Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Reactivity of Frustrated Lewis Pairs with BOC protected diazocarboxylates: FLP Capture of Diazene

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Experimental

General information for synthesis

All manipulations were performed under inert conditions using either standard Schlenk or Glove box technique, unless noted otherwise. Molecular sieves were vacuum dried for 3 days at 200 ^{o}C. Dichloromethane (DCM, CH_2Cl_2) and *n*-hexanes (C_6H_{14}) were collected from an MBRAUN Solvent Purification System, deoxygenated by bubbling Ar for 20 min, and stored over 3 Å molecular sieves. All the deuterated solvents such as acetonitril-d_3 (CD_3CN) and dichloromethane-d_2 (CD_2Cl_2) were used as received and stored over 3 Å molecular sieves. Glassware and stir bars for reactions were dried for overnight in oven at 110 ^{o}C. ^{1}H (500 MHz), ^{19}F (471 MHz), ^{19}F{^{1}H} (471 MHz), ^{31}P{^{1}H} (202 MHz), and ^{13}C{^{1}H} (126 MHz) NMR spectra were run at 298 K on Bruker 500 spectrometers. The chemical shifts (δ, ppm) for ^{1}H and ^{13}C{^{1}H} NMR spectra are given relative to solvent signals, whereas external reference standards used for ^{31}P (85% H_3PO_4), ^{31}P{^{1}H} (85% H_3PO_4), ^{19}F ($CFCl_3$) and ^{19}F{^{1}H} ($CFCl_3$) NMR spectra. These NMR data are written as: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. HRESI-MS analysis was performed on Thermo Scientific Q-Exactive Plus spectrometer.

Single-crystal *X*-ray diffraction data were collected on a Bruker D8 QUEST diffractometer using Cu (60W, Diamond, μKα = 12.894 mm^{-1}) micro-focus *X*-ray sources. Using Olex2,[1] the structures were solved with the XT structure solution program[2] employing Intrinsic Phasing and refined with the XL refinement package[3] with the Least Squares minimization.

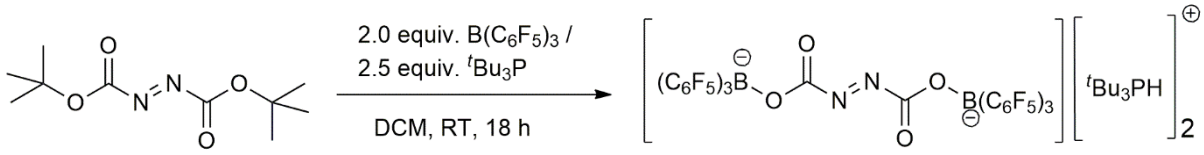
$B(C_6F_5)_3$[4] was prepared by following literature method. $P(NMe_2)_3$ was freshly distilled and used. All other reagents were purchased from commercial sources and were used without further purification.

Synthetic procedures and characterization data

General procedure

All the reactions were run on 0.10 mmol scale. Unless otherwise noted, to a solution mixture of $B(C_6F_5)_3$ (2.0 equiv.) and the corresponding bases (2.0 equiv.) in DCM was added a solution of di-(*t*-butyl)azodicarboxylate (1.0 equiv.) in DCM drop wise, bubbling of gas along with colour change was noted in all cases. The reaction was left for magnetic stirring at room temperature for 18 h. After 18 h, all the volatiles were removed *in vacuo*, the solid residue obtained was then washed with hexanes several times (3 x 3 mL). For recrystallization, the solid residue was dissolved in DCM and layered with hexane (1:3) and left at -30 ^{o}C overnight.

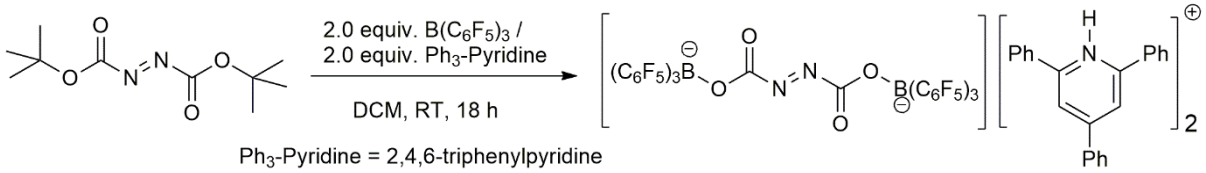
Synthesis of Compound 1



To an open top PTFE (4 mL) vial containing a solution of $B(C_6F_5)_3$ (102.4 mg, 0.20 mmol, 2.0 equiv.) in DCM was added a solution of $^{t}Bu_3P$ (50.5 mg, 0.25 mmol, 2.5 equiv.) in DCM (0.5 mL). Finally, a solution of di-(*tert*-butyl)azodicarboxylate (23.0 mg, 0.10 mmol, 1.0 equiv.) in DCM (0.5 mL) was added drop wise, bubbling of gas along with colour change from yellow to orange was noted. The reaction mixture was then left under magnetic stirring at room temperature for 18 h. After removing all the volatiles, the orange residue obtained was washed with hexane (3 x 3 mL), drying under vacuum afford compound **1** in 88% (136 mg) yield. Orange color *X*-ray quality crystals were grown by dissolving compound **1** in DCM and layering with hexane (1:3) at -30 °C overnight. ^{1}H NMR (500 MHz, CD_3CN) δ 5.41 (d, *J* = 44 Hz, 1H), 1.61 (d, *J* = 15.6 Hz, 27H); $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_3CN) δ 55.7; ^{31}P NMR (202 MHz, CD_3CN) δ 55.7 (dm, *J* = 44 Hz); ^{19}F NMR (471 MHz, CD_3CN) δ -135.39 (dd, *J* = 22.8, 7.7 Hz), -162.11 (t, *J* = 19.6 Hz), -167.58 (td, *J* = 22.8, 7.5 Hz). ^{11}B NMR (160 MHz, CD_3CN) δ -3.3; ^{13}C NMR (126 MHz, CD_3CN) δ 163.1, 148.9 (d, *J* = 241.0 Hz), 140.9, 137.5 (d, *J* = 251.9 Hz), 38.0 (d, *J*

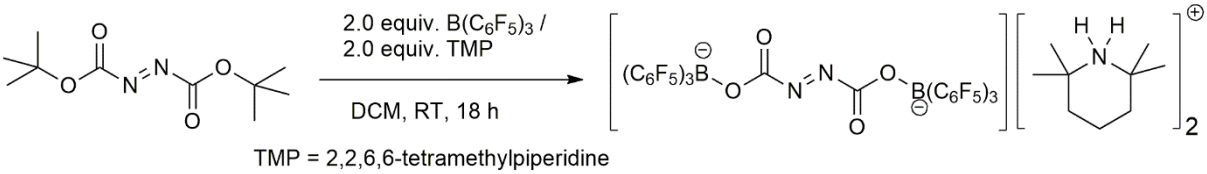
= 28.1 Hz), 30.2; HRESI-MS (+) m/z: 203.1925 $[M+H]^+$ (calcd.: 203.1923 for $[C_{12}H_{28}P]^+$); HRESI-MS (-) m/z: 569.9777 $[M]^{2-}$ (calcd.: 569.9788 for $[C_{38}B_2F_{30}N_2O_4]^{2-}$).

Synthesis of Compound 2



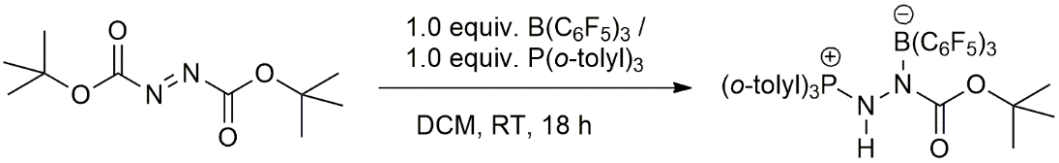
Compound **2** was prepared by following the general procedure described above. Yield = 79% (139 mg). ^{1}H NMR (500 MHz, CD_3CN) δ 12.72 (s, 1H), 8.37 (s, 2H), 8.06 (ddt, *J* = 18.1, 6.9, 1.7 Hz, 6H), 7.80 – 7.62 (m, 9H); ^{19}F NMR (471 MHz, CD_3CN) δ -135.43 (dd, *J* = 22.4, 7.6 Hz), -162.10 (t, *J* = 19.6 Hz), -165.79 – -169.55 (m); ^{11}B NMR (160 MHz, CD_3CN) δ -3.3; ^{13}C NMR (126 MHz, CD_3CN) δ 163.1, 155.0, 148.0, 138.5, 136.3, 132.9, 130.5, 130.2, 129.2, 122.4; HRESI-MS (+) m/z: 308.1435 $[M+H]^+$ (calcd.: 308.1434 for $[C_{23}H_{18}N]^+$); HRESI-MS (-) m/z: 569.9775 $[M]^{2-}$ (calcd.: 569.9788 for $[C_{38}B_2F_{30}N_2O_4]^{2-}$).

Synthesis of Compound 3



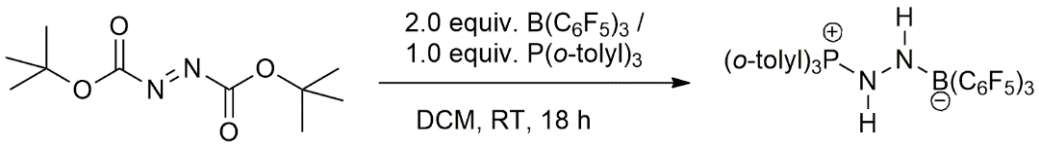
Compound **3** was prepared following the described general procedure above. Yield = 83% (118 mg). ^{1}H NMR (500 MHz, CD_3CN) δ 6.23 (t, *J* = 48.7 Hz, 2H), 2.03 – 1.74 (m, 2H), 1.64 (p, *J* = 4.5 Hz, 4H), 1.37 (s, 12H); ^{19}F NMR (471 MHz, CD_3CN) δ -135.41 (dd, *J* = 22.9, 7.7 Hz), -162.07 (t, *J* = 19.6 Hz), -167.58 (td, *J* = 23.0, 7.7 Hz); ^{11}B NMR (160 MHz, CD_3CN) δ -3.5; ^{13}C NMR (126 MHz, CD_3CN) δ 163.2, 148.9 (d, *J* = 245.0 Hz), 140.0 (d, *J* = 246.3 Hz), 137.6 (d, *J* = 216.0 Hz), 59.3, 35.3, 27.4, 16.6; HRESI-MS (+) m/z: 142.1591 $[M+H]^+$ (calcd.: 142.1591 for $[C_9H_{20}N]^+$); HRESI-MS (-) m/z: 569.9775 $[M]^{2-}$ (calcd.: 569.9788 for $[C_{38}B_2F_{30}N_2O_4]^{2-}$).

Synthesis of Compound 4



Compounds **4** was following the same general procedure described above. Yield = 69% (65.4 mg). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.87 (br. s, 3H), 7.60 (t, *J* = 7.6 Hz, 3H), 7.43 (br. s, 3H), 7.29 (t, *J* = 6.9 Hz, 3H), 5.33 (s, 1H), 1.93 (s, 9H), 0.90 (s, 9H); ^{31}P{^{1}H} NMR (202 MHz, CD_2Cl_2) δ 34.5; ^{19}F NMR (471 MHz, CD_2Cl_2) δ -134.33 (d, *J* = 22.8 Hz), -162.46 (t, *J* = 20.4 Hz), -167.12 (t, *J* = 20.8 Hz); ^{11}B NMR (160 MHz, CD_2Cl_2) δ -7.7; ^{13}C NMR (126 MHz, CD_2Cl_2) δ 186.6, 149.1, 142.4, 137.7, 135.5, 133.6, 132.9, 132.8, 126.3, 81.3, 27.3, 21.6; HRESI-MS (+) m/z: 947.5644 $[M+H]^+$ (calcd.: 947.2050 for $[C_{44}H_{32}BF_{15}N_2O_2P]^+$).

Synthesis of Compound 5



Compounds **5** was prepared by following the general procedure described above. Yield = 63% (53.2 mg). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.67 (t, *J* = 7.6 Hz, 3H), 7.50 (dd, *J* = 15.2, 7.9 Hz, 3H), 7.44 (t, *J* = 6.6 Hz, 3H), 7.35 (td, *J* = 7.8, 2.6 Hz, 3H), 4.55 (d, *J* = 29.6 Hz, 1H), 4.28 (s, 1H), 2.13 (s, 9H); ^{31}P{^{1}H} NMR (202 MHz, CD_2Cl_2) δ 40.5; ^{19}F NMR (471 MHz, CD_2Cl_2) δ -133.48 (d, *J* = 22.2 Hz), -161.83 (t, *J* = 20.3 Hz), -163.93 – -168.79 (m); ^{11}B NMR (160 MHz, CD_2Cl_2) δ -7.2; ^{13}C NMR (126 MHz, CD_2Cl_2) δ 148.5 (d, *J* = 237.2 Hz), 144.2 (d, *J* = 9.1 Hz), 140.0, 137.1 (d, *J* = 247.3 Hz), 135.3 (d, *J* = 2.3 Hz), 135.2, 133.8 (d, *J* = 11.5 Hz), 127.5 (d, *J* = 12.9 Hz), 119.5 (d, *J* = 97.4 Hz), 22.4 (d, *J* = 3.7 Hz); HRESI-MS (+) m/z: 847.1151 $[M+H]^+$ (calcd.: 847.1526 for $[C_{39}H_{24}BF_{15}N_2P]^+$).

NMR spectra of all compounds

Compound 1

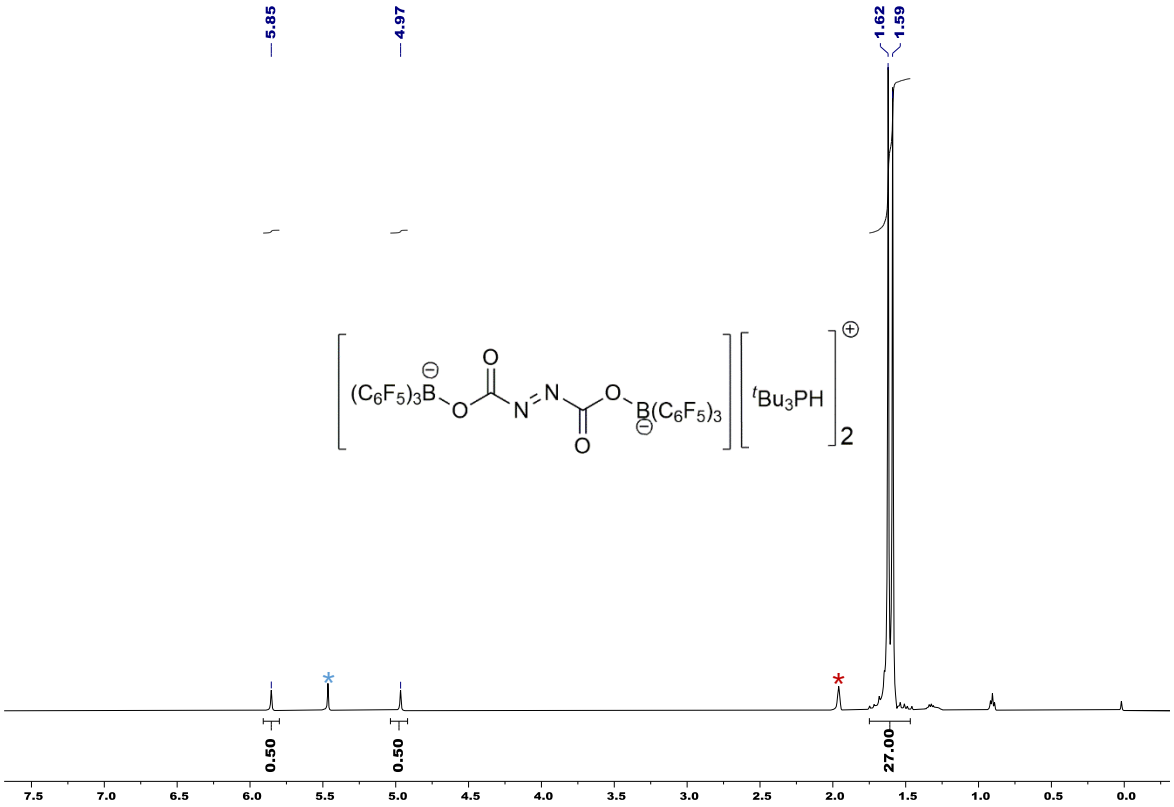


Figure S01. ^{1}H NMR (500 MHz, CD_3CN) spectrum of the compound **1** (*=CD_3CN, *=DCM).

