Supporting information

Using Frustrated Lewis pairs to explore C-F bond activation

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Contents

[PhC(O)CF$_2$C(OSiMe$_2$tBu)CF$_3$Ph] **1**

Figure S1: ^{1}H NMR (500 MHz, CDCl$_3$) spectrum of **1**.

Figure S2: ^{13}C NMR (100 MHz, CDCl$_3$) spectrum of **1**.

Figure S3: 19F{H} NMR (377 MHz. CDCl3) spectrum for 1.

[PhC(CF₂)OP(MeNCH₂CH₂)₃N][BFPh₃] 2

$[PhC(CF_2)OP(MeNCH_2CH_2)_3N][BFPh_3]$ 2
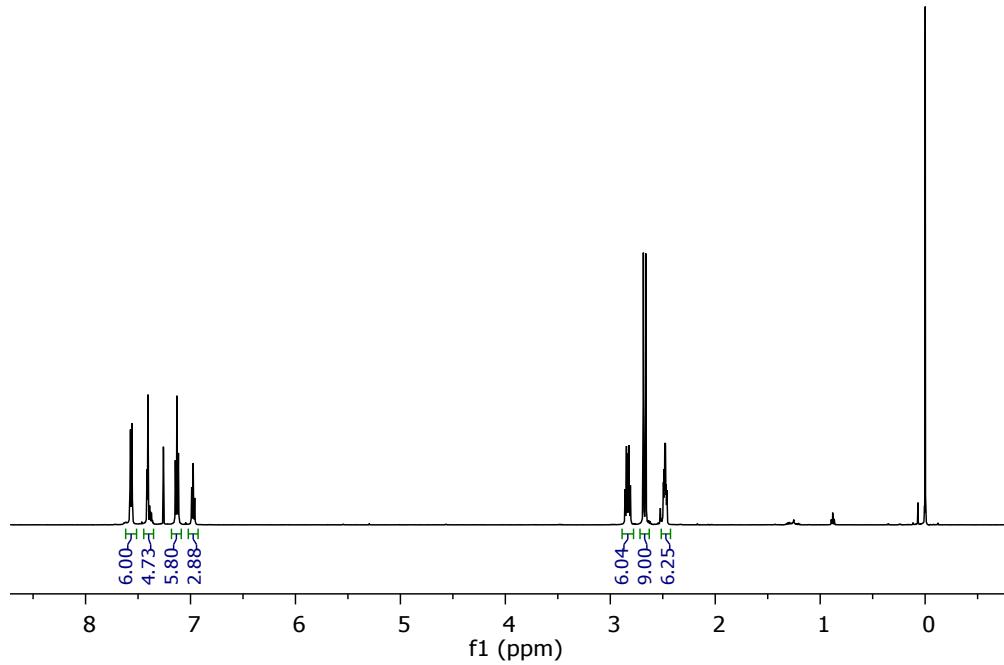
Figure S4: 1H NMR (500 MHz, CDCl3) spectrum of 2
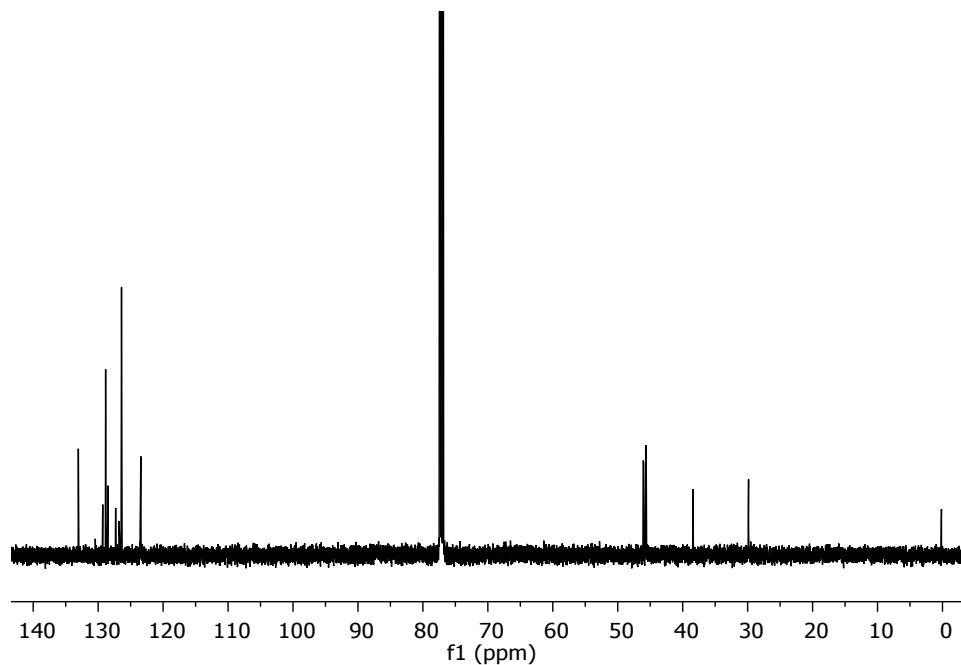
Figure S5 : 13C NMR (100 MHz, CDCl3) spectrum of 2

A (d)	B (d)
-97.24	-111.13
J(70.25)	J(70.07)
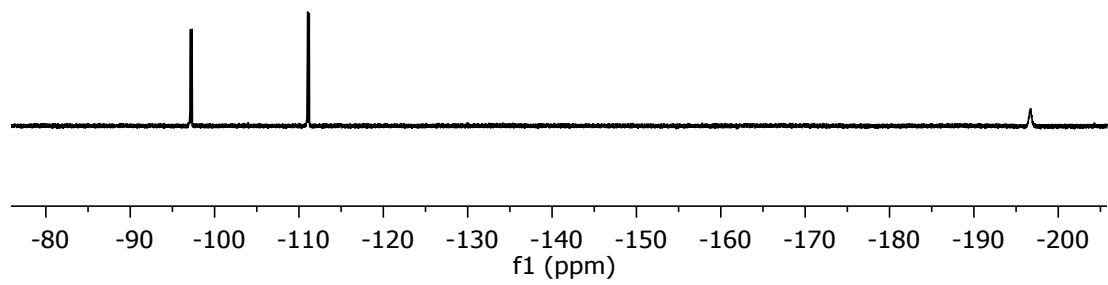
Figure S6: 19F NMR (377 MHz, CDCl3) spectrum of 2.
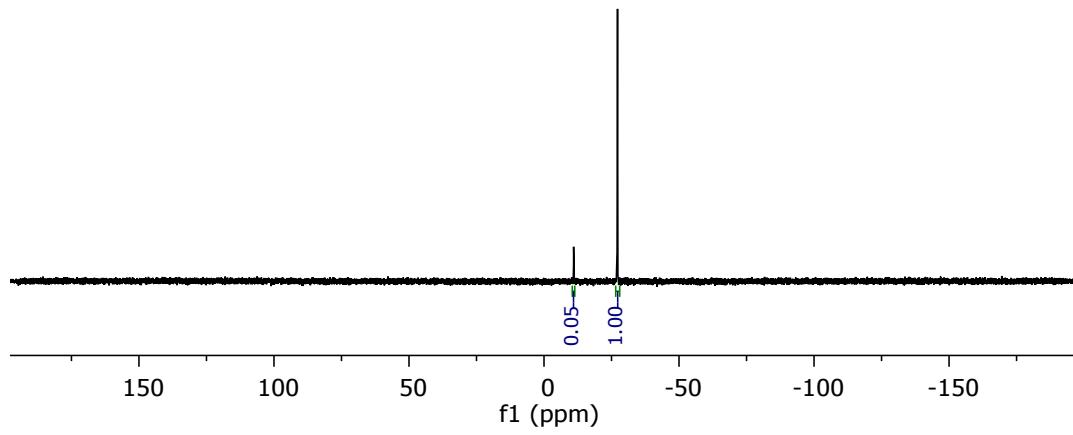
Figure S7: 31P{1H} NMR (162 MHz, CDCl3) spectrum of 2. (Peak at -10.9 ppm corresponds to HP[(MeNCH2CH2)3N]+)
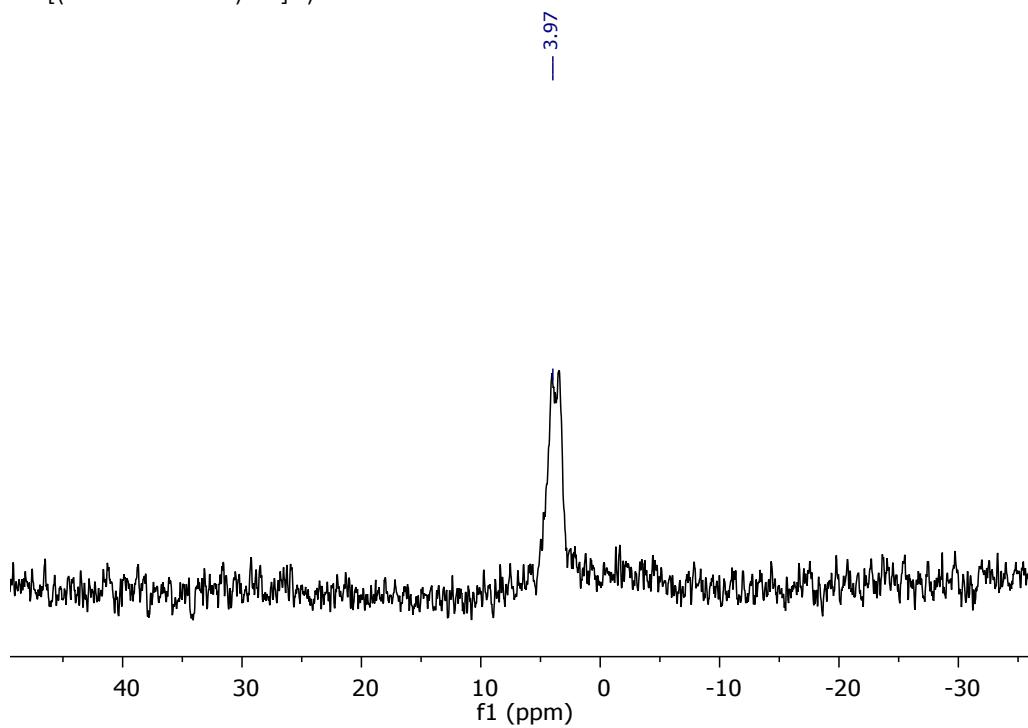
Figure S*8*: 11B NMR (128 MHz, CDCl3) spectrum of 2.

