	PSO	DSO	FC	SD	^{1p}J(P-N)
FH3P+:N-base					
NH3	-2.1	-0.1	14.6	-1.6	10.8
NClH2	-1.2	-0.1	9.7	-1.3	7.2
NFH2	-0.5	-0.1	7.1	-0.9	5.6
NF2H	0.1	-0.1	-9.8	-0.3	-10.1
NF3	0.0	-0.1	-30.8	0.0	-30.9
NCNH2	-1.1	-0.1	15.4	-0.4	13.8
NCCH3	-1.0	-0.1	5.3	-0.4	3.8
NP	-0.4	-0.1	7.6	-0.3	6.8
NCOH	-1.0	-0.1	-3.9	-0.3	-5.3
NCCl	-0.8	-0.1	-11.1	-0.3	-12.3
NCH	-0.7	-0.1	-18.5	-0.2	-19.5
NCF	-0.7	-0.1	-26.3	-0.2	-27.3
NCCN	-0.6	-0.1	-29.4	-0.1	-30.1
N2	-0.2	-0.1	-30.9	0.0	-31.2

Table S4. Spin-spin coupling constants $^1J(P-F_{ax})$ and their components (Hz) for complexes of F_4P^+, F_3HP^+, $F_2H_2P^+$, and FH_3P^+ with nitrogen bases

F_4HP^+:N-base	PSO	DSO	FC	SD	$^1J(P-F_{ax})$
NH_3	-191.6	1.6	-869.6	16.2	-1043.4
NFH_2	-200.1	1.6	-885.4	15.6	-1068.3
NP	-189.8	1.6	-854.1	16.5	-1025.8
NCH	-202.9	1.6	-872.7	16	-1058.1
NCF	-207.3	1.6	-878.8	15.8	-1068.8
N_2	-250.5	1.5	-1041.7	13.1	-1277.6
F_4P^+	-257.4	1.4	-1075.7	12.8	-1318.9
F_3HP^+:N-base					
NH_3	-187.8	1.2	-873.8	19.3	-1041.2
$NClH_2$	-193.4	1.2	-877.8	19.2	-1050.8
NFH_2	-201.6	1.2	-888.8	18.9	-1070.3
NF_2H	-230.9	1.2	-933.2	18.9	-1144.0
$NCNH_2$	-91.5	0.4	-735.6	41.7	-785.0
$NCCH_3$	-97.9	0.4	-751.5	41.6	-807.4
NP	-94.5	0.4	-749.0	40.7	-802.5
NCOH	-101.0	0.3	-762.3	42.2	-820.7
NCCl	-105.7	0.3	-775.4	42.1	-838.5
NCH	-110.8	0.3	-790.2	42.1	-858.6
NCF	-112.8	0.3	-799.5	42.6	-869.4
NCCN	-118.2	0.3	-814.2	42.1	-889.9
N_2	-130.6	0.3	-873.2	42.1	-961.4
F_3HP^+	-269.8	1.0	-1065.7	16.1	-1318.4

$F_2H_2P^+$:N-base

NH_3	-159.7	0.7	-812.3	24.8	-946.4
NH_2Cl	-170.9	0.8	-823.8	25.2	-968.7
NH_2F	-178.7	0.8	-832.8	25.2	-985.6
NHF_2	-212.9	0.7	-897.4	25.0	-1084.5
NF_3	-230.5	0.7	-942.9	24.2	-1148.4
$NCNH_2$	-173.0	0.7	-810.7	26.4	-956.5
$NCCH_3$	-181.8	0.7	-825.1	26.6	-979.7
NP	-174.7	0.7	-820.8	26.1	-968.7
$NCOH$	-188.5	0.7	-836.2	26.8	-997.1
$NCCl$	-195.9	0.7	-851.9	26.5	-1020.5
NCH	-203.8	0.7	-869.6	26.3	-1046.4
NCF	-208.4	0.7	-880.3	26.2	-1061.9
$NCCN$	-214.7	0.7	-896.6	25.7	-1084.9
N_2	-232.9	0.6	-951.3	24.2	-1159.4
$F_2H_2P^+$	-241.6	0.6	-982.6	22.7	-1200.9

FH_3P^+:N-base

NH_3	-187.8	1.2	-873.8	19.3	-1041.2
$NClH_2$	-193.4	1.2	-877.8	19.2	-1050.8
NFH_2	-201.6	1.2	-888.8	18.9	-1070.3
NF_2H	-230.9	1.2	-933.2	18.9	-1144.0
$NCNH_2$	-91.5	0.4	-735.6	41.7	-785.0
$NCCH_3$	-97.9	0.4	-751.5	41.6	-807.4
NP	-94.5	0.4	-749.0	40.7	-802.5
$NCOH$	-101.0	0.3	-762.3	42.2	-820.7
$NCCl$	-105.7	0.3	-775.4	42.1	-838.5
NCH	-110.8	0.3	-790.2	42.1	-858.6
NCF	-112.8	0.3	-799.5	42.6	-869.4
$NCCN$	-118.2	0.3	-814.2	42.1	-889.9
N_2	-130.6	0.3	-873.2	42.1	-961.4
FH_3P^+	-269.8	1.0	-1065.7	16.1	-1318.4

Full references 36 and 50

(36) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Gaussian, Inc., 2009.

(50) Stanton, J. F.; Gauss, J.; Watts, J. D.; Nooijen, M.; Oliphant, N.; Perera, S. A.; Szalay, P. G.; Lauderdale, W. J.; Gwaltney, S. R.; Beck, S.; Balkova, A.; Bernholdt, D. E.; Baeck, K.-K.; Tozyczko, P.; Sekino, H.; Huber, C.; Bartlett, R. J. ACES II is a program product of the Quantum Theorey Project, University of Florida. Integral packages included are VMOL (J. Almlöf and Taylor PR); VPROPS (P. R. Taylor); ABACUS (T Helgaker, H. J. Aa. Jensen, P. Jørgensen, J. Olsen, and P. R. Taylor). Brillouin-Wigner perturbation theory was implement by J. Pittner.