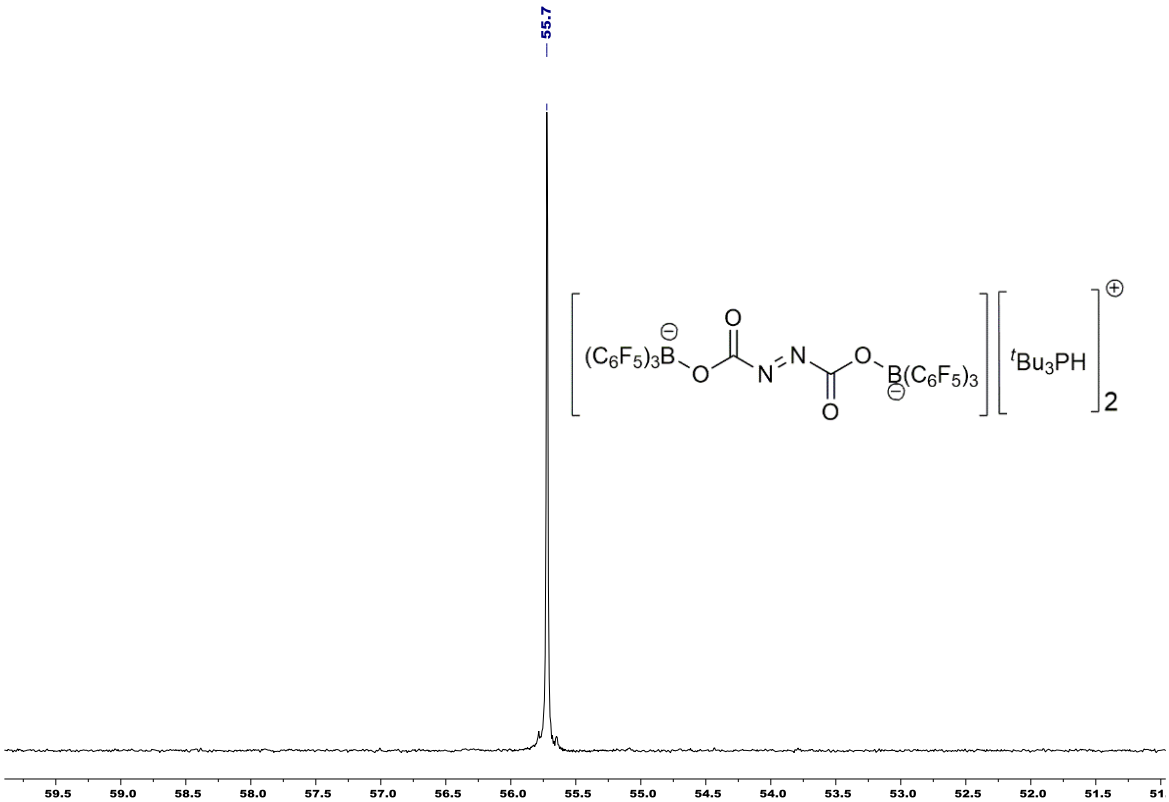


Figure S02. $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_3CN) spectrum of the compound **1**.

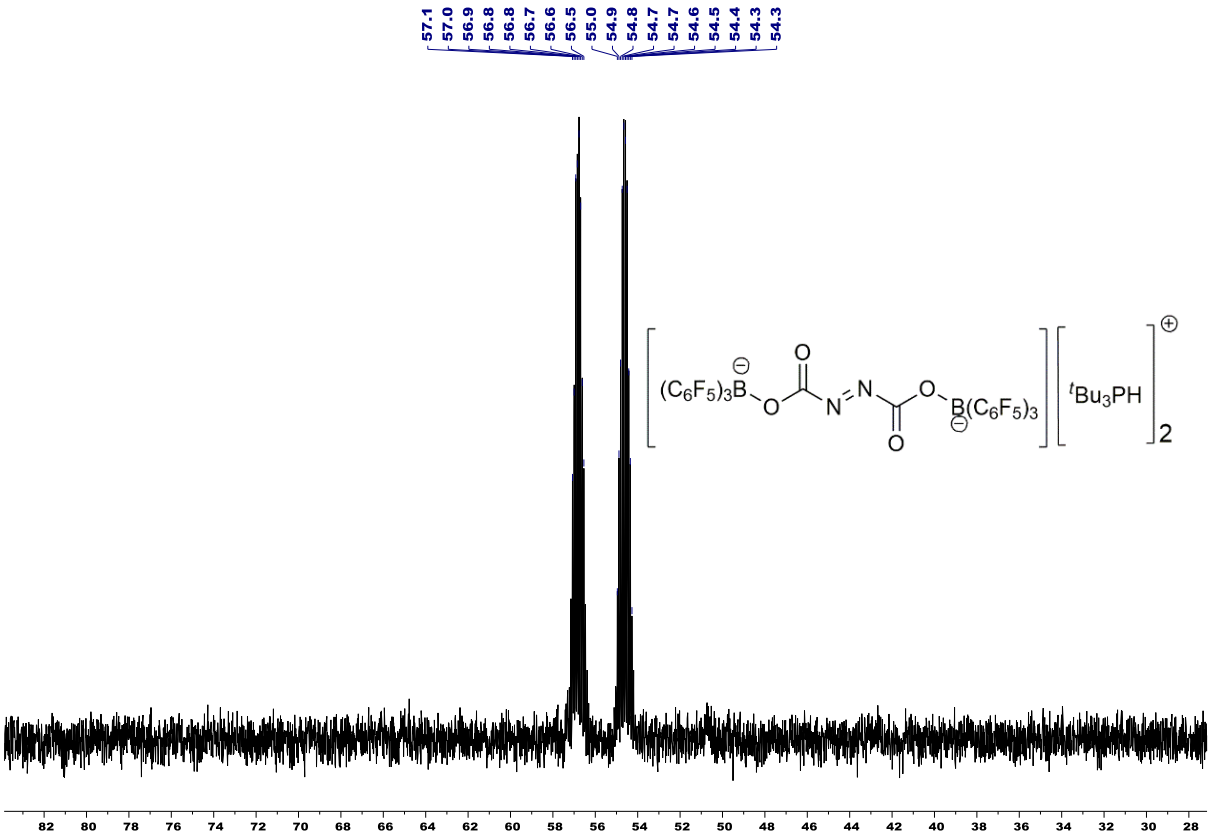


Figure S03. ^{31}P NMR (202 MHz, CD_3CN) spectrum of the compound **1**.

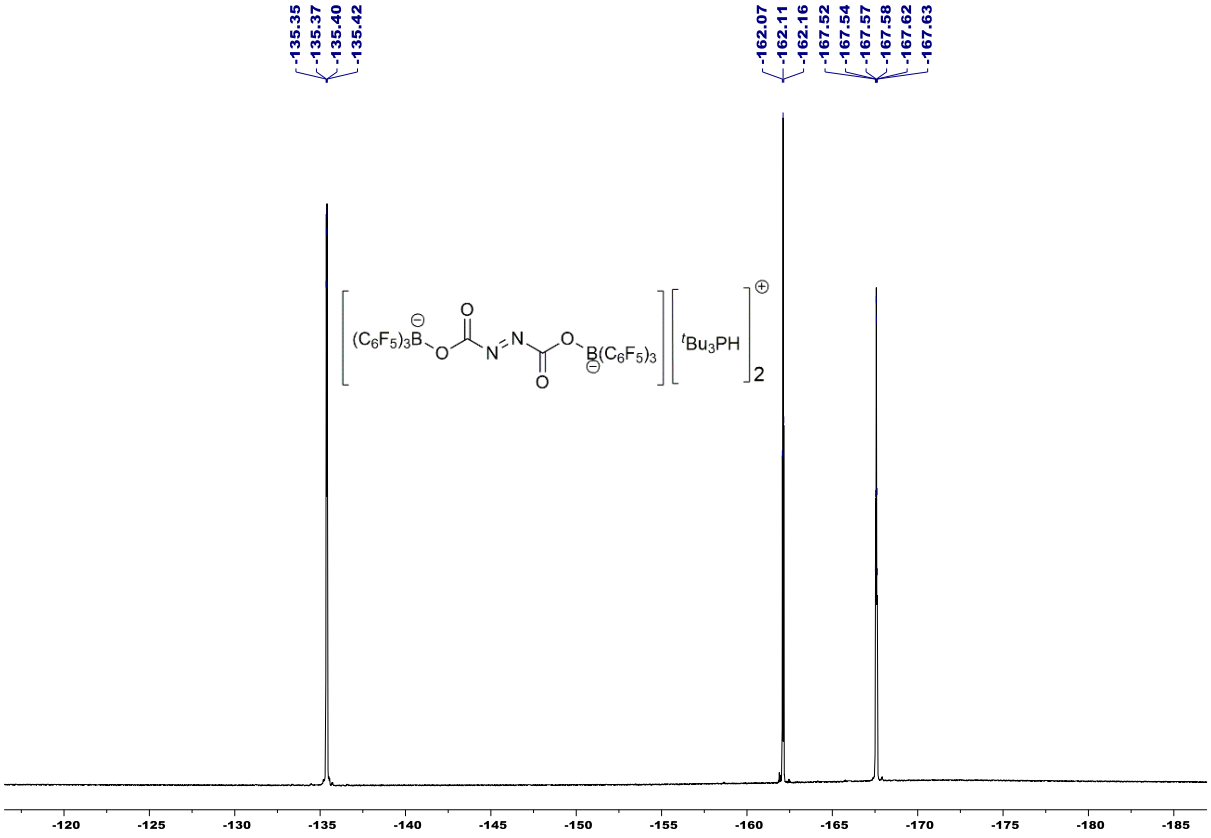


Figure S04. ^{19}F NMR (471 MHz, CD_3CN) spectrum of the compound **1**.

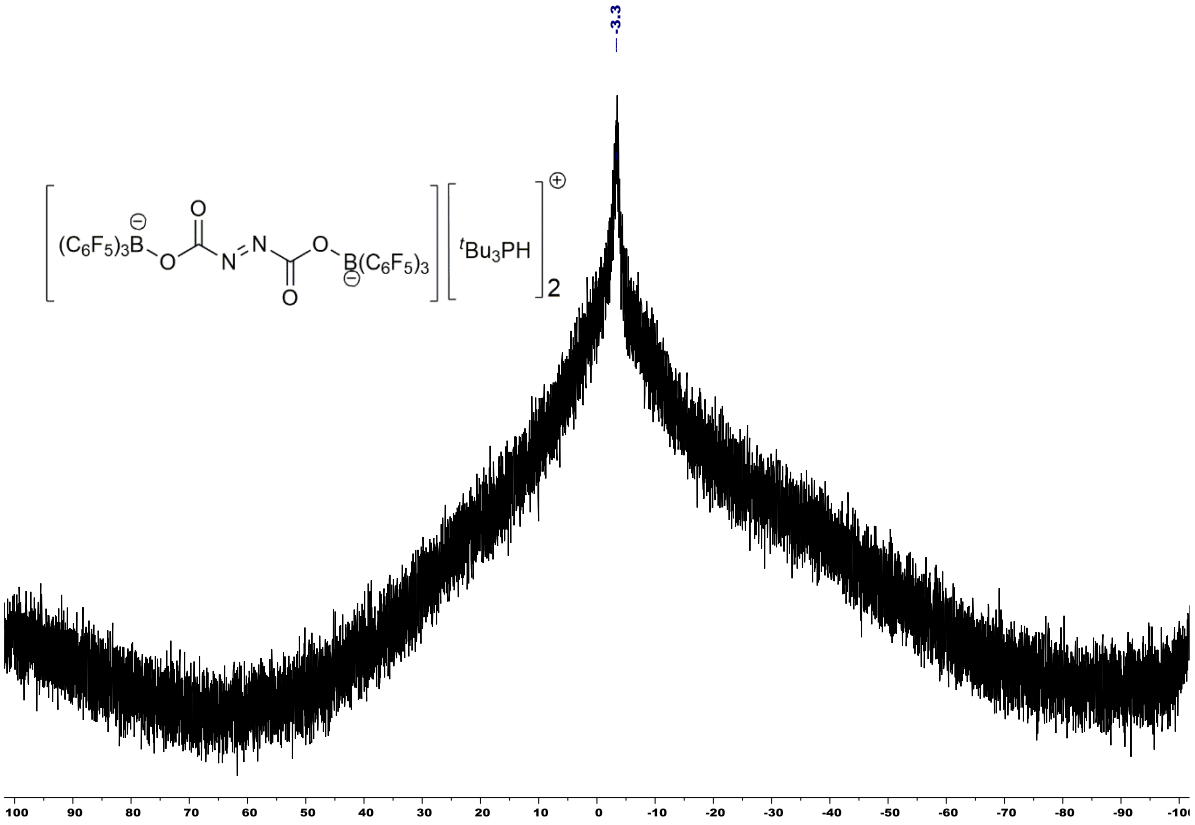


Figure S05. ^{11}B NMR (160 MHz, CD_3CN) spectrum of the compound **1**.