$[PhC(CF_2)OP(MeNCH_2CH_2)_3N][O_3SCF_3]$ 3
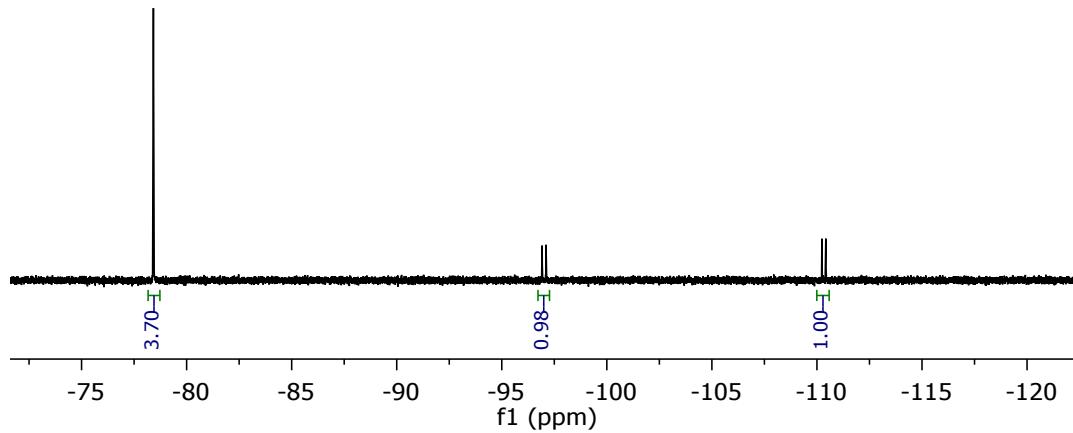
Figure S9: 19F{1H} NMR (377 MHz, CDCl3) spectrum of 3.
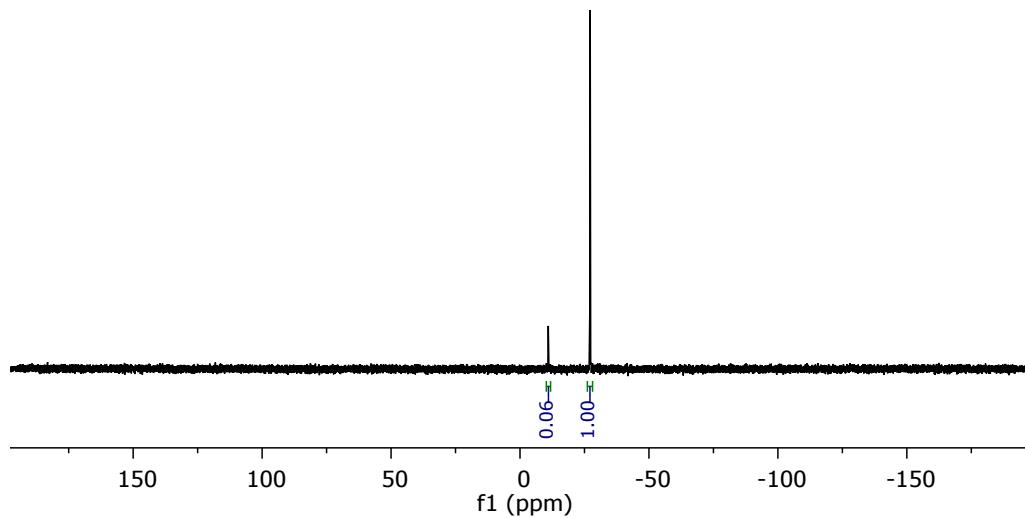
Figure S10: 31P{1H} NMR (162 MHz, CDCl3) spectrum of 3

[PhC(CF(H))OP(MeNCH$_2$CH$_2$)$_3$N][O$_3$SCF$_3$] 3

B (dd)
6.77
J(77.47, 0.85)

A (d)
7.14
J(79.01)
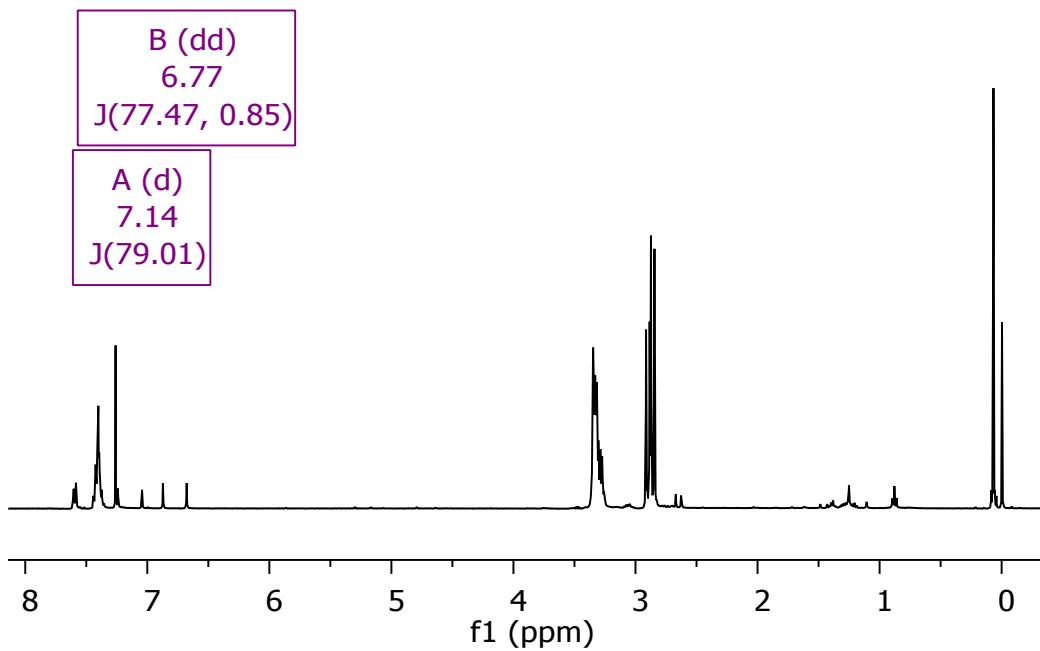
Figure S11: 1H NMR (400 MHz, CDCl3) spectrum of 4.
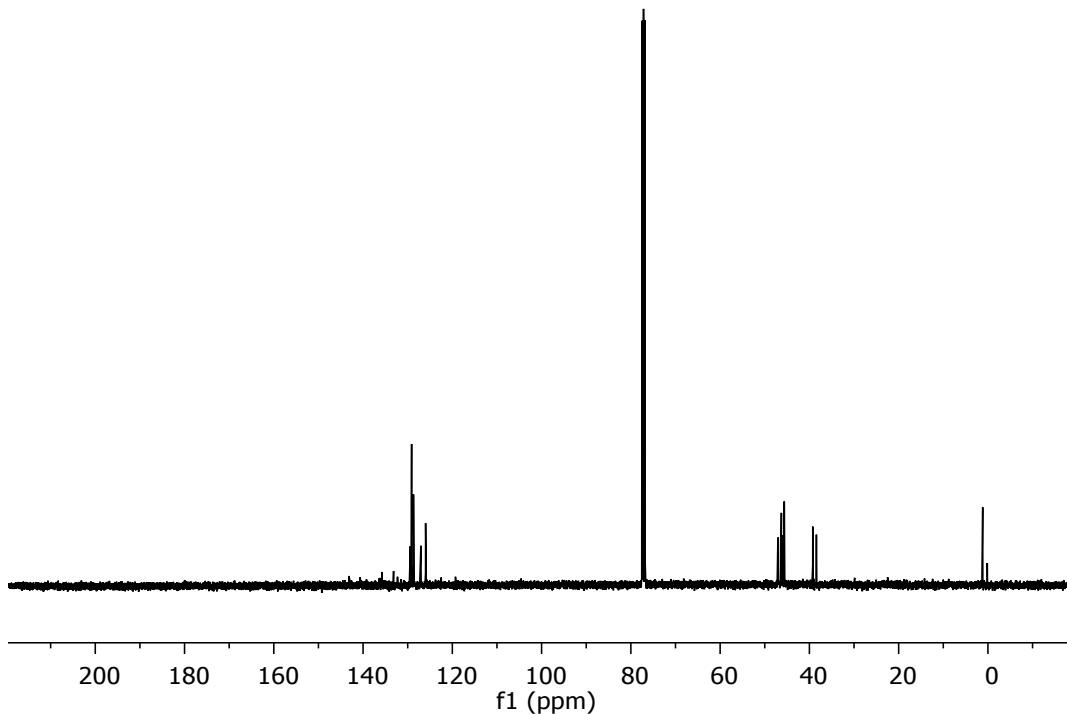
Figure S12 13C NMR (100 MHz, CDCl3) spectrum of 4.
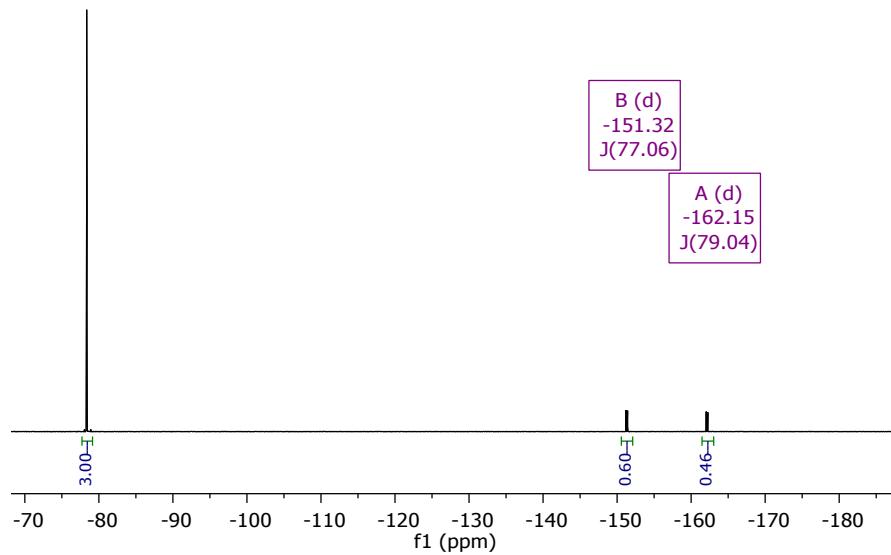
Figure S13: 19F NMR (377 MHz, CDCl3) spectrum of 4.