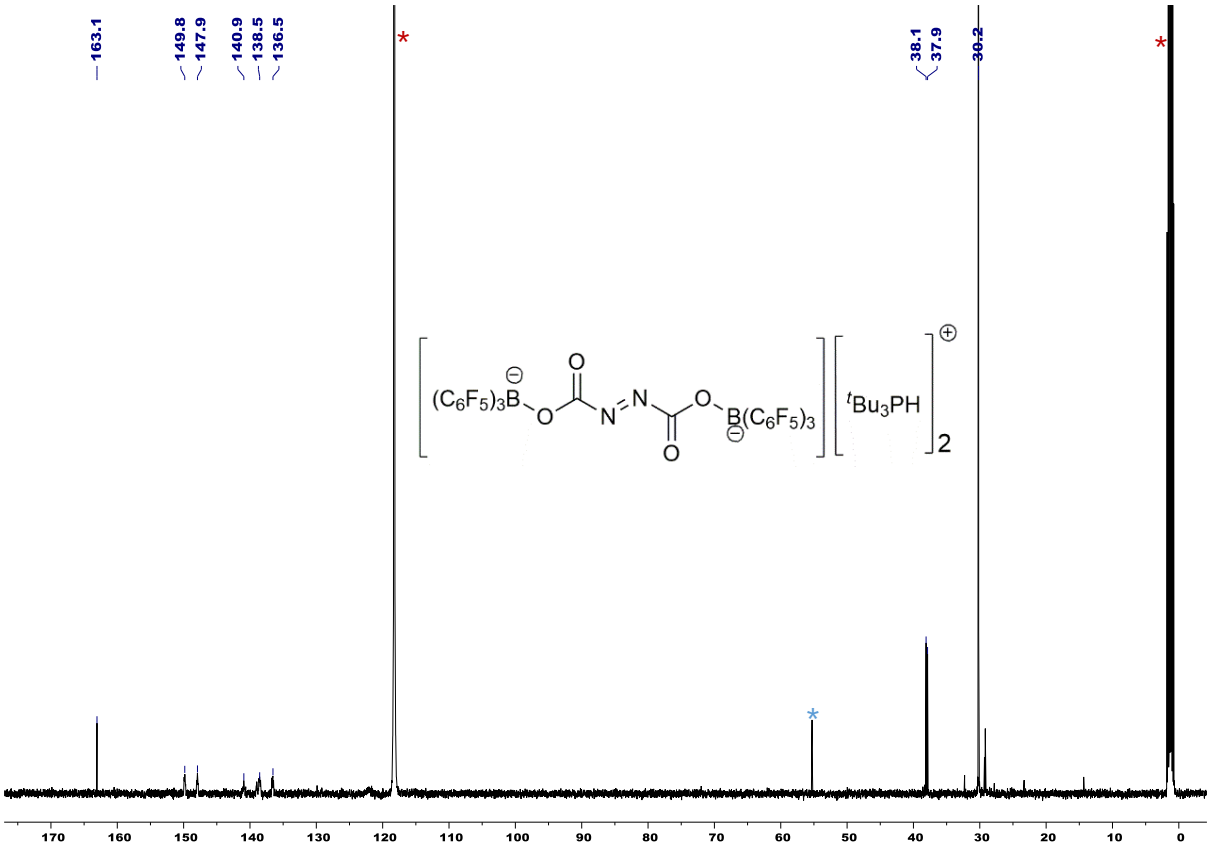


Figure S06. ^{13}C NMR (126 MHz, CD_3CN) spectrum of the compound **1** (*=CD_3CN, *=DCM).

Compound 2

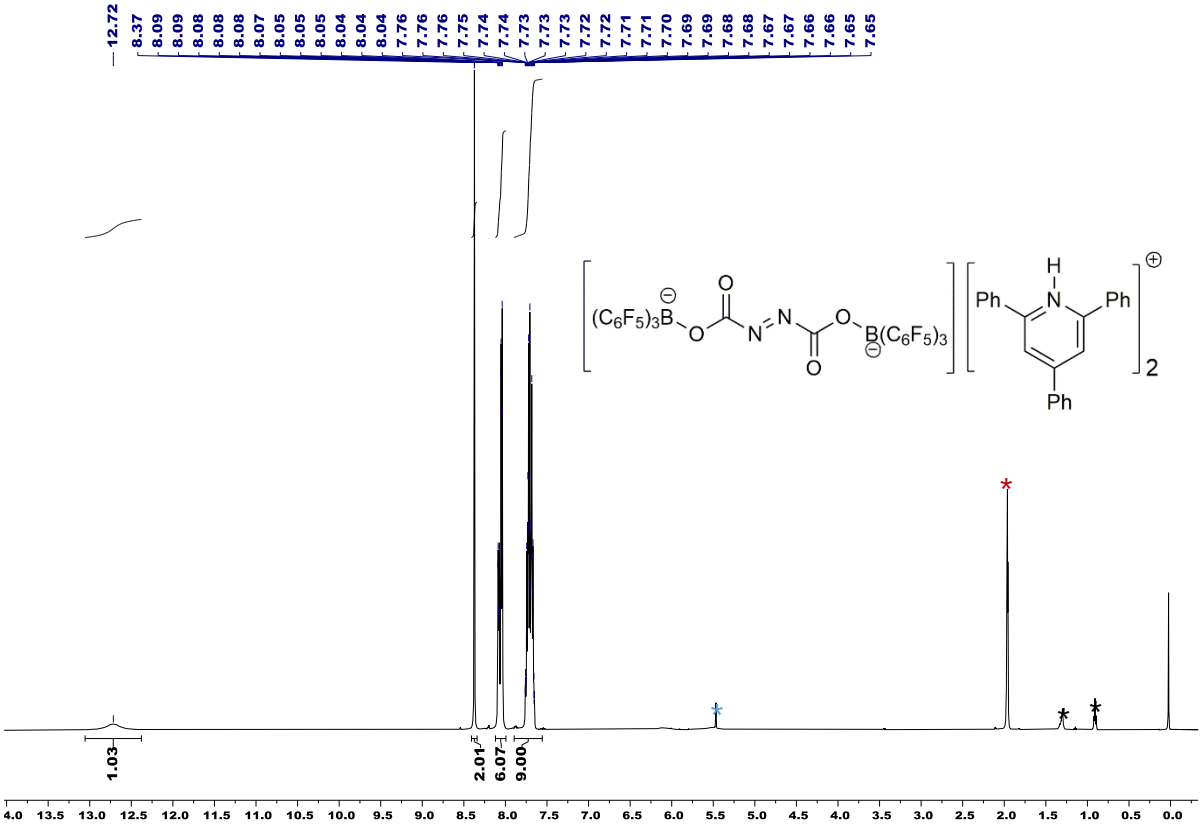


Figure S07. ^{1}H NMR (500 MHz, CD_3CN) spectrum of the compound **2** (*=CD_3CN, *=DCM, *=hexane).

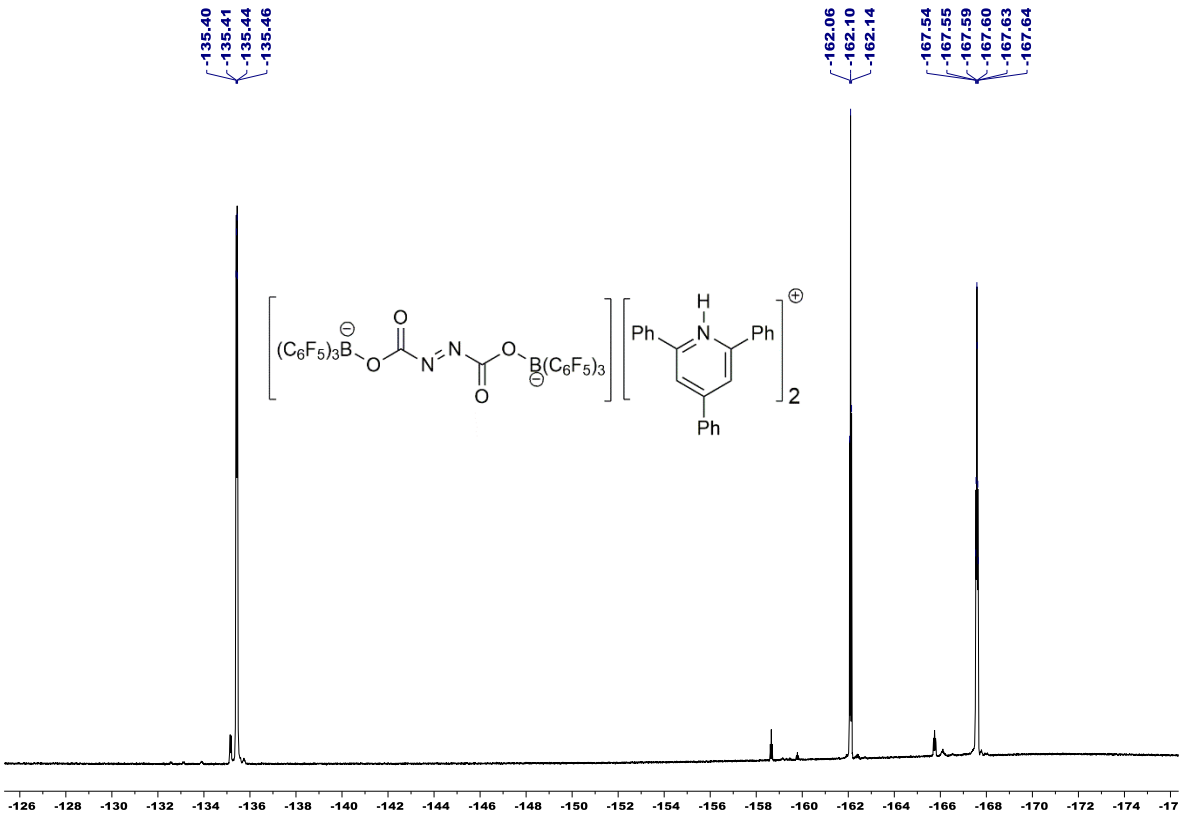


Figure S08. ^{19}F NMR (471 MHz, CD_3CN) spectrum of the compound **2**.

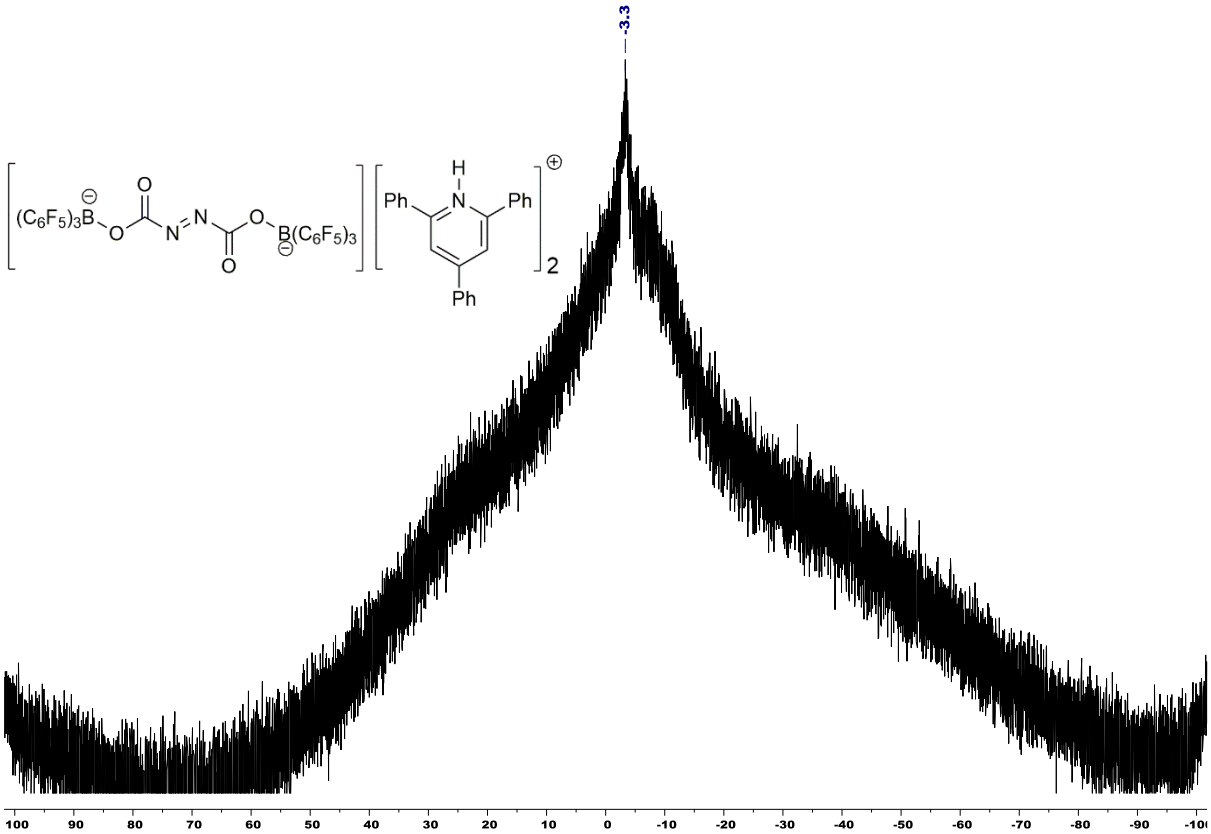


Figure S09. ^{11}B NMR (160 MHz, CD_3CN) spectrum of the compound **2**.

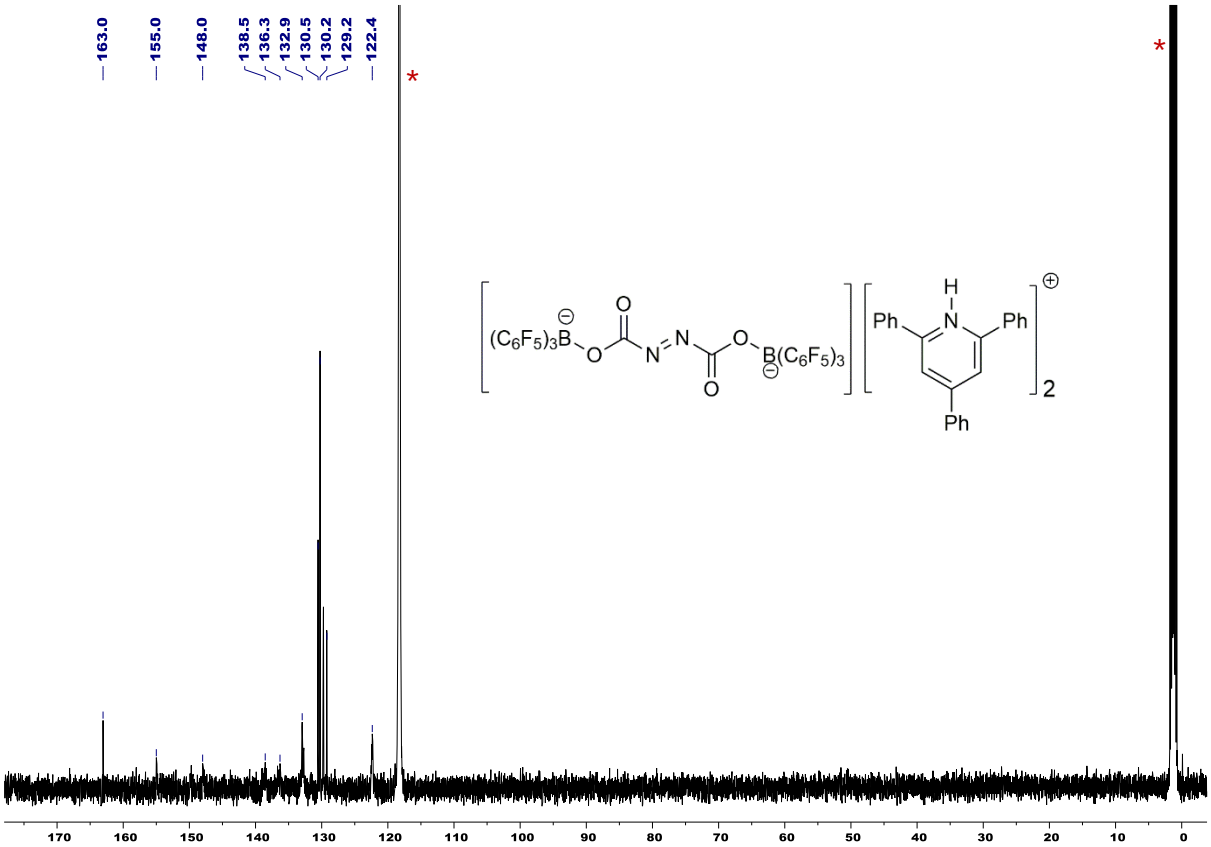


Figure S10. ^{13}C NMR (126 MHz, CD_3CN) spectrum of the compound **2** (*=CD_3CN).

Compound 3

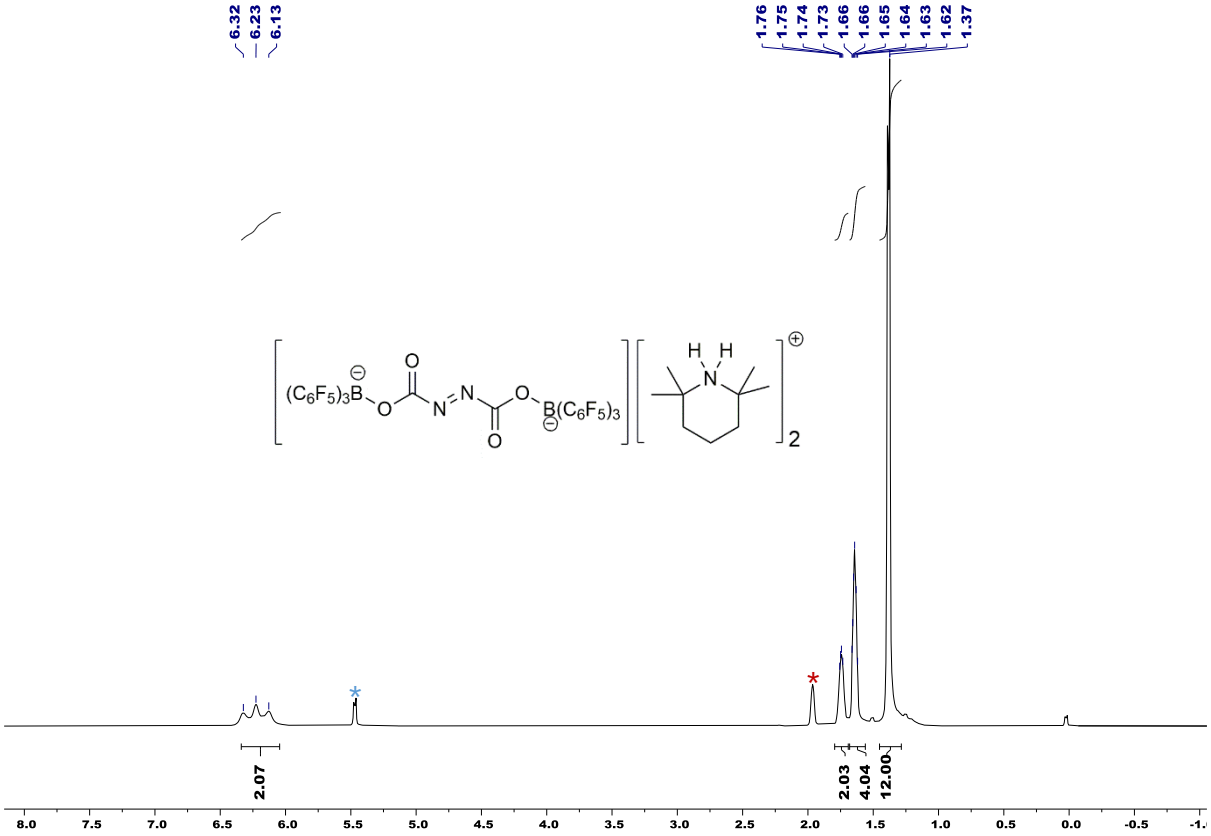


Figure S11. ^{1}H NMR (500 MHz, CD_3CN) spectrum of the compound **3** (*=CD_3CN, *=DCM).

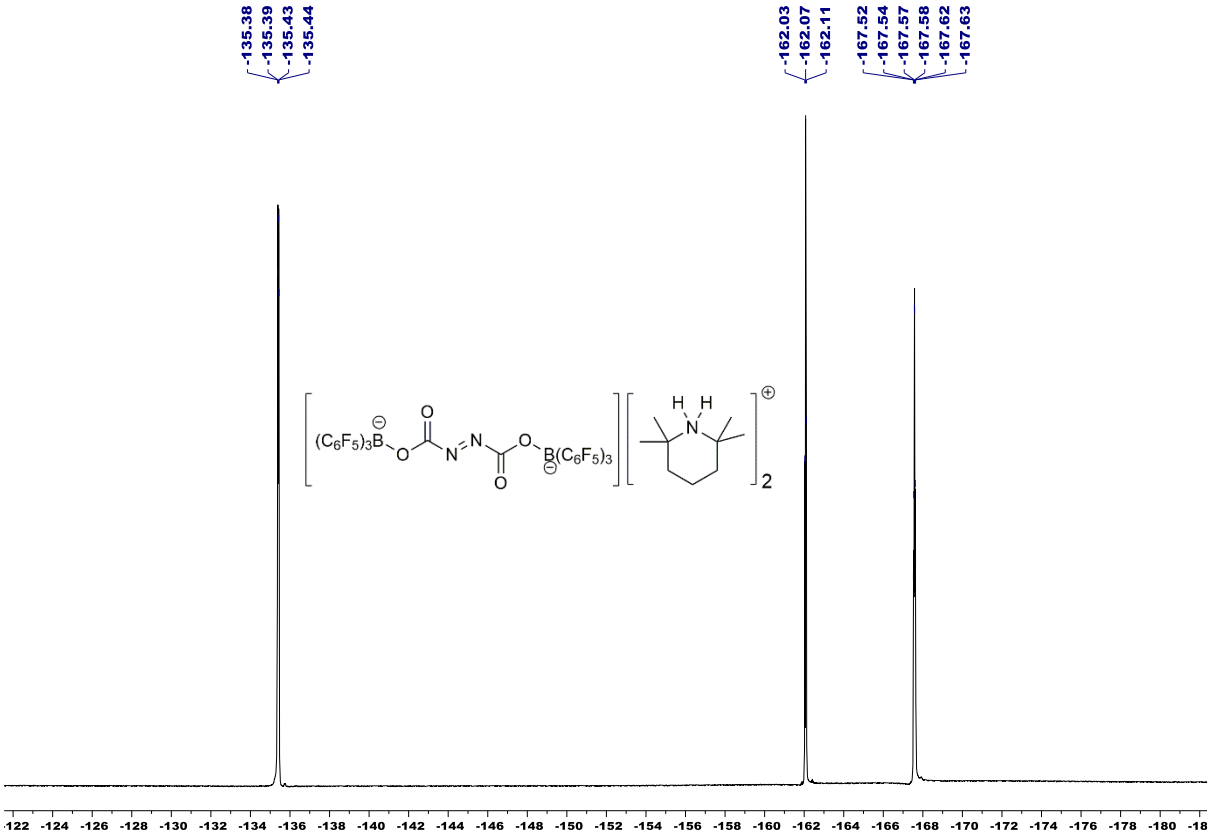


Figure S12. ^{19}F NMR (471 MHz, CD_3CN) spectrum of the compound **3**.

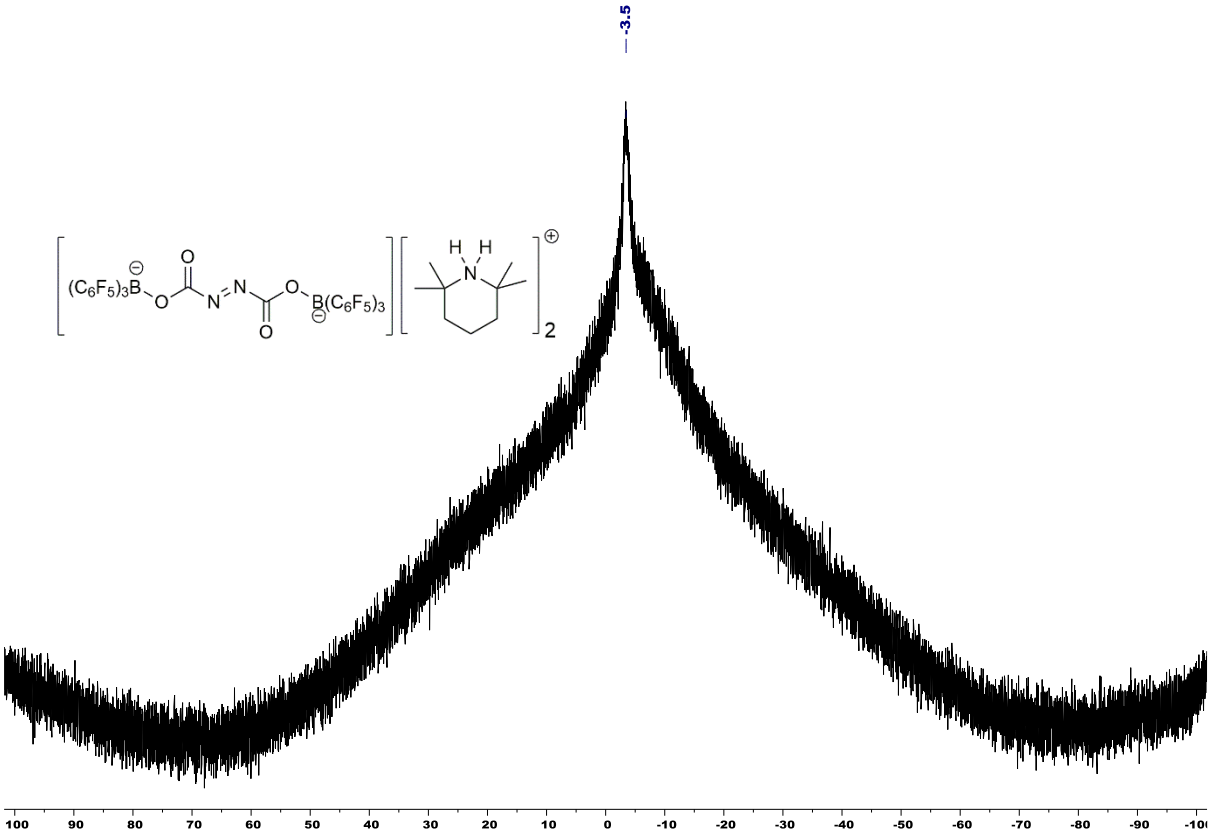


Figure S13. ^{11}B NMR (160 MHz, CD_3CN) spectrum of the compound **3**.

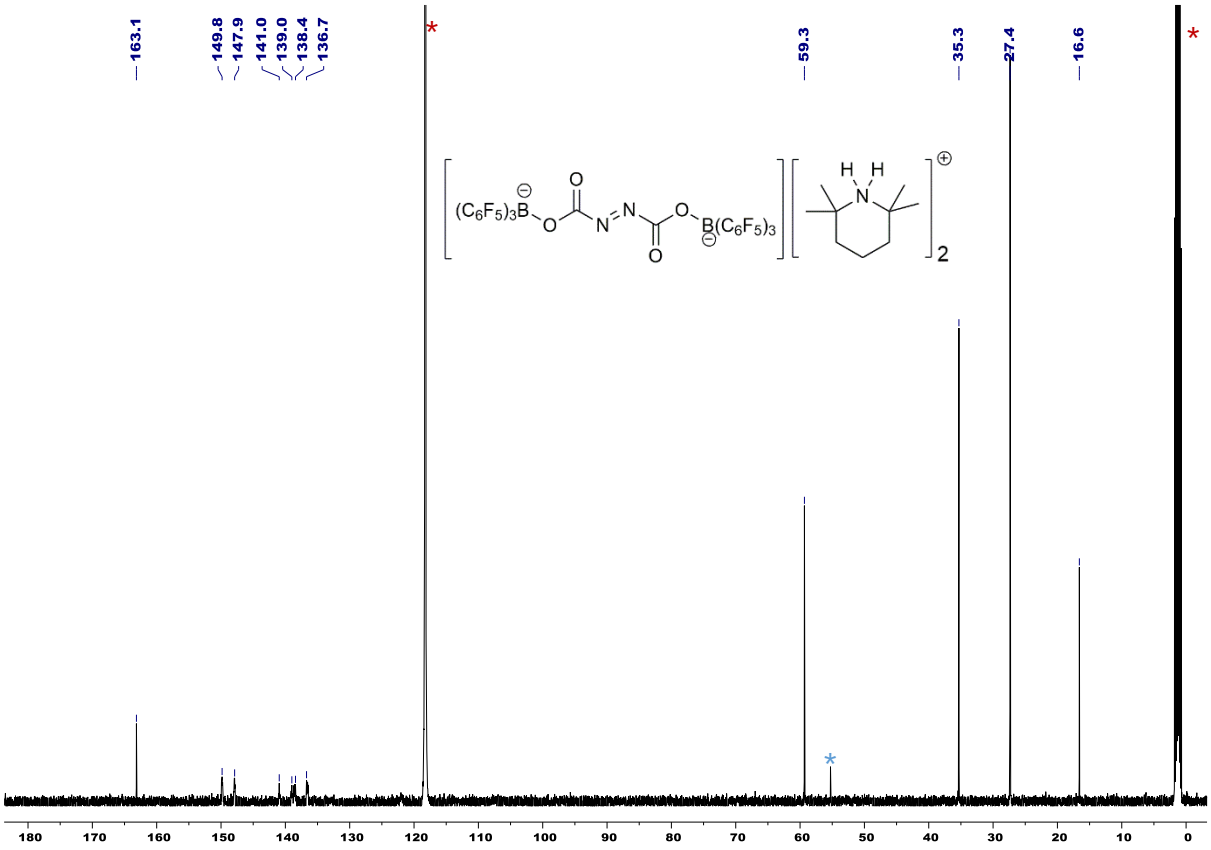


Figure S14. ^{13}C NMR (126 MHz, CD_3CN) spectrum of the compound **3** (*=CD_3CN, *=DCM).