B (d)
-151.32
J(77.06)

A (d)
-162.15
J(79.04)
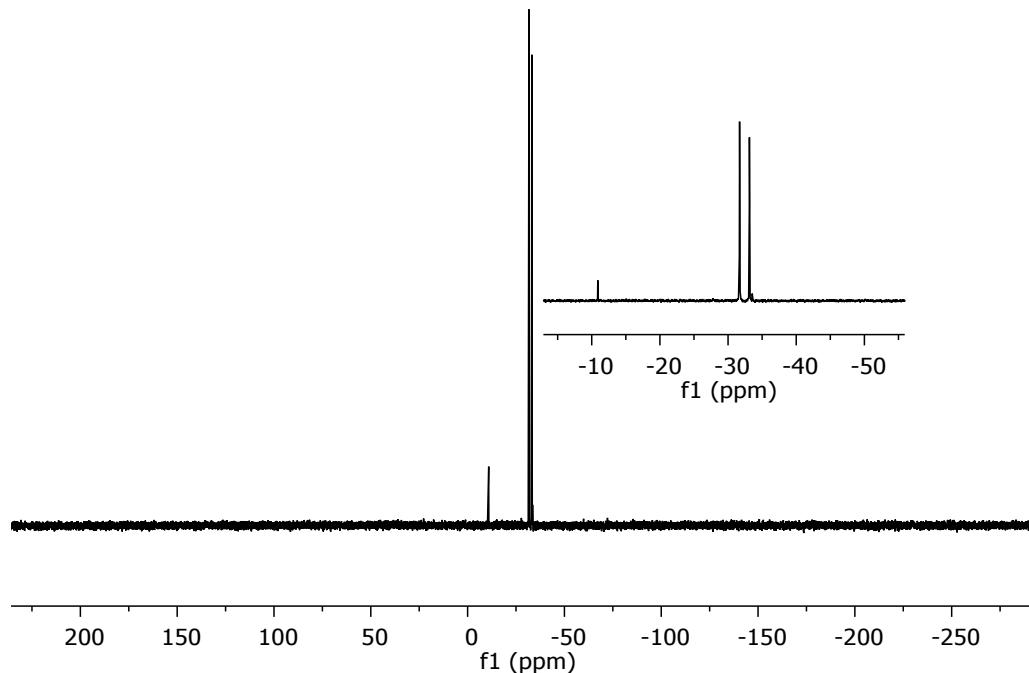
Figure S14: 31P NMR (162 MHz, CDCl3) spectrum of 4.

[PhC(CH$_2$)OP(MeNCH$_2$CH$_2$)$_3$N][O$_3$SCF$_3$] 5
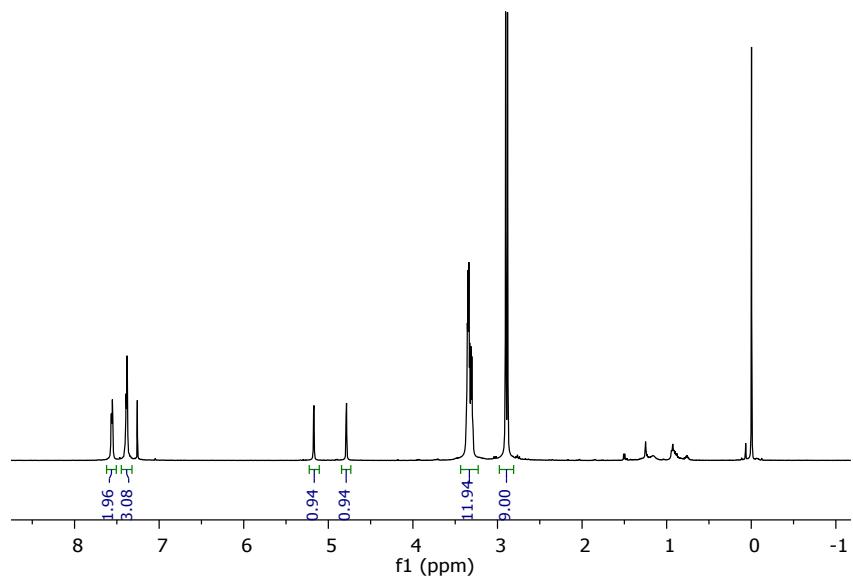
Figure S15: 1H NMR (500 MHz, CDCl3) spectrum of 5.
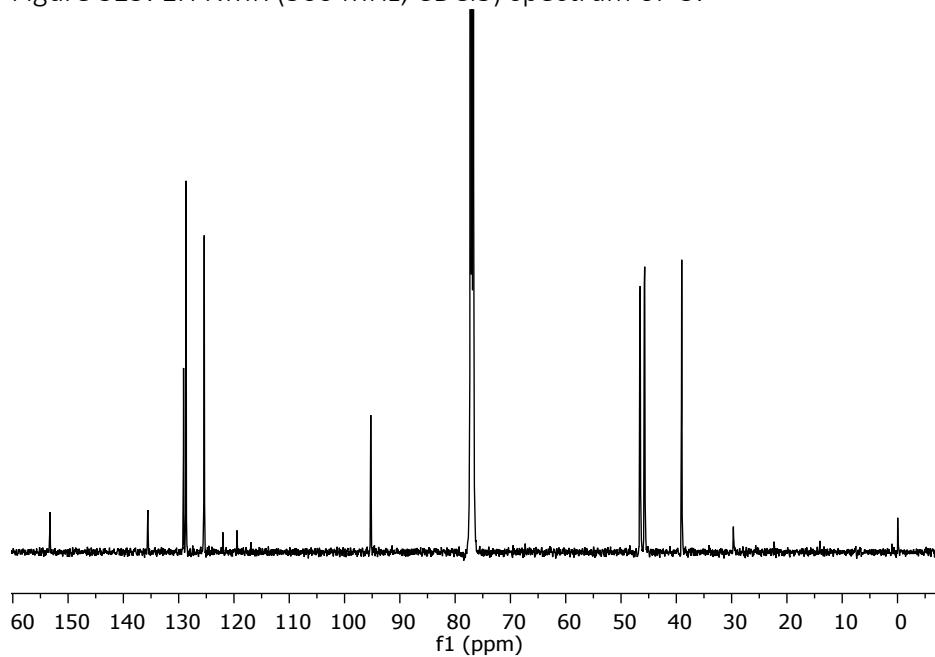
Figure S16: 13C NMR (500 MHz, CDCl3) spectrum of 5.
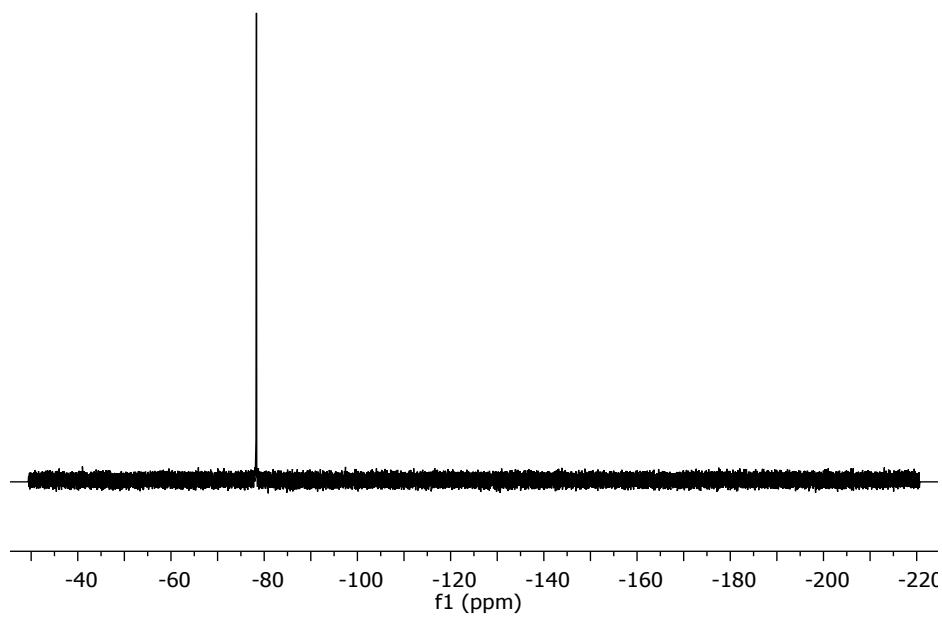
Figure S17: 19F NMR (377 MHz, CDCl3) spectrum of 5.
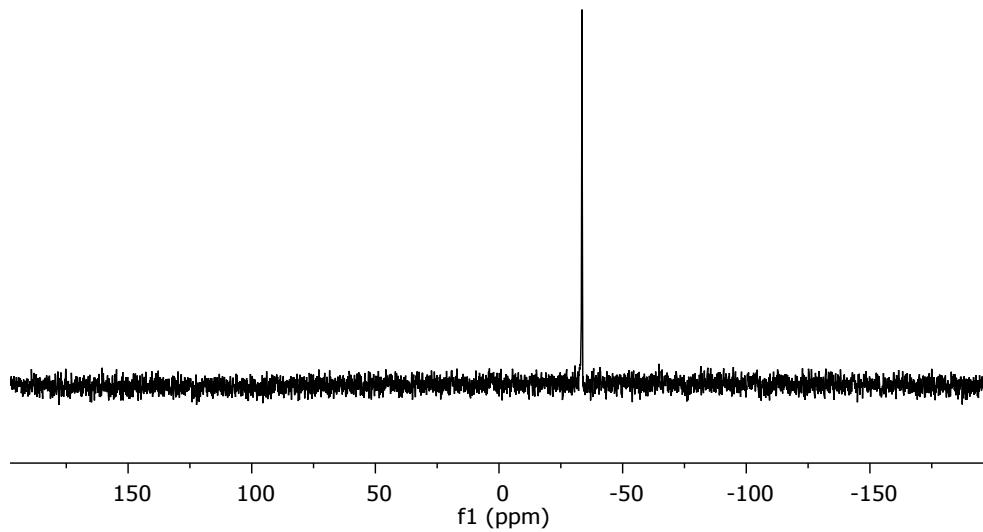
Figure S18: 31P{1H} NMR (162 MHz, CDCl3) spectrum of 5.

[HP(MeNCH$_2$CH$_2$)$_3$N][PhC(CH$_2$)OB(C$_6$F$_5$)$_3$] 6
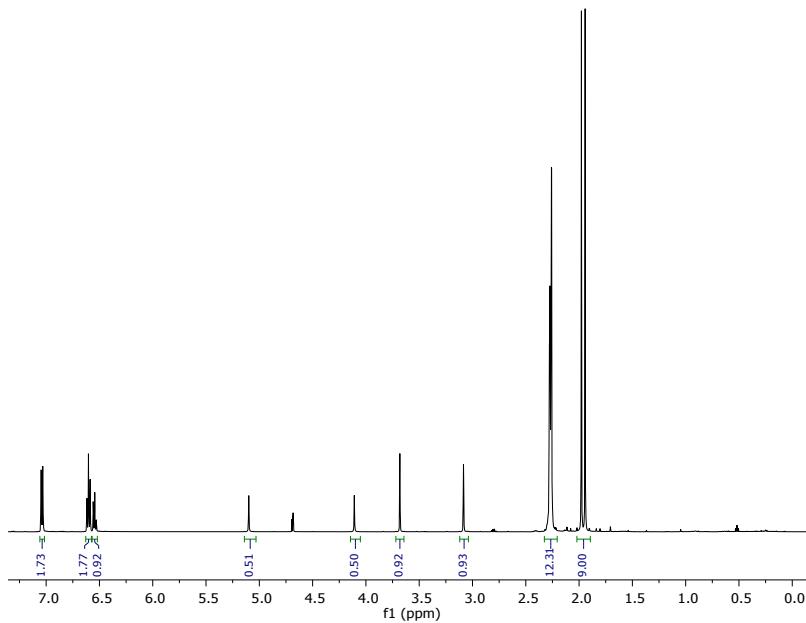
Figure S19: 1H NMR (500 MHz, CD2Cl2) spectrum of 6
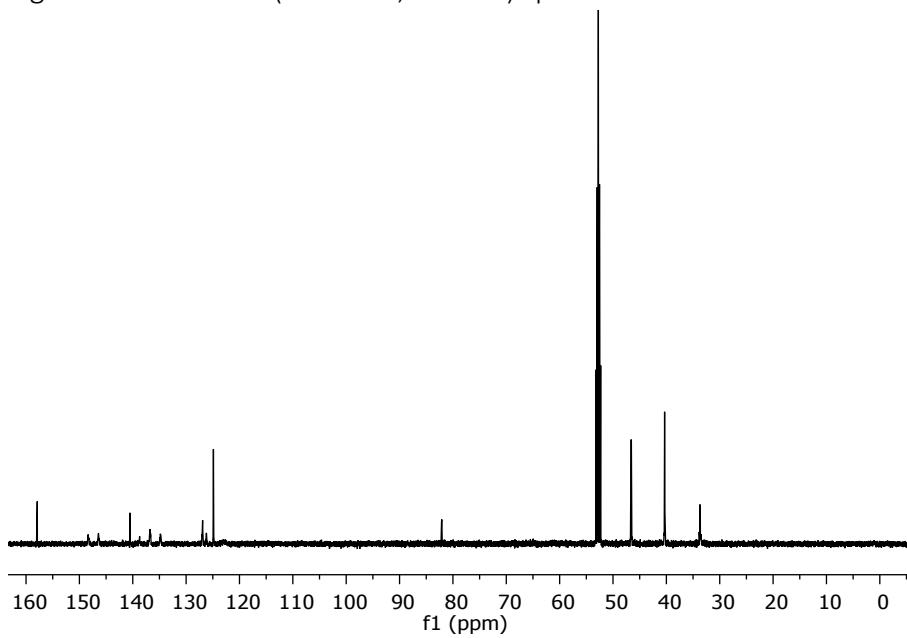
Figure S20: 13C NMR (100 MHz, CD2Cl2) spectrum of 6
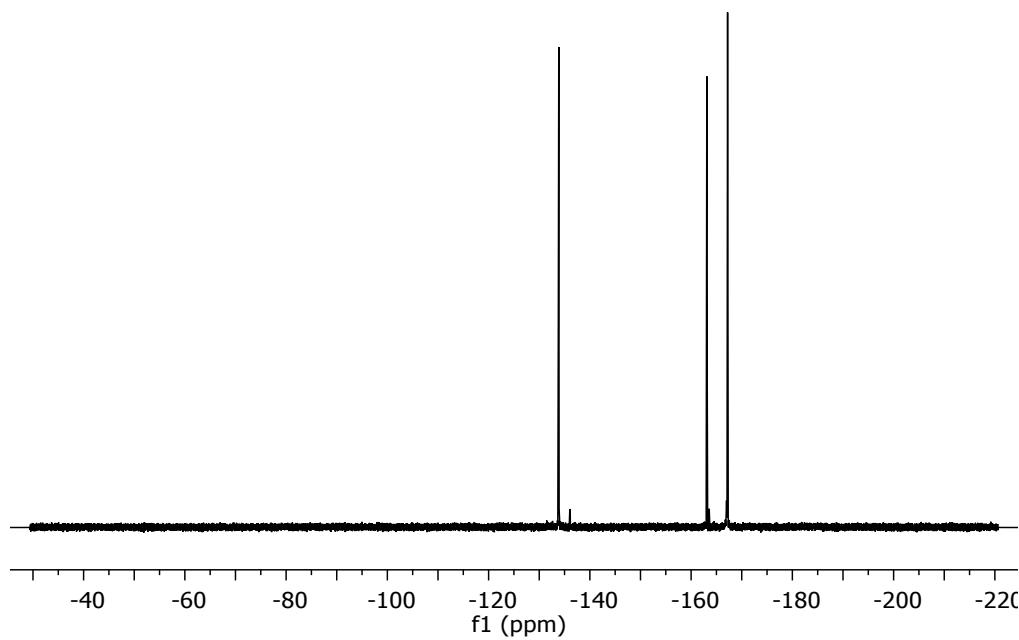
Figure S21: 19F NMR (377 MHz, CD2Cl2) spectrum of 6.
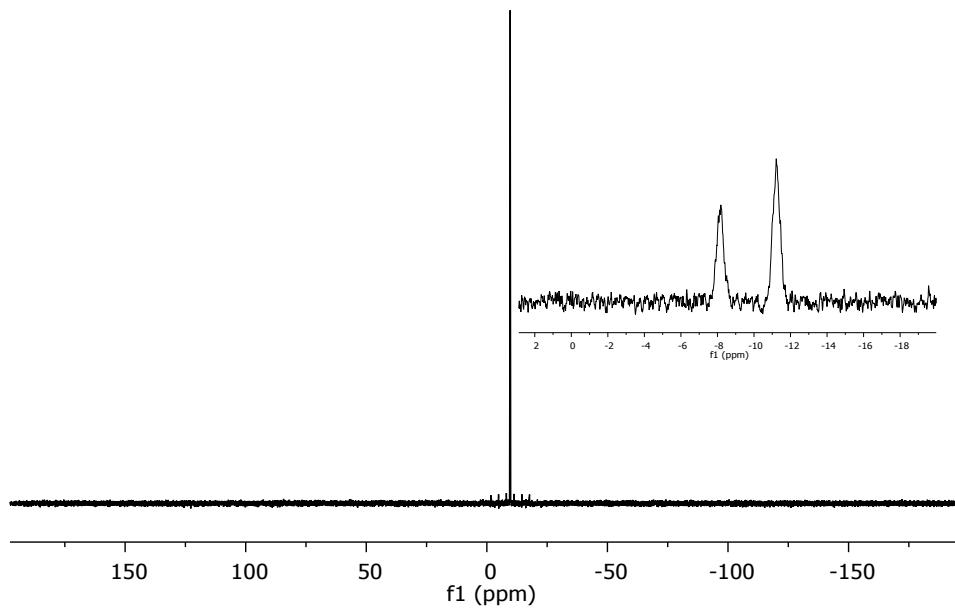
Figure S22: 31P NMR (162 MHz, CDCl3) spectrum of 6.
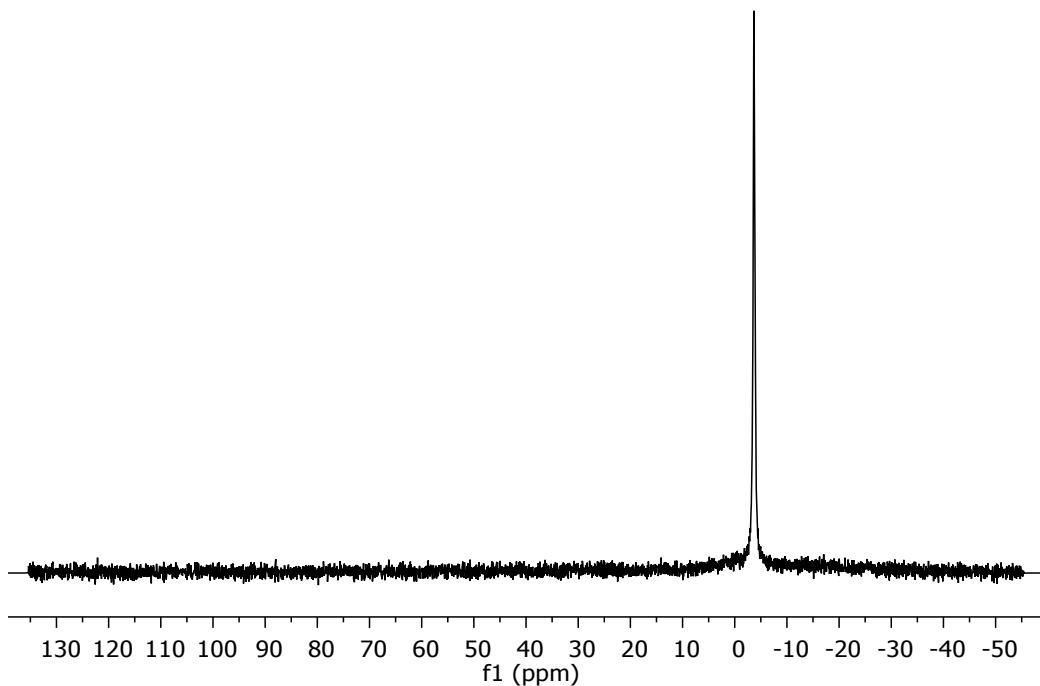
Figure S23: 11B NMR (128 MHz, CD2Cl2) spectrum of 6.