Compound 4

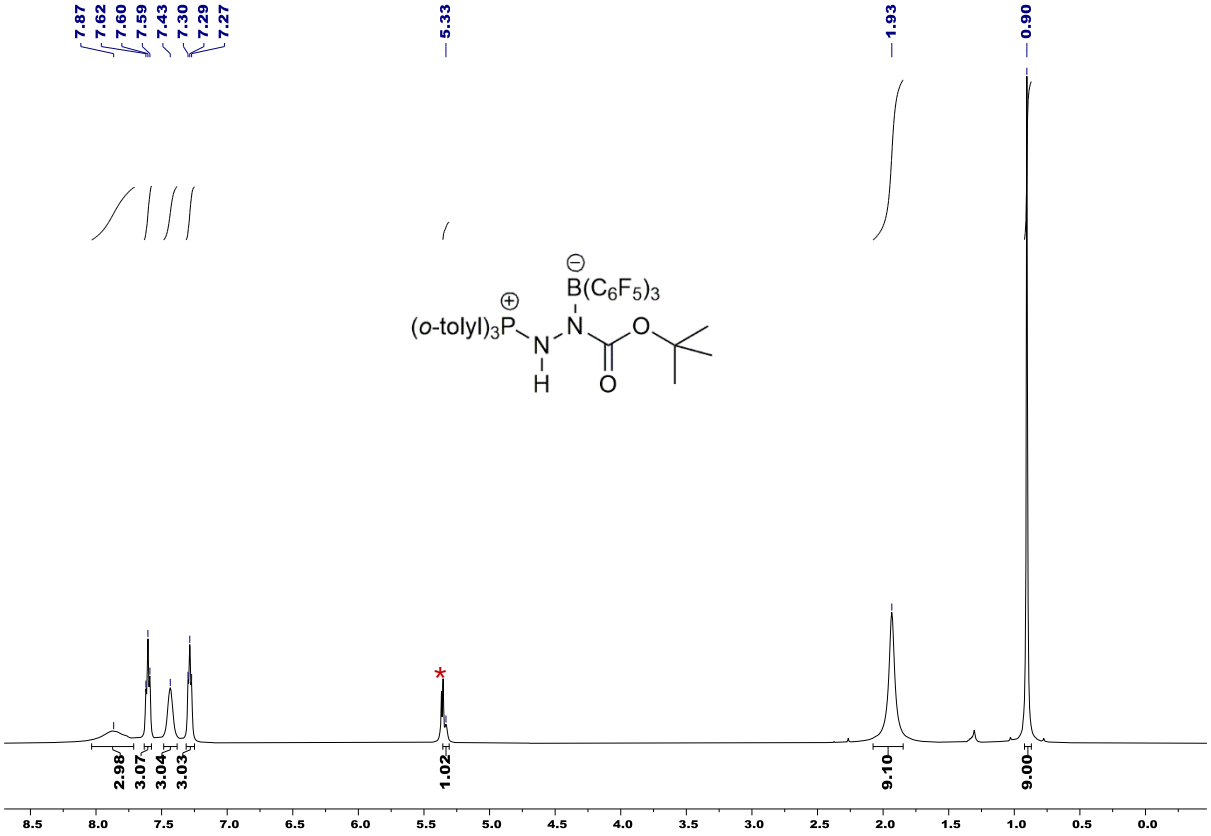


Figure S15. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of the compound **4** (*=CD_2Cl_2).

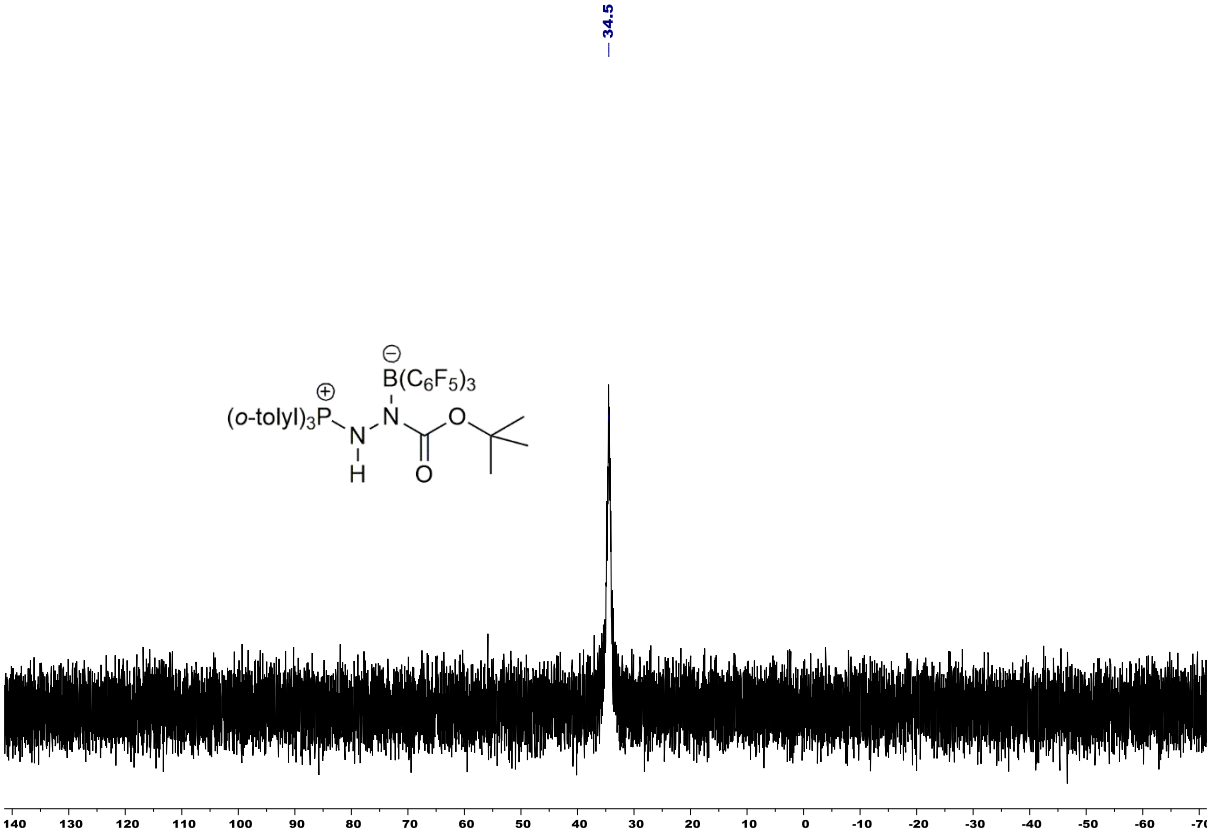


Figure S16. $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2) spectrum of the compound **4**.

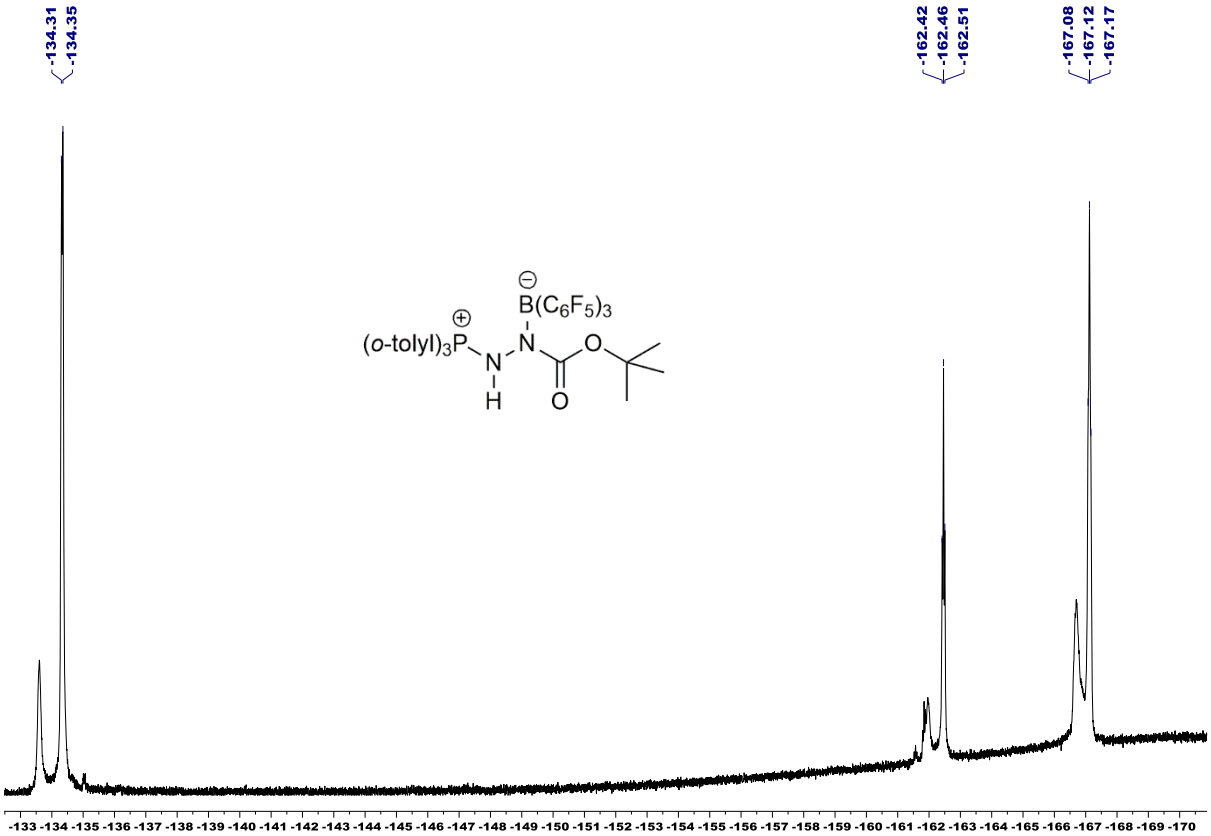


Figure S17. ^{19}F NMR (471 MHz, CD_2Cl_2) spectrum of the compound **4**.

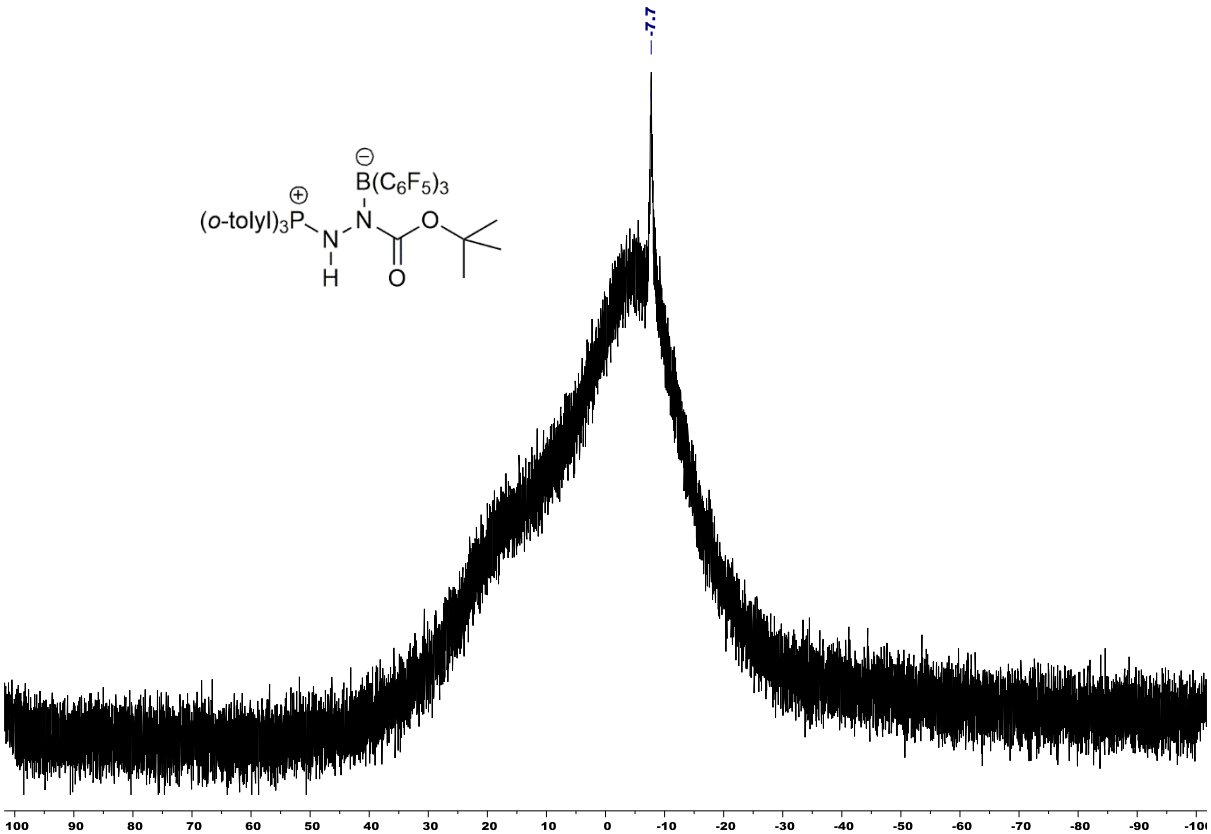


Figure S18. ^{11}B NMR (160 MHz, CD_2Cl_2) spectrum of the compound **4**.

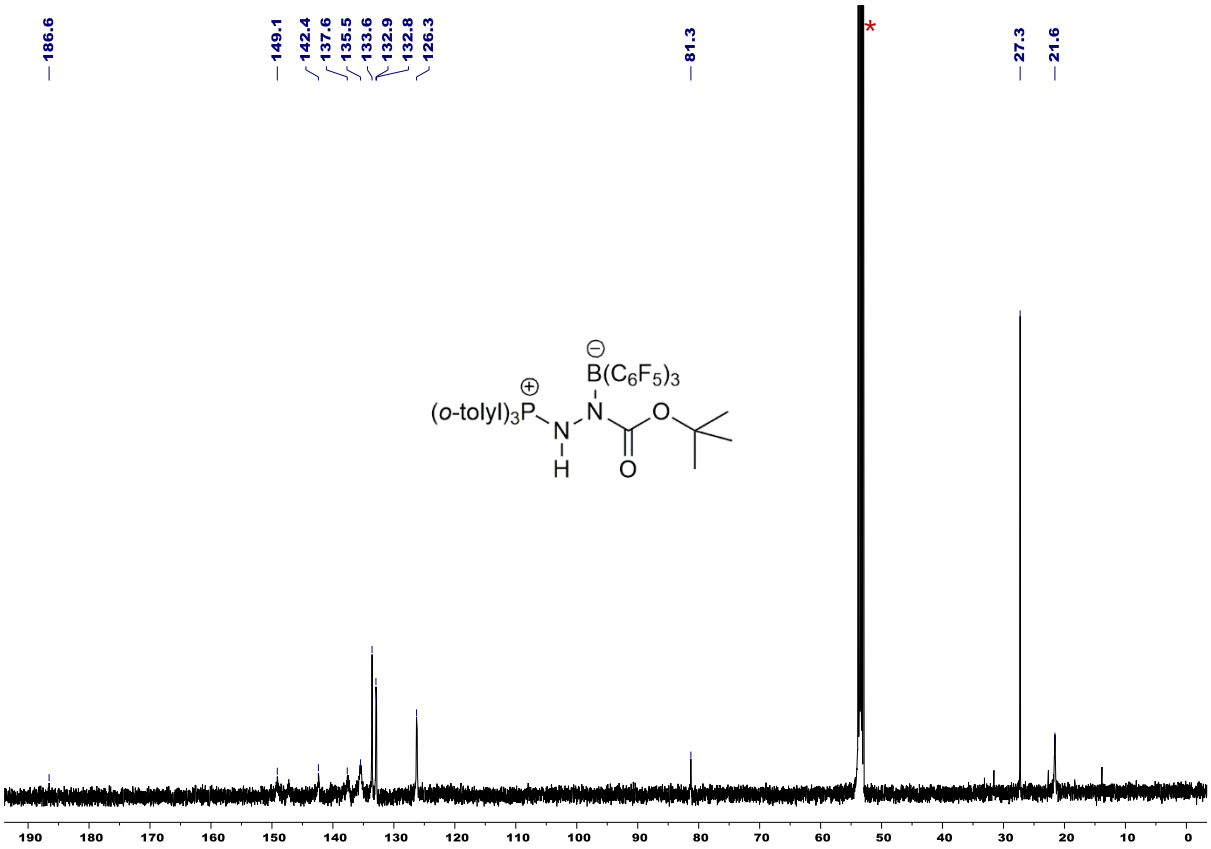


Figure S19. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of the compound **4** (*=CD_2Cl_2).