Computations

Calculations were carried out with the Gaussian 09 package,[7] All geometry optimizations were performed with the PBE1PBE functional. The optimizations also implemented Grimme's D3 empirical dispersion with Beck-Johnson damping (GD3BJ)[8] alongside SMD solvent correction. Def2-SVPP basis set was used for all the atoms. Frequency calculations at the same level of theory, with the same corrections, were performed to identify the number of imaginary frequencies and provide the thermal corrections of Gibbs free energy. Intrinsic Reaction Coordinates (IRC) were performed for transition state structures to determine corresponding two minima.

Single-point energy calculations were performed at the PBE1PBE/Def2-TZVPP level of theory alongside the SMD solvent correction and Grimme's GD3BJ. The Gibbs energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energies in solution. All the solution-phase free energies reported in the paper correspond to the reference state of 1 mol/L, 298K.

All geometry optimization and frequency calculations were performed using Gaussian 09. The PBE0 functional with def2-SVPP basis set was used. Stefan Grimme's D3 dispersion with added Becke-Johnson damping function for the empirical dispersion correction was implemented alongside the SMD model for solvent correction. The single-point energy calculations were performed with the same functional, empirical dispersion correction, and solvent corrections as

the geometry and frequency calculations, but the basis set used was def2-TZVPP. Minimum stationary states were identified by the absence of imaginary frequencies, whilst the transition states resulted in a single imaginary frequency.

Compound	Single point energy (Hartree)	Thermal correction to Gibbs Free Energy (Hartree)	Sum of Electronic and Thermal Enthalpy (Hartree)
1	-682.194021429	0.079532	-682.1144894
2	-915.410104705	0.272955	-915.1371497
3	-719.260113261	0.235419	-719.0246943
TS1	-1597.61033494	0.380213	-1597.230122
4	-1597.61298337	0.381474	-1597.231509
5	-1597.62420599	0.379641	-1597.244565
TS2	-2316.88643402	0.635210	-2316.251224
6	-1497.69719234	0.382257	-1497.314935
7	-819.229559691	0.233689	-818.9958707