Compound 5

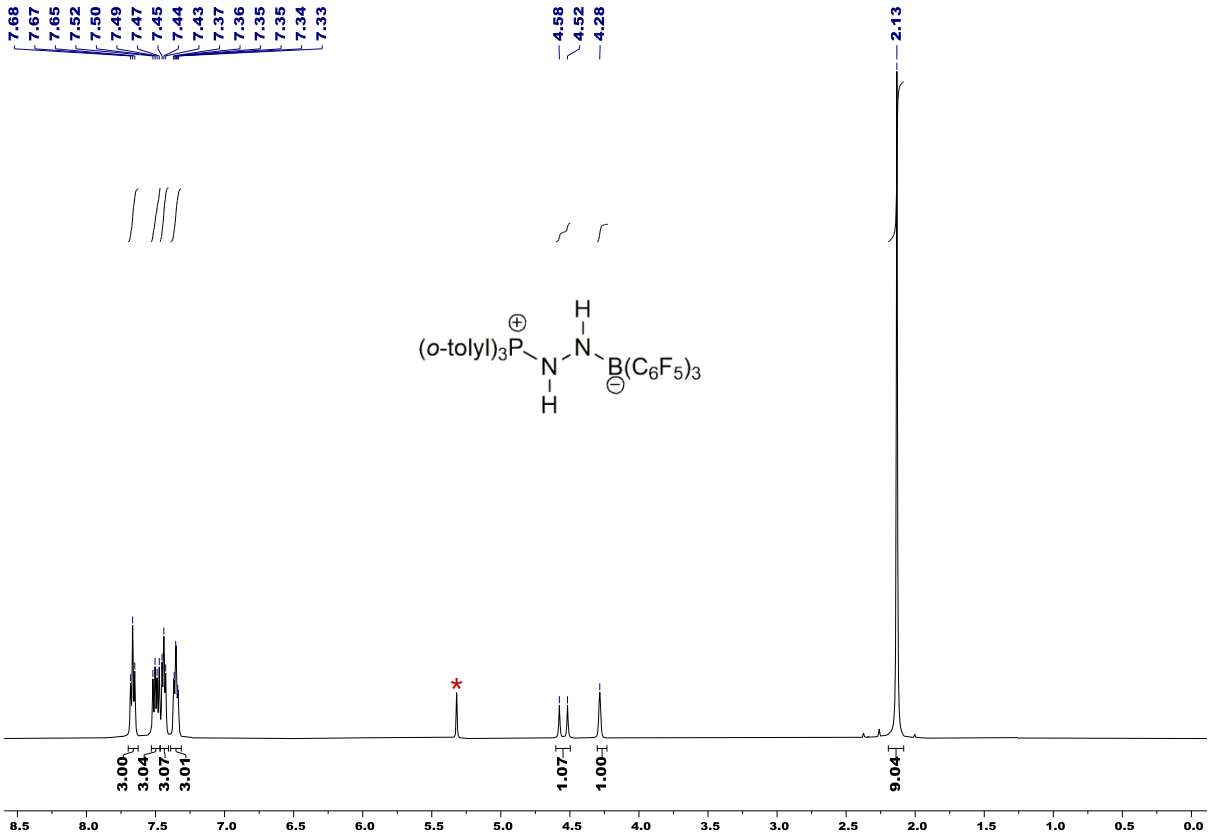


Figure S20. ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of the compound **5** (*=CD_2Cl_2).

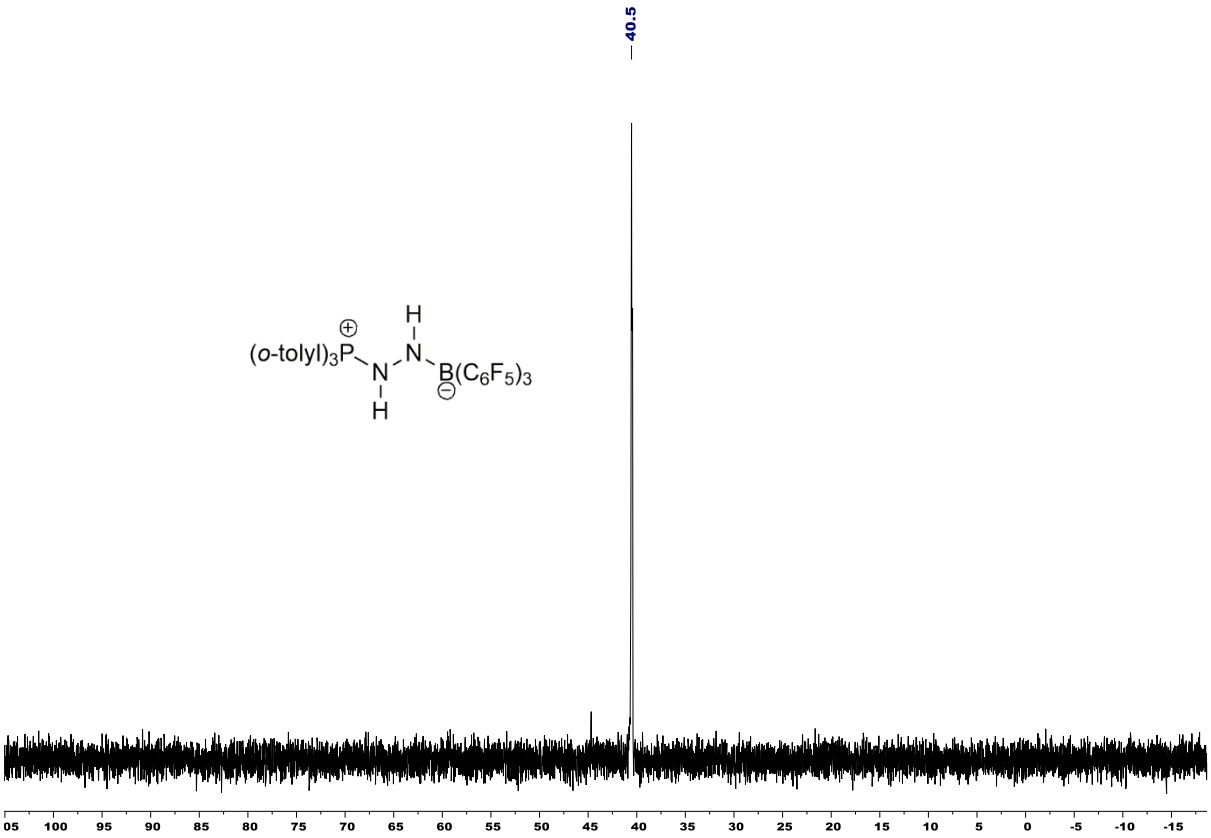


Figure S21. $^{31}P\{^{1}H\}$ NMR (202 MHz, CD_2Cl_2) spectrum of the compound **5**.

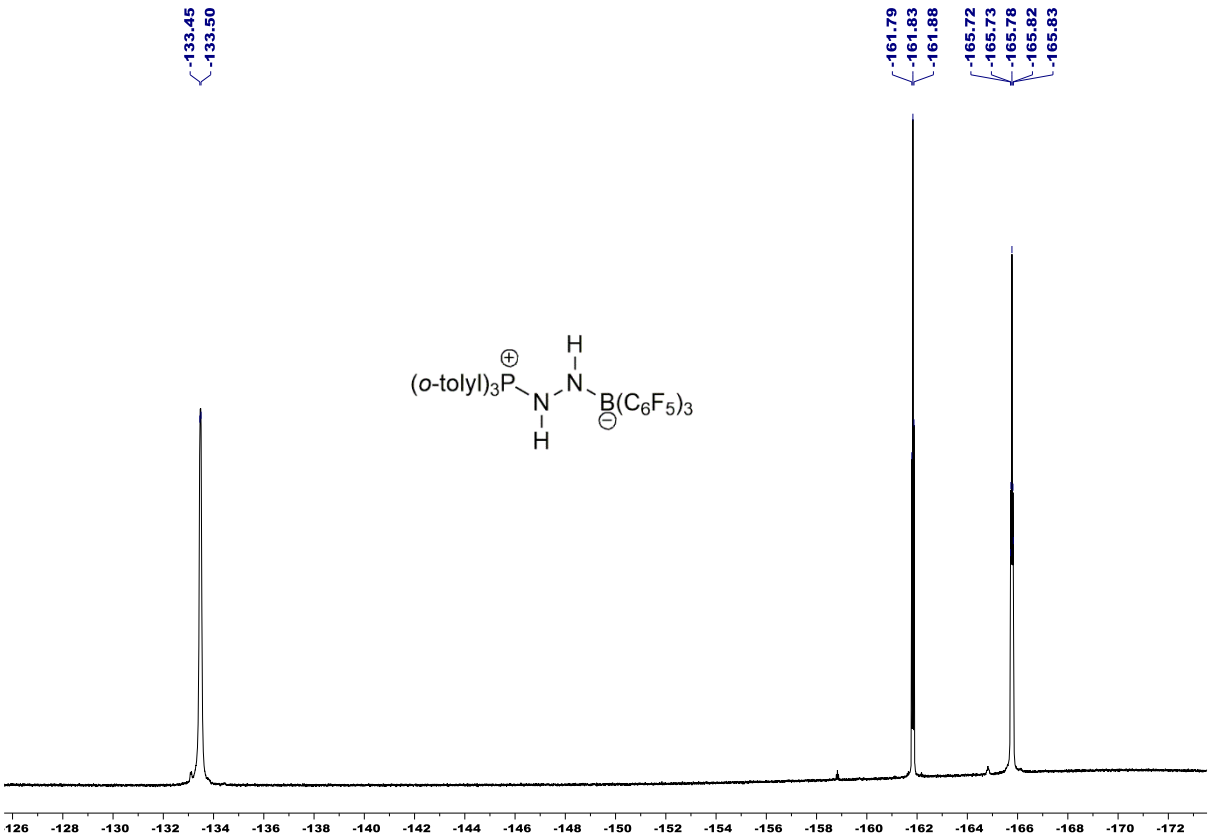


Figure S22. ^{19}F NMR (471 MHz, CD_2Cl_2) spectrum of the compound **5**.

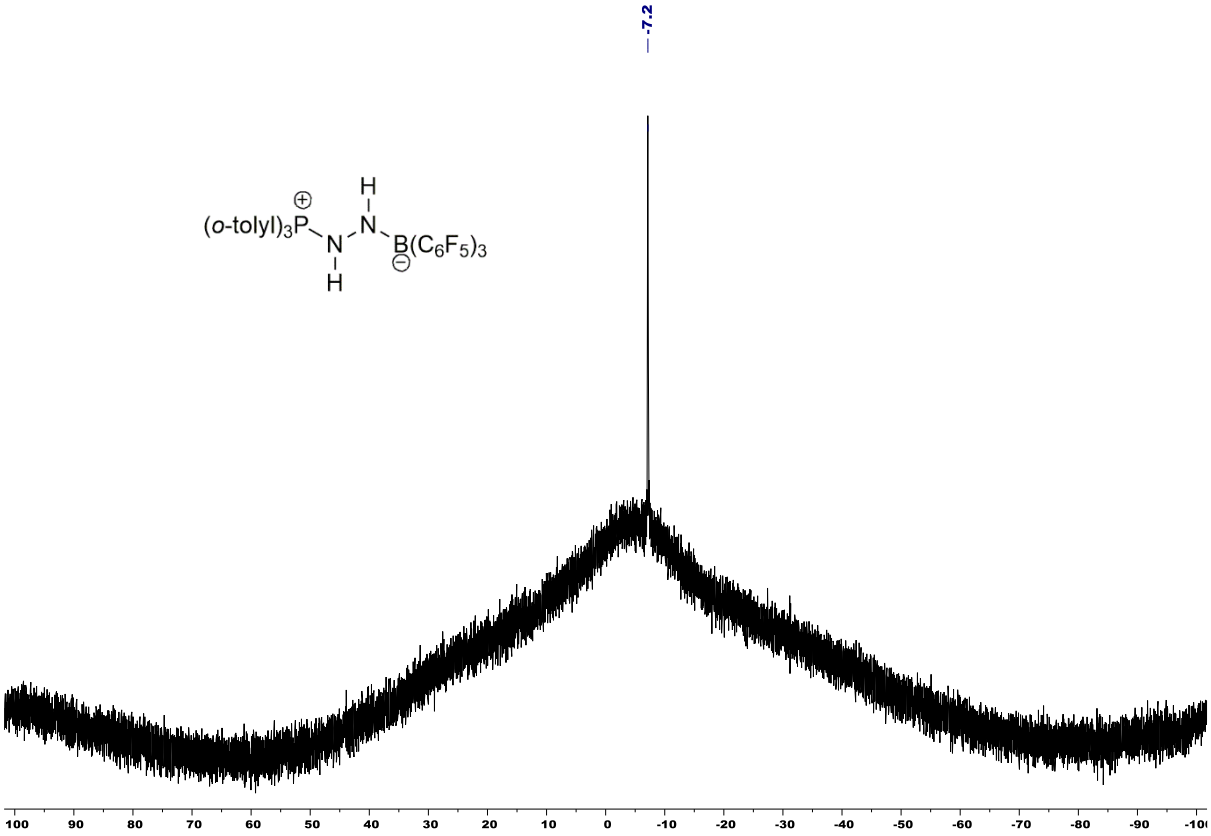


Figure S23. ^{11}B NMR (160 MHz, CD_2Cl_2) spectrum of the compound **5**.

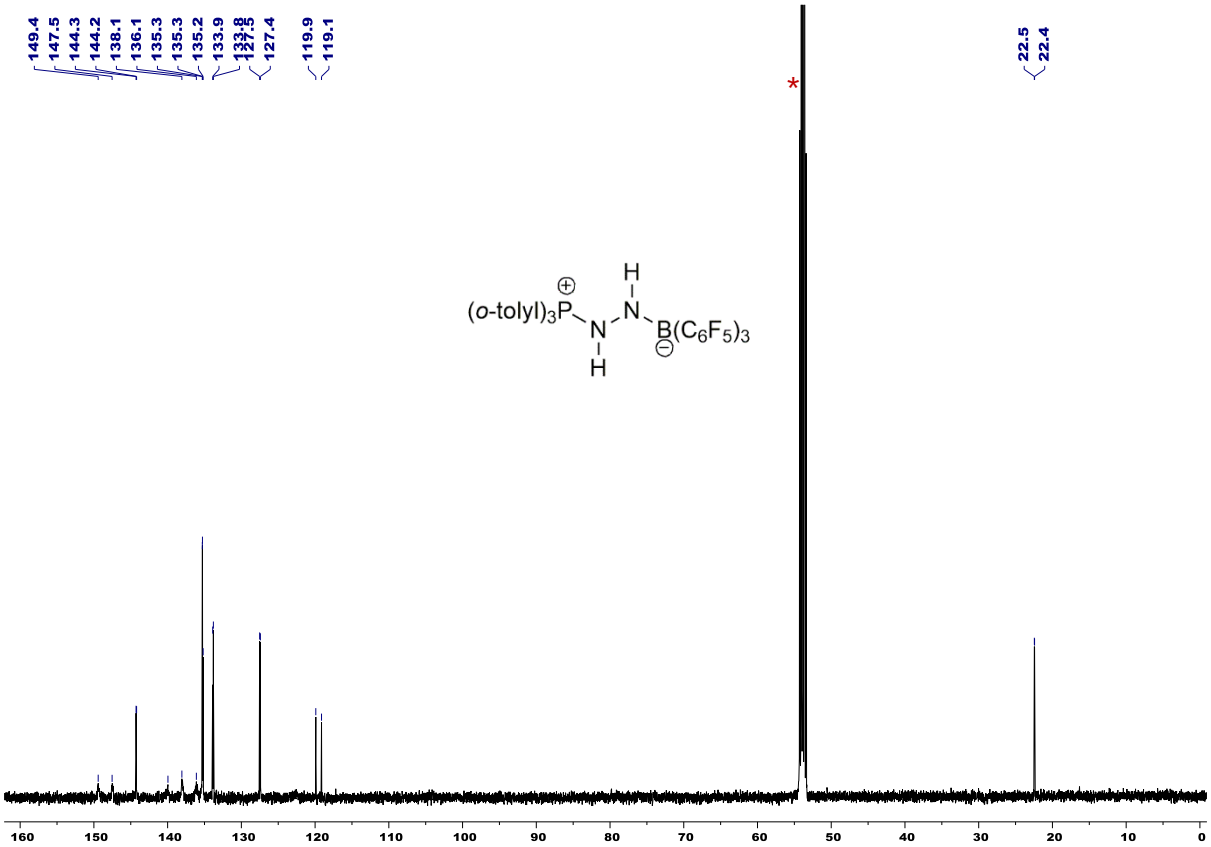


Figure S24. ^{13}C NMR (126 MHz, CD_2Cl_2) spectrum of the compound **5** (*=CD_2Cl_2).

HRESI-MS spectra of all compounds

Compound 1

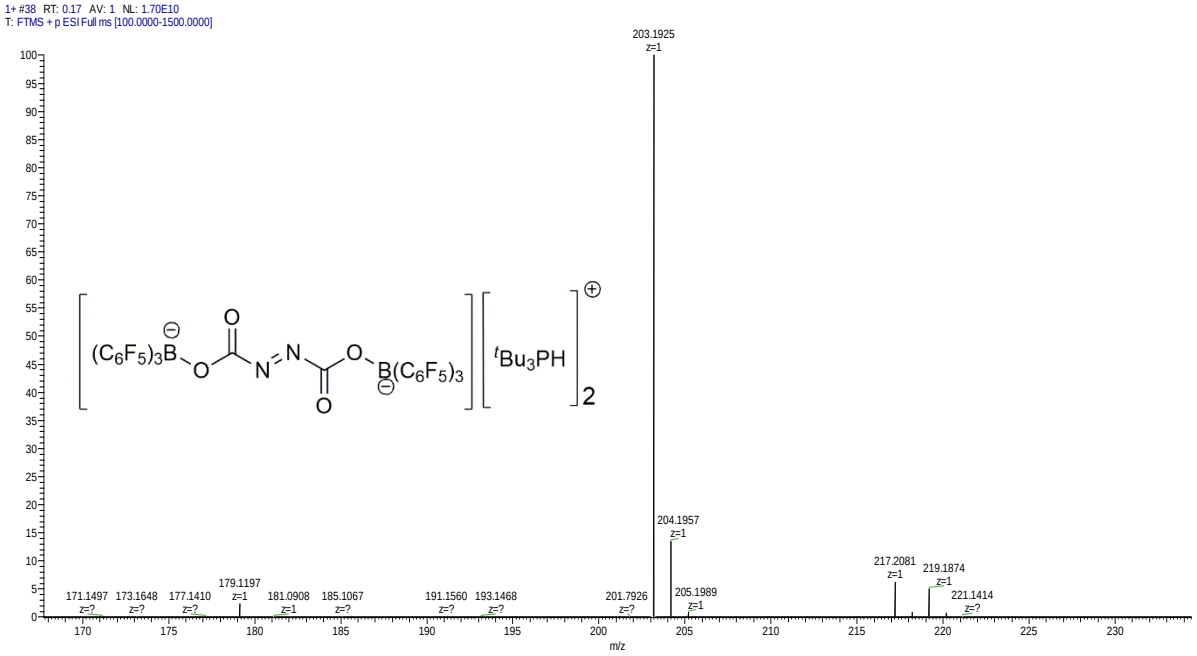


Figure S25. HRESI-MS (+ive mode) spectrum of the compound **1**.

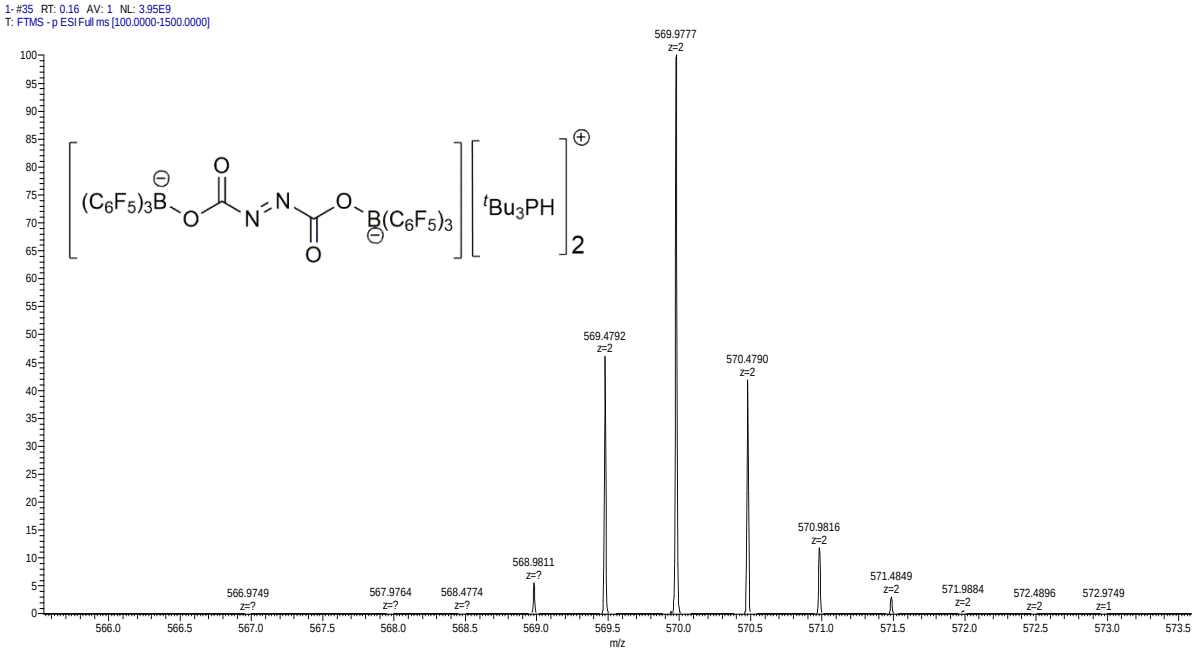


Figure S26. HRESI-MS (-ive mode) spectrum of the compound **1**.

Compound 2

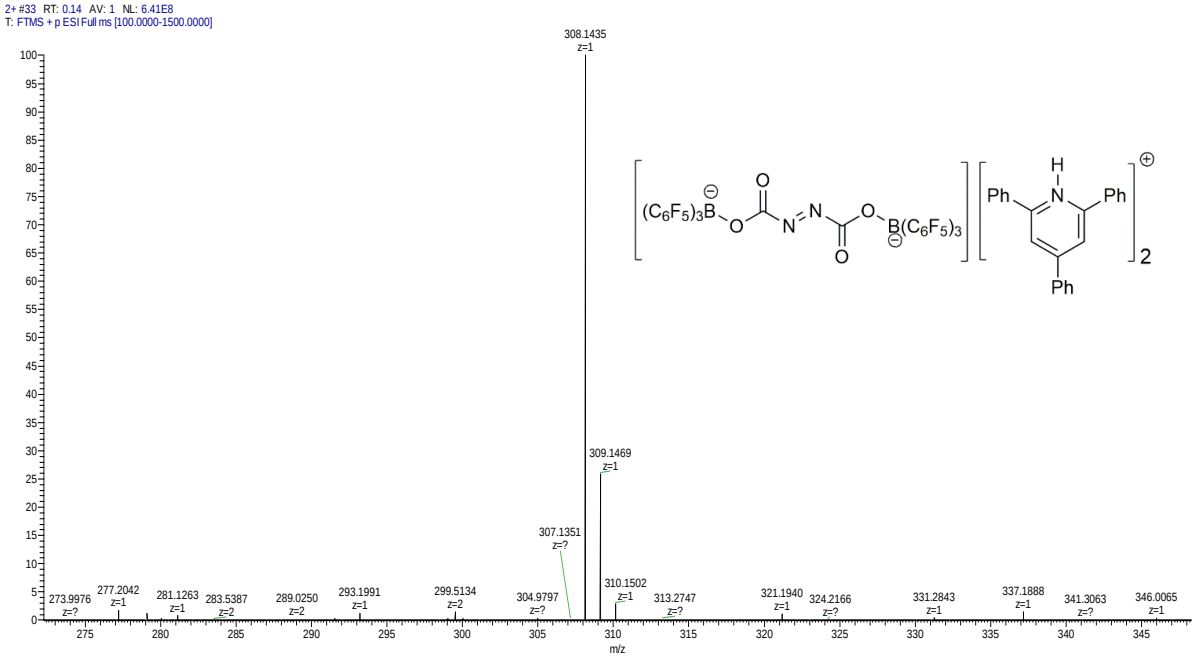


Figure S27. HRESI-MS (+ive mode) spectrum of the compound **2**.

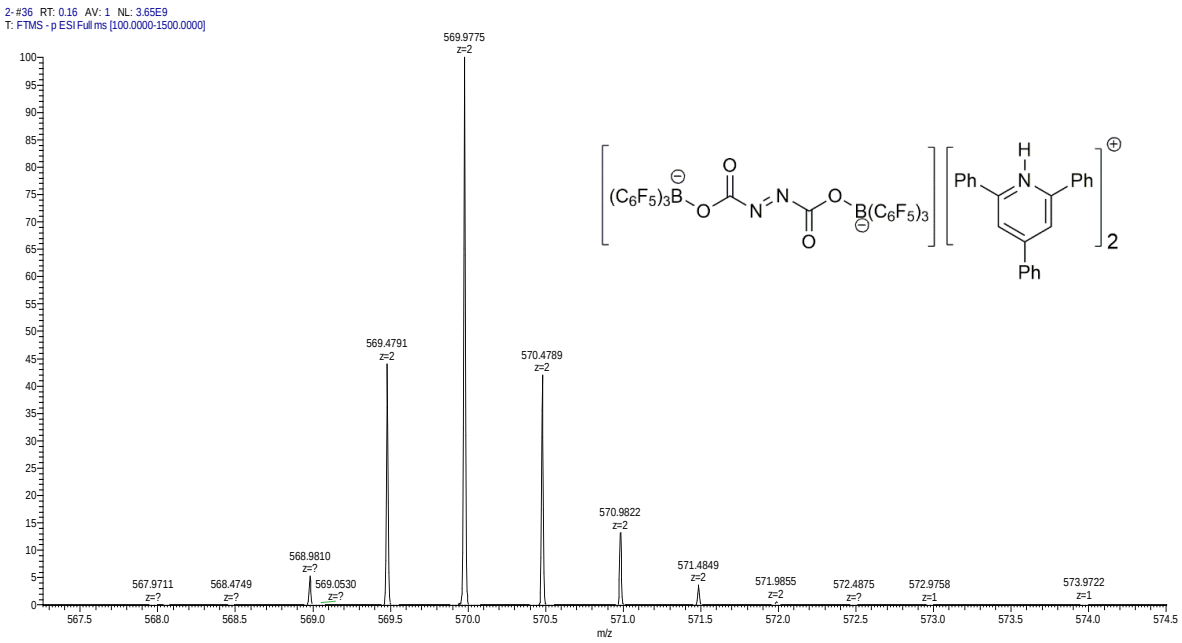


Figure S28. HRESI-MS (-ive mode) spectrum of the compound **2**.

Compound 3

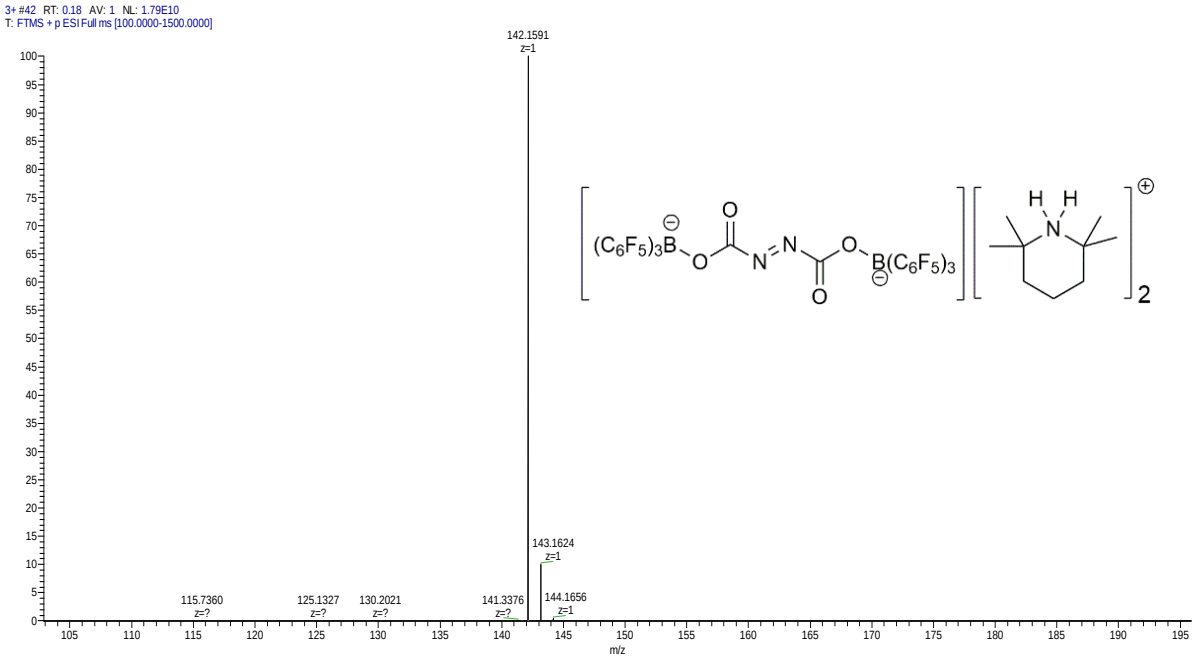


Figure S29. HRESI-MS (+ive mode) spectrum of the compound **3**.