Table S 1: Thermodynamic intermediates and transition state calculation energies
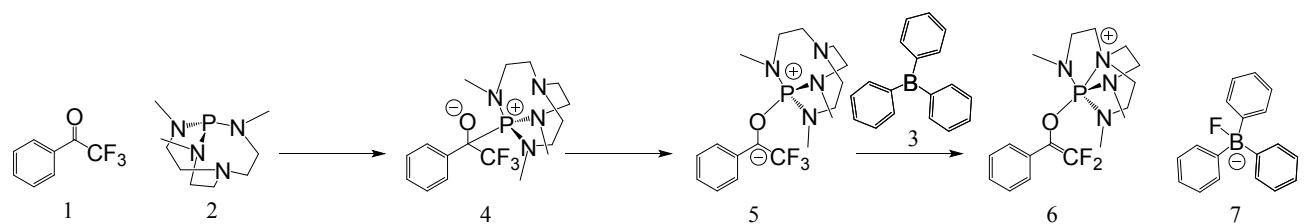
Scheme S1: Proposed mechanism for DFEP[FB(C₆H₅)₃]
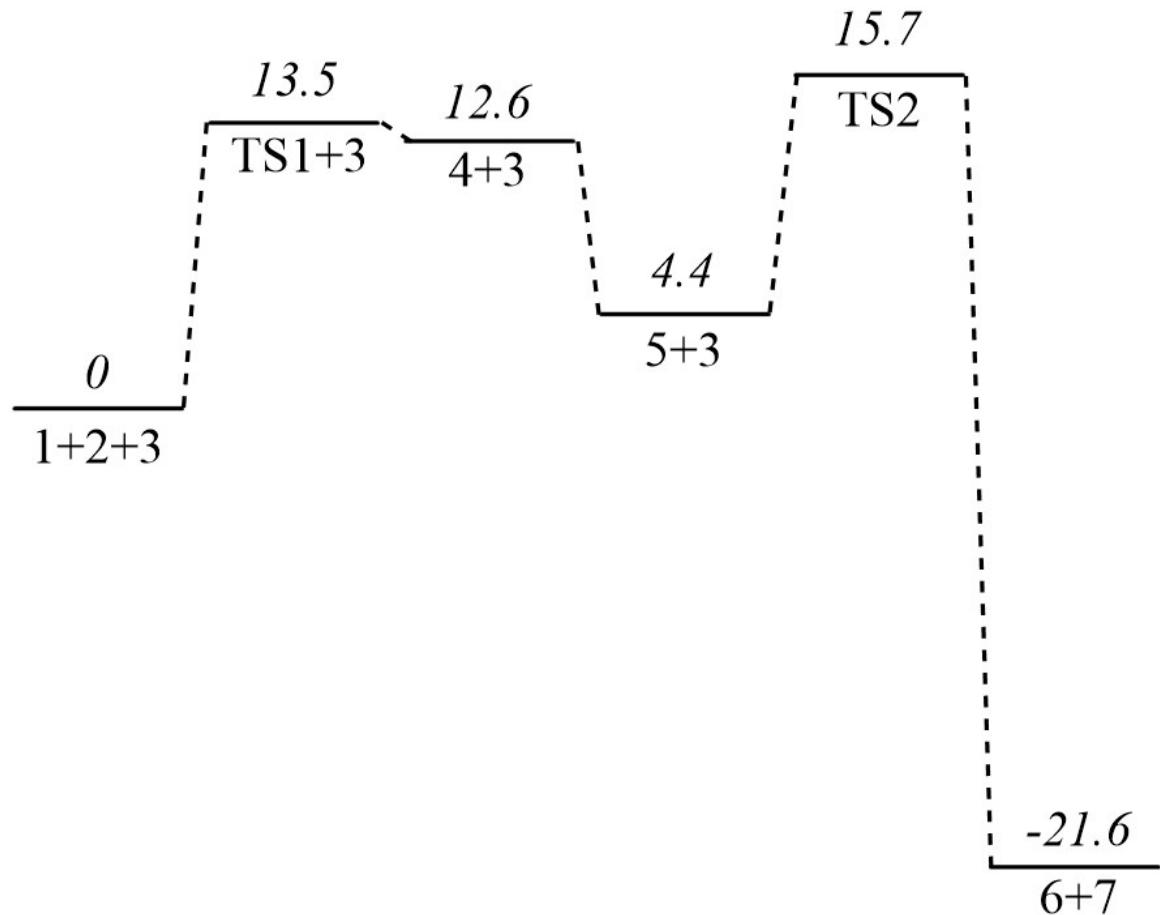
Figure S24: Thermodynamic and kinetic prediction using DFT for generation of DFEP[FBPh₃]. Energy's for stationary points, italicized, in kcal/mol.

1
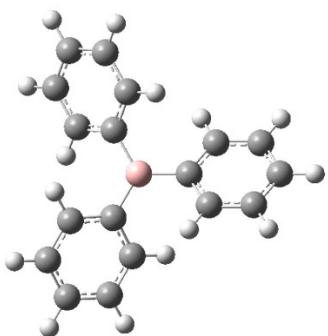
3
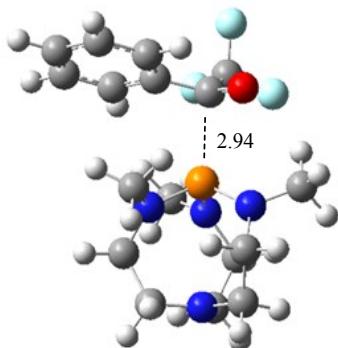
2
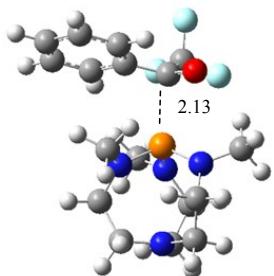
TS1
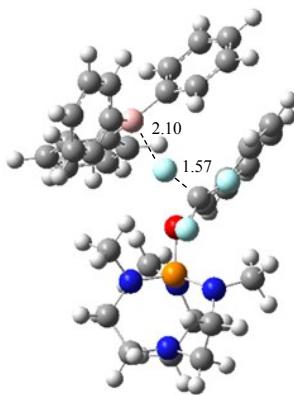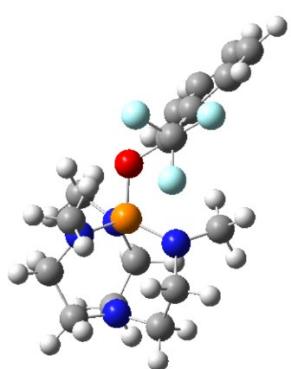
4
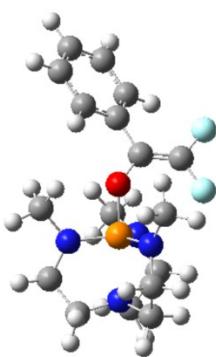
5
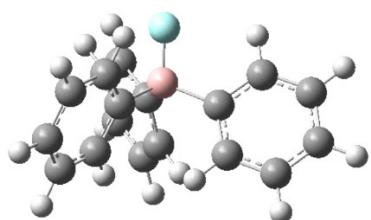
TS2

Figure S*25*: Approximated structures (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-SVPP) used for calculation thermodynamic profile for DFEP[FBPH$_3$] formation. The computational approximations' coordinates for all the atoms are listed in the X, Y, Z Cartesian. The elemental symbols (i.e. P, N, O, C, B, F, H) are all for ground state electronic configurations. Therefore, the elemental symbols P, N, O, C, B, F, and H correspond to 15, 9, 8, 7, 6, 5, and 1 atomic numbers, respectively, in the singlet electronic configuration.

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **1**

C	-4.22270200	0.06235800	1.49168600	H	-4.66903700	3.44600900	1.50427300
C	-2.83106200	0.01396100	1.48988400	H	-5.97694700	1.32271000	1.49894300
C	-2.09001200	1.20702900	1.49262500	C	-0.61238200	1.25552400	1.49055100
C	-2.76325200	2.43981700	1.49717900	O	0.02904300	2.27755400	1.47940800
C	-4.15136900	2.48246500	1.49985000	C	0.17470700	-0.07883900	1.50552600
C	-4.88308600	1.29160700	1.49698700	F	1.47721500	0.15053700	1.51330700
H	-4.79613500	-0.86890500	1.48899300	F	-0.12579500	-0.80059200	2.58839100
H	-2.33859100	-0.96023200	1.48547800	F	-0.11019300	-0.81557500	0.42839800
H	-2.17303100	3.35977600	1.49922900				

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **2**

P	2.93932600	1.30957700	5.88622200	H	0.54844300	-1.00342000	5.23424000
N	2.64177000	1.43144000	2.51661700	H	2.49254400	-0.90517300	4.00593200
N	1.37344000	0.97237100	5.26380300	H	4.17026200	-1.39054900	3.72176600
N	3.30830700	2.82309800	5.15959200	H	-0.32712100	1.55010700	4.22662000
N	3.93670300	0.22014400	5.00716800	H	0.96286200	2.76171100	4.27263800
C	4.02982900	2.97557200	3.91805700	H	2.48719100	3.74411600	6.84109400
C	0.63156300	-0.09901100	5.87366200	H	2.01398700	4.52224500	5.30926000
C	3.51067000	-0.50966500	3.83640300	H	3.66890100	4.74883600	5.95406900
C	0.76967100	1.67940300	4.15893700	H	0.97674400	0.20854100	2.57830200
C	2.85058300	4.01051300	5.83081500	H	0.64367500	1.86098600	2.02842500
C	1.23477200	1.26680500	2.76040800	H	4.51980600	0.60540200	2.27316900
C	3.49568200	0.27552900	2.52242400	H	3.19335400	-0.43261400	1.71915600
C	3.22642400	2.73909200	2.63666200	H	2.41423500	3.48405200	2.56295500
C	5.28939600	0.04232000	5.46397600	H	3.90840200	2.93748700	1.78016500
H	4.45415000	3.99706800	3.89157000	H	5.40713300	0.51562800	6.45685000
H	4.89152400	2.28296900	3.91122600	H	5.54350600	-1.03163500	5.57344000
H	1.13568800	-0.40840800	6.80845800	H	6.04852500	0.49931500	4.79432700
H	-0.39734900	0.21894400	6.13829400				

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **3**

B	-0.49401600	0.22117600	0.00302600	C	3.89936300	0.22027700	-0.00370100
C	1.07302200	0.22096300	0.00080300	H	3.74622000	-1.36872400	1.45604900
C	1.80642000	-0.67811300	0.80061300	H	3.74233400	1.80937600	-1.46294100
C	1.80430100	1.11973100	-0.80128700	H	4.99418600	0.21999200	-0.00546500
C	3.20033600	-0.67127600	0.81269300	C	-1.27720900	1.56596900	-0.17964800
H	1.27128000	-1.38869900	1.43888300	C	-2.51589300	1.60697600	-0.85054600
C	3.19817200	1.11219800	-0.81783700	C	-0.77037900	2.78219800	0.32023100
H	1.26745400	1.83056800	-1.43784200	C	-3.20824700	2.80377200	-1.02809800