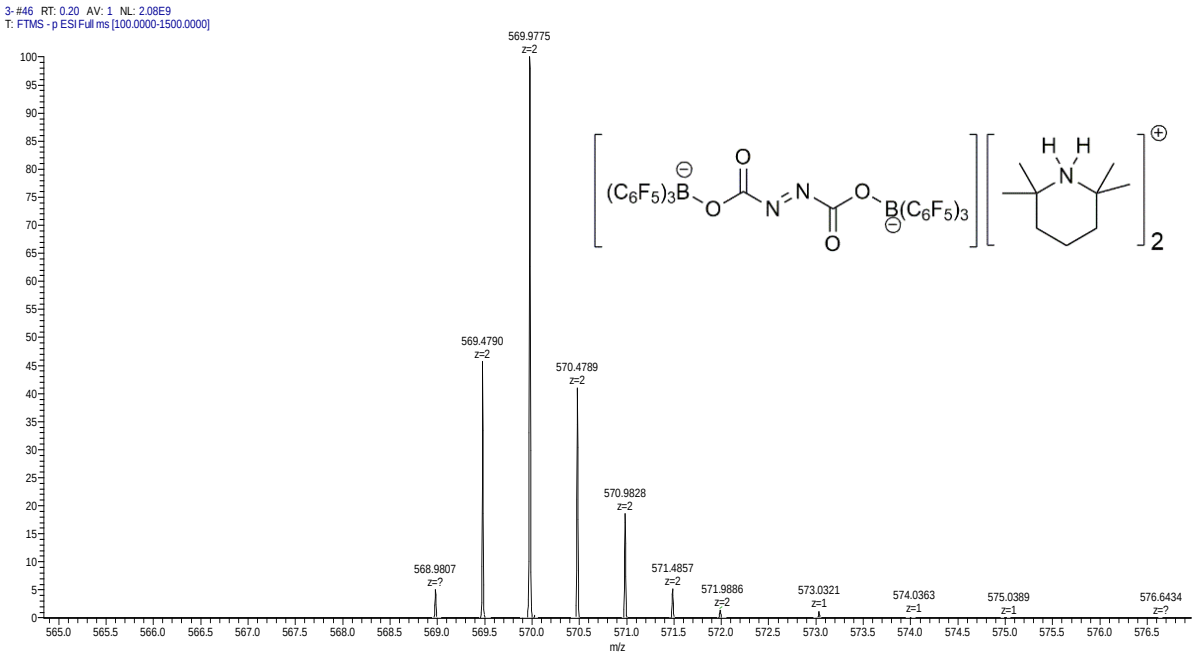


Figure S30. HRESI-MS (-ive mode) spectrum of the compound **3**.

Compound 4

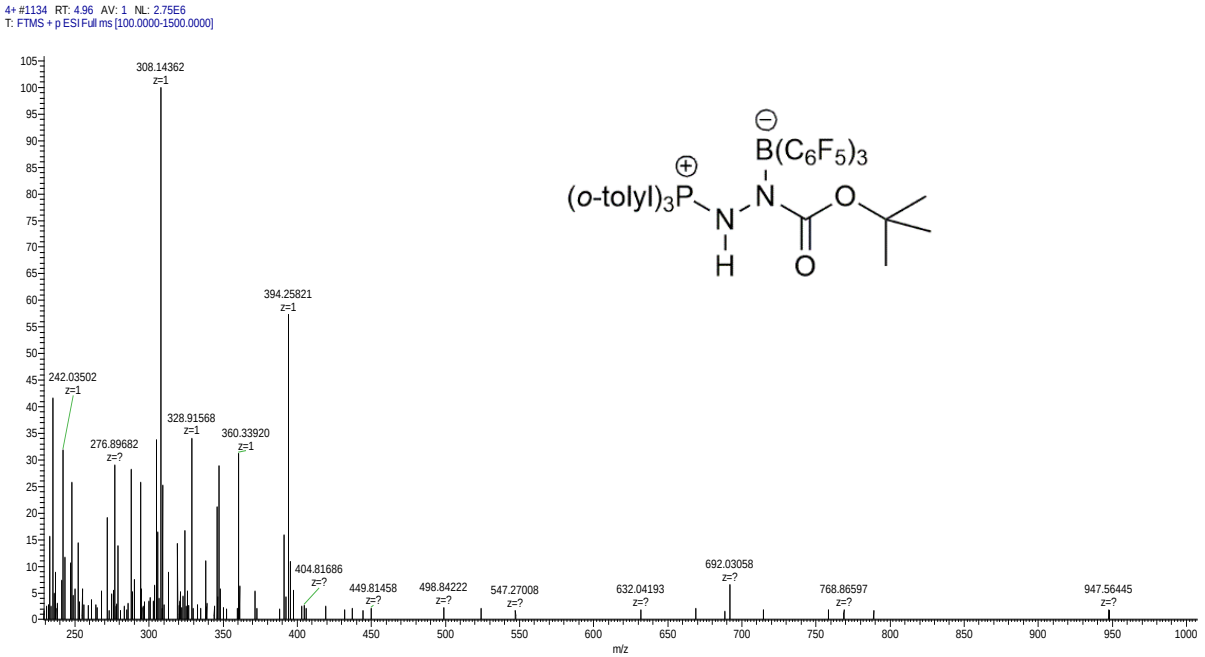


Figure S31. HRESI-MS (+ive mode) spectrum of the compound **4**.

Compound 5

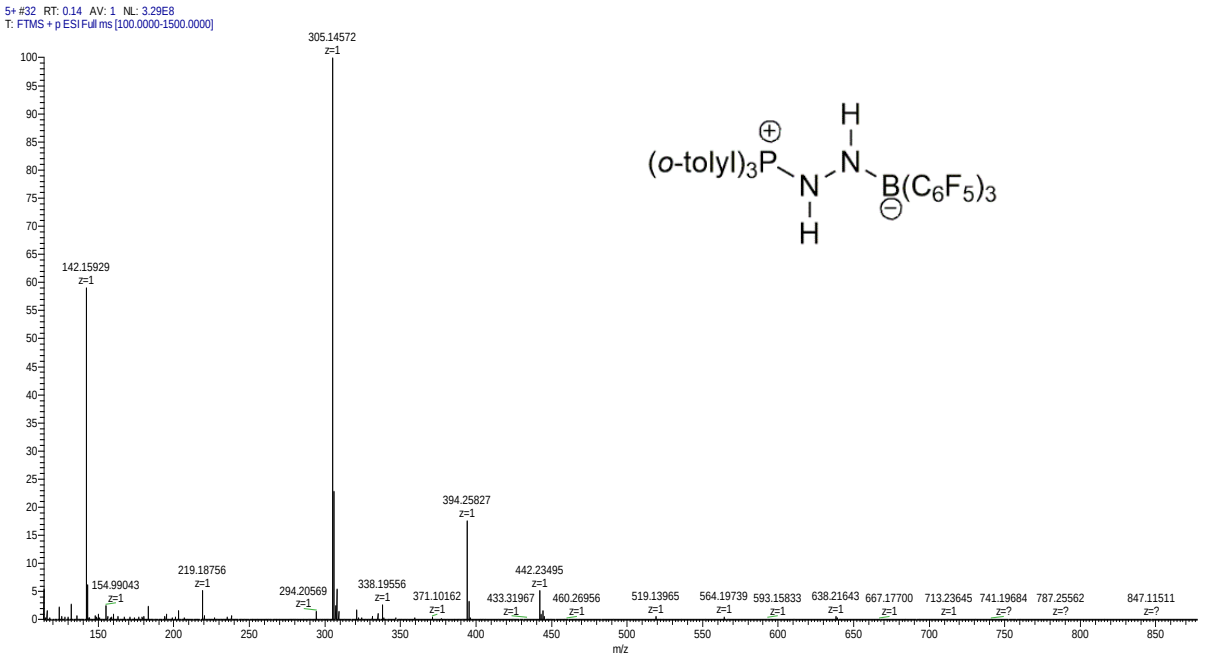


Figure S32. HRESI-MS (+ive mode) spectrum of the compound **5**.

Thermal ellipsoid plots

Compound 1

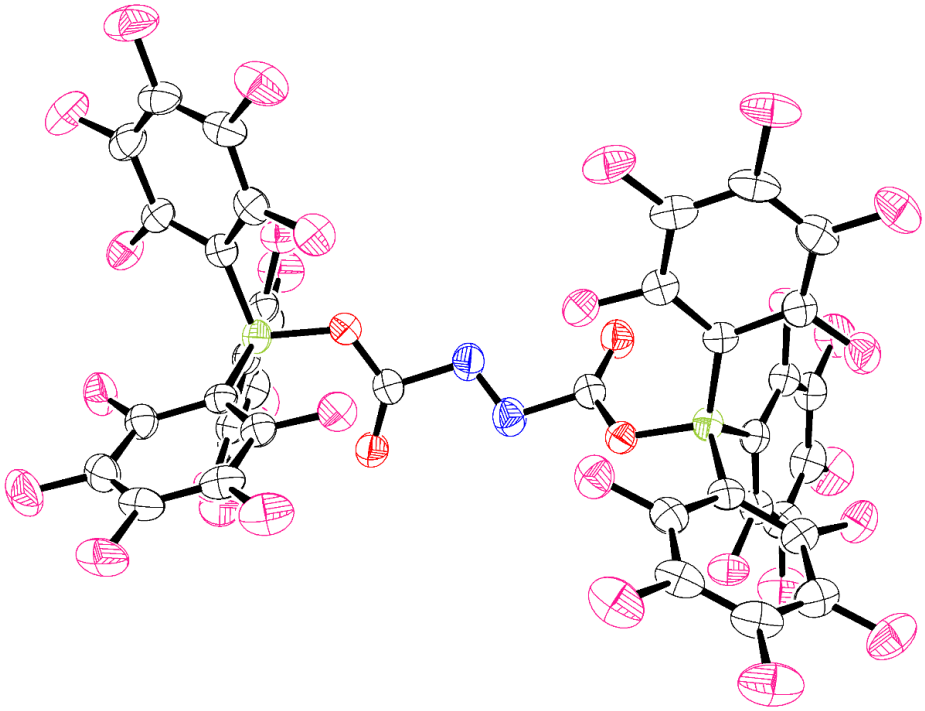


Figure S33. Thermal ellipsoid plot for **1** with the anisotropic displacement parameters depicted at the 50% probability level. Cation parts and hydrogen atoms are omitted for clarity.

Compound 4

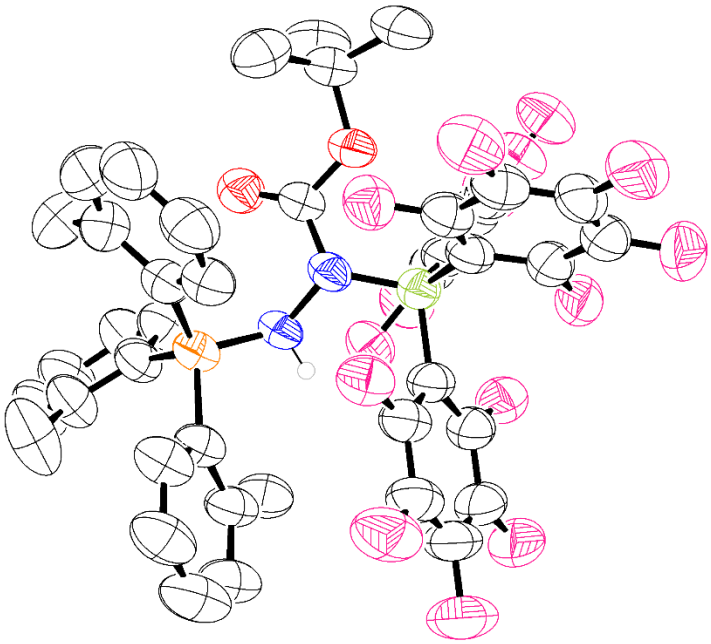


Figure S34. Thermal ellipsoid plot for **4** with the anisotropic displacement parameters depicted at the 50% probability level. Hydrogen atoms expect that linked to the N atoms are omitted for clarity.

Compound 5

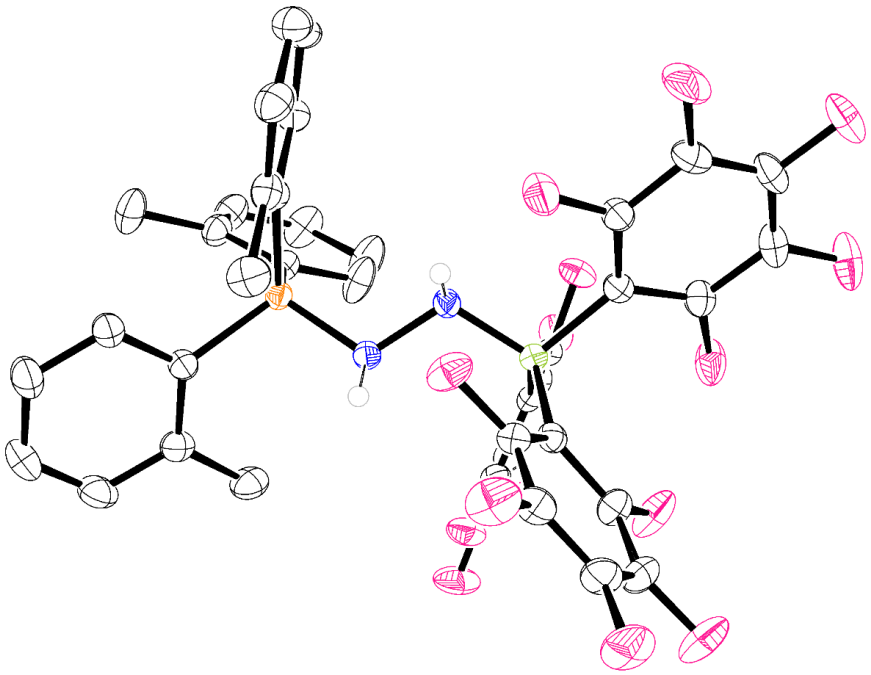


Figure S35. Thermal ellipsoid plot for **5** with the anisotropic displacement parameters depicted at the 50% probability level. Hydrogen atoms expect that linked to the N atoms are omitted for clarity.

Experimental references

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DFT computational details

Supporting information (DFT part)

Computational Details

The quantum chemical DFT calculations have been performed with the TURBOMOLE 7.4 suite of programs[1] The initial structures generated according to their Lewis structures are checked with the CREST method using the xTB program for low-lying conformers as input.[2] The structures are fully optimized at the TPSS-D3/def2-SVP + COSMO level of theory, which combines the TPSS meta-