H	-2.93815500	0.68159000	-1.25542400	C	-2.51419700	-1.16411500	0.86153700
C	-1.47043800	3.97853100	0.17201100	C	-1.47150200	-3.53601800	-0.16305200
H	0.18748400	2.78671700	0.85034300	H	0.18501600	-2.34458100	-0.84544800
C	-2.68905300	3.99194400	-0.50977300	C	-3.20635800	-2.36076100	1.04084400
H	-4.16055900	2.81131100	-1.56781600	H	-2.93536900	-0.23859400	1.26724700
H	-1.06254800	4.90702600	0.58405900	C	-2.68855200	-3.54910800	0.52152600
H	-3.23584500	4.93173700	-0.63793800	H	-1.06472400	-4.46464800	-0.57589300
C	-1.27704500	-1.12343000	0.18778900	H	-4.15743400	-2.36805000	1.58274000
C	-0.77159700	-2.33982600	-0.31308900	H	-3.23521100	-4.48878500	0.65110300

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **TS1**

P	-0.13318700	-0.37481800	0.10527800	H	2.13290300	0.01646300	3.25140000
N	0.06959800	-0.05112600	3.30176800	H	1.37933800	1.52052900	3.80829900
N	1.31294700	0.34512200	0.58452600	H	-0.87584000	-1.85516900	3.65136900
N	-1.34929900	0.61004300	0.74599000	H	0.81071600	-1.81025400	4.19650600
N	-0.24920000	-1.84237200	0.94345300	H	-1.01443600	1.70454200	3.30570300
C	-2.02441500	0.30862200	1.99311100	H	-1.82323100	0.36095500	4.13063700
C	2.57617900	-0.10248300	0.03936400	H	-2.06389000	-2.31485900	-0.01348500
C	0.58961000	-2.15186400	2.08526800	H	-0.98695900	-3.71380900	0.26674300
C	1.38397500	1.30052400	1.67600100	H	-1.89573700	-2.97661300	1.62304200
C	-1.55304900	1.93082800	0.18976300	C	-3.79450600	0.39284600	-2.58061600
C	1.27743000	0.69120500	3.07486200	C	-2.58756700	-0.22631600	-2.25988500
C	0.12831200	-1.48338900	3.38200800	C	-1.36851600	0.37760400	-2.59445200
C	-1.19959000	0.61756300	3.24708600	C	-1.38901600	1.60621200	-3.26487600
C	-1.34217800	-2.75493300	0.69083600	C	-2.59384500	2.22636600	-3.58801900
H	-2.96875600	0.88238600	2.01543300	C	-3.80367500	1.62280800	-3.24175300
H	-2.31166800	-0.75525200	2.00894300	H	-4.73787200	-0.08879300	-2.30490600
H	2.40527700	-0.78040300	-0.80649600	H	-2.60770000	-1.18097000	-1.73210500
H	3.16108600	0.75579600	-0.33895400	H	-0.42965000	2.06674800	-3.51468100
H	3.18904900	-0.63362800	0.79529500	H	-2.58924400	3.18777800	-4.11152000
H	1.62764700	-1.84806400	1.87308200	H	-4.75339300	2.10840400	-3.48734200
H	0.60769700	-3.25003800	2.20904800	C	0.00829500	-0.17811900	-2.27683900
H	2.34162500	1.84276700	1.58089600	O	1.01085900	0.52861400	-2.47524000
H	0.59199900	2.05810900	1.56065700	C	0.19381300	-1.66638000	-2.64925500
H	-0.79929500	2.13765000	-0.58600300	F	1.35184100	-2.15312200	-2.19629500
H	-1.44588300	2.71033700	0.96825600	F	-0.76595500	-2.49720600	-2.22382700
H	-2.55520600	2.03599100	-0.26828600	F	0.22385900	-1.77145300	-3.98693700

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **4**

0 1				C	0.15000800	-1.32787200	2.87501000
P	-0.14309500	-0.78338100	-0.48696100	C	-0.96384800	0.85091500	2.40511400
N	0.22883800	0.06072100	2.52020400	C	-1.58048800	-2.88034800	0.55377800
N	1.38952700	-0.17895400	-0.21114000	H	-2.74688700	1.10651500	1.18573900
N	-1.22263300	0.42126400	-0.04448300	H	-2.28471000	-0.57363800	1.46271000
N	-0.37180500	-2.08153600	0.55935100	H	2.31377300	-1.70955500	-1.31559200
C	-1.87770400	0.42804100	1.25096900	H	3.19039100	-0.16862100	-1.30253900
C	2.58012200	-0.85252600	-0.68674400	H	3.19907600	-1.21396400	0.15827600
C	0.48920100	-2.26877700	1.71722400	H	1.54047300	-2.12334200	1.42237300
C	1.61157500	0.95709100	0.66876700	H	0.39868500	-3.32173300	2.03852800
C	-1.29233400	1.63747200	-0.83123500	H	2.61727100	1.35495500	0.44695000
C	1.49744600	0.62547300	2.15681200	H	0.90349300	1.76518600	0.42660400

H	-0.55324500	1.60286700	-1.64691300	C	-1.45621300	0.48433200	-4.07950400
H	-1.06280900	2.52325900	-0.20902400	C	-2.61313200	1.07221700	-4.58750300
H	-2.29477900	1.77466600	-1.27730100	C	-3.86247300	0.69362200	-4.09358300
H	2.28597800	-0.09431700	2.43663700	H	-4.91407500	-0.59079300	-2.70614600
H	1.70439700	1.55473700	2.72987900	H	-2.87150500	-1.63411900	-1.82281700
H	-0.87502600	-1.53613500	3.22838600	H	-0.46172700	0.77067300	-4.43214700
H	0.82803200	-1.56740200	3.72230200	H	-2.54031100	1.83313900	-5.37156000
H	-0.66281000	1.90400400	2.26736400	H	-4.77472700	1.15684900	-4.48289100
H	-1.56158700	0.81769100	3.34105000	C	-0.16068700	-1.03609500	-2.60406000
H	-2.30108600	-2.50387900	-0.18508200	O	0.87443100	-0.44034500	-3.03692500
H	-1.36220200	-3.93779600	0.31589700	C	-0.10493800	-2.56879100	-2.83459000
H	-2.07743000	-2.84246100	1.54114400	F	1.00492300	-3.11908200	-2.32348100
C	-3.93974500	-0.28358700	-3.09944500	F	-1.13628500	-3.26501300	-2.32879000
C	-2.77833900	-0.87268900	-2.59906600	F	-0.08614000	-2.81628200	-4.15024400
C	-1.52084000	-0.48875200	-3.07793100				

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **5**

P	0.03720300	0.00220800	-0.03754600	H	-2.88944600	1.39225400	-1.12290100
O	0.06492300	0.01485600	1.57019400	H	-2.25708000	-0.77881700	-1.66388600
N	0.15830200	-0.02088300	-2.82171800	H	-1.89685500	-2.50625200	-1.75624200
N	-0.85592000	1.28044300	-0.56668000	H	-0.97179100	2.98959400	-1.74641600
N	1.64681600	0.03415600	-0.39910800	H	0.66627200	2.35146200	-1.53482000
N	-0.63879800	-1.43473200	-0.49573500	H	2.20738200	1.14723600	1.29636200
C	-0.72309200	0.84540900	2.42092500	H	2.73940300	1.86474700	-0.25644100
C	2.13975600	-0.66400500	-1.58167500	H	3.54426700	0.40064600	0.39719900
C	-1.83523600	0.24838100	3.06128300	H	-1.57052000	1.05767100	-3.20477000
C	-2.25973100	1.42250800	-0.21354400	H	-0.09916700	1.82381600	-3.84415300
C	-1.43151700	-1.50794300	-1.71522500	H	0.12977000	-2.07279600	-3.10146300
C	-3.72417600	0.21928500	4.64521800	H	-1.24217500	-1.23591100	-3.85614900
C	-0.38433400	2.05786000	-1.70027400	H	1.97499800	0.96176600	-2.99382800
C	2.57570700	0.91658000	0.28933600	H	1.96957900	-0.65243700	-3.73861500
C	-2.62217400	0.85691400	4.09152900	H	0.48851700	-2.48016400	0.93965700
C	-2.27607100	-1.05092800	2.65748600	H	-1.01768000	-3.28886500	0.43253200
C	-4.13377500	-1.05430500	4.22914200	H	0.40481900	-3.27765000	-0.65993800
C	-0.50478400	1.24490300	-2.99010700	H	-2.35627300	1.84595100	4.46497900
C	-0.58549700	-1.24476400	-2.96289100	H	-4.28207400	0.73841700	5.43371500
C	1.59521900	-0.06652700	-2.87402400	H	-5.00467500	-1.54492400	4.67349700
C	-0.16565200	-2.68253300	0.07789200	H	-3.66277000	-2.67084400	2.86883300
C	-3.38311100	-1.67190000	3.22466900	H	-1.71885000	-1.57471000	1.87971800
H	3.23999500	-0.62359200	-1.56077700	C	0.00787200	2.04263000	2.78329500
H	1.86127000	-1.73061100	-1.52445200	F	0.44054700	2.76922400	1.70531400
H	-2.58344000	0.60806400	0.45237100	F	1.19023600	1.83550100	3.47486400
H	-2.43126700	2.37831900	0.31082000	F	-0.69336200	2.89486900	3.5444090

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **TS2**

P	2.47280500	1.80858200	5.77815200	N	2.64660600	3.38315000	5.27311600
O	2.00638300	2.07913100	7.30384100	N	3.90101300	0.96954200	5.98983200
N	3.22491800	1.51448000	3.39389500	C	0.83460400	1.62995900	7.94490400
N	1.27621800	0.86746000	5.12354700	C	3.60067300	3.72689800	4.22497400

Atom	X	Y	Z
C	1.03298100	0.73093800	9.04126600
C	0.98089400	-0.43810800	5.69264600
C	4.33247100	0.05378900	4.94938000
C	0.30614300	-0.48563700	11.04228400
C	0.90224200	1.07876800	3.73972800
C	2.17460200	4.53065200	6.04029900
C	0.04395500	0.40687900	10.00982800
C	2.29624800	0.09962900	9.20423900
C	1.55459600	-1.10282000	11.17918800
C	2.10455200	0.77099500	2.85298600
C	4.45759700	0.78756500	3.61705300
C	3.33663800	2.89712300	2.98539000
C	4.93565500	1.57020500	6.81597100
C	2.54381900	-0.79236400	10.24381500
H	3.48291000	4.79696600	3.99422300
H	4.64085700	3.58677800	4.57892400
H	1.53979000	-0.59546000	6.62718100
H	-0.09489000	-0.52244200	5.92466600
H	1.26073100	-1.24405500	4.98768700
H	3.60901900	-0.77479200	4.85819200
H	5.29226200	-0.39371500	5.25252200
H	0.03923400	0.43601900	3.50507000
H	0.57686900	2.12392800	3.59811400
H	1.55834400	4.21892100	6.88744300
H	1.57945000	5.19657000	5.39013200
H	3.03431900	5.09916800	6.43926800
H	2.33360100	-0.30593100	2.90378500
H	1.90927900	1.02089500	1.79326700
H	5.28847700	1.50946300	3.67231600
H	4.68286300	0.08381300	2.79332100
H	2.37701700	3.20906000	2.54366800
H	4.12497900	3.05319200	2.22410700
H	4.49385900	2.32601800	7.48216400
H	5.41109500	0.79933000	7.44746200
H	5.72015100	2.05958300	6.20704200
H	-0.94061900	0.87263800	9.96281200
H	-0.48831400	-0.69421800	11.76731900
H	1.75078800	-1.80140200	11.99801600
H	3.53574600	-1.25184600	10.32236900
H	3.09157700	0.32463700	8.49030900
C	-0.30221200	2.41976900	7.68530800
F	-1.47386900	1.92486200	8.07336800
F	-0.42728800	2.88357200	6.43149800
F	-0.35785700	3.81267600	8.40058700
C	-0.41769000	3.93760000	11.18281100
C	1.73738500	4.99619000	9.87552600
C	-0.71348400	6.17057700	9.66759400
B	0.17132500	4.92809200	10.09849300
C	-1.52299500	2.22921700	13.15179400
C	-0.20708800	2.67532500	13.26793900
C	0.33495500	3.51307500	12.29063200
C	-1.74739500	3.48293900	11.09814300
C	-2.29389500	2.63457600	12.05875000
C	2.39067900	6.21807500	9.63306800
C	3.77653300	6.29309600	9.47797700
C	4.54969800	5.13414300	9.55894200
C	-2.35713100	7.89147200	10.23980300
C	-2.24318000	8.44865000	8.96654400
C	-1.36878500	7.87434300	8.03961600
C	-0.61140300	6.75910900	8.39268300
C	-1.60705700	6.76213200	10.57674500
C	2.54314700	3.84498500	9.95535000
C	3.92641500	3.90687700	9.79854600
H	4.52205900	2.99099600	9.86734000
H	5.63701700	5.18677900	9.43939100
H	4.25557900	7.26112000	9.29729100
H	1.80148800	7.13890500	9.57459200
H	2.07362700	2.87334300	10.13090400
H	-1.71563200	6.33258300	11.57831400
H	0.06820400	6.32161300	7.65419100
H	-3.03872000	8.33406300	10.97376200
H	-2.83498200	9.32872700	8.69412800
H	-1.27688600	8.30294100	7.03605300
H	1.37067000	3.85049000	12.39911500
H	0.40487800	2.36362100	14.12066900
H	-1.94936000	1.56533200	13.91106600
H	-3.32757000	2.28727900	11.95856800
H	-2.36304300	3.79177800	10.24762300

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **6**

Atom	X	Y	Z
P	2.79629500	1.51008800	5.18447400
F	0.93787900	3.49377800	6.74113100
O	2.97386100	1.53294800	6.85482200
F	0.21743300	2.91780300	8.69132500
N	2.59070300	1.47973700	3.07953100
N	1.16808100	1.06583800	5.19317700
N	3.24439500	3.10890600	4.94397100
N	3.93162000	0.29858700	4.94527400
C	2.03461200	1.71100600	7.82797000
C	3.66646800	3.52656900	3.61962400
C	2.17564500	0.81611400	8.99352700
C	0.80643100	-0.19488500	5.82752000
C	3.88203100	-0.43246100	3.69395600
C	1.24892100	-0.49845800	10.81181400
C	0.40983500	1.40977800	4.01019900
C	3.76680400	3.98611400	5.98097000
C	1.07031900	0.35839200	9.72784800
C	1.10265800	2.67292700	7.75206000
C	3.45810800	0.38091300	9.36225100
C	2.52848700	-0.91892900	11.17690200
C	1.23731800	0.96223900	2.82038300
C	3.65888900	0.58891100	2.60312700

C	2.74954000	2.86694100	2.62537100
C	4.78463200	-0.23174900	5.99461500
C	3.63184200	-0.47778000	10.44518100
H	3.58014000	4.62211600	3.54117300
H	4.72891300	3.26557200	3.44042400
H	1.56501900	-0.49642300	6.56453400
H	-0.15610100	-0.08776400	6.35694300
H	0.71505200	-1.01167800	5.08600700
H	3.09120500	-1.20846800	3.69489300
H	4.84270900	-0.94542500	3.53225300
H	-0.56676500	0.90450100	4.03602500
H	0.21772900	2.49651500	3.97945800
H	3.48339400	3.65935000	6.98579300
H	3.37192100	5.00463900	5.82274300
H	4.87179200	4.02928100	5.93247600
H	1.28022600	-0.13740300	2.79023100
H	0.86727800	1.32867700	1.84927900
H	4.57231500	1.18820600	2.47151700
H	3.38287600	0.14140100	1.63426000
H	1.76434000	3.35422600	2.65211300
H	3.13262300	2.89789700	1.59290400
H	5.14142000	0.57186800	6.65217800
H	4.27957400	-0.99668200	6.61329200
H	5.66489700	-0.69534100	5.51937200
H	0.05950700	0.65941800	9.44378200
H	0.37547300	-0.84866200	11.37031100
H	2.66468900	-1.59411500	12.02709200
H	4.63989800	-0.80170300	10.72172600
H	4.32542400	0.72736900	8.79630100

Optimized (SMD(DCM)/PBE0-GD3BJ/def2-TZVPP//SMD(DCM)/PBE0-GD3BJ/def2-svpp) Cartesian coordinates for **7**

F	-1.61222600	-6.74007800	13.13567000
C	-3.06782100	-6.37161400	15.13794200
C	-1.10417800	-8.21295000	15.09602500
C	-0.48752900	-5.59501800	15.05705100
B	-1.56941700	-6.72942300	14.59043400
C	-5.66460400	-5.64003900	16.04588100
C	-4.79351000	-6.34179000	16.88170900
C	-3.52241300	-6.70168800	16.42628700
C	-3.96931200	-5.66964400	14.31853300
C	-5.24543800	-5.30745200	14.75592700
C	-0.52294600	-8.45561900	16.35260100
C	-0.17519900	-9.74100700	16.77631100
C	-0.39206700	-10.83701400	15.93877800
C	0.44694600	-4.02800900	16.69778100
C	1.48599700	-3.69322100	15.82736700
C	1.54046700	-4.30169500	14.57125700
C	0.56904900	-5.23491200	14.20198700
C	-0.52044300	-4.95903700	16.31001100
C	-1.30562600	-9.33550800	14.27392600
C	-0.95796900	-10.62629000	14.67946700
H	-1.12890400	-11.47593000	14.00841100
H	-0.11758200	-11.84662000	16.26276000
H	0.27589900	-9.88814400	17.76420600
H	-0.32239200	-7.61014200	17.02150700
H	-1.74680300	-9.18997700	13.28142100
H	-1.33640500	-5.18847200	17.00562100
H	0.62793100	-5.70056000	13.21162000
H	0.38540500	-3.55394200	17.68396800
H	2.24459400	-2.96076900	16.12347900
H	2.34712500	-4.04605900	13.87460700
H	-2.86645900	-7.27054300	17.09619400
H	-5.11036200	-6.61795300	17.89383200
H	-6.66386400	-5.35913300	16.39541700
H	-5.91993800	-4.76226400	14.08567500
H	-3.65910800	-5.40305900	13.30201500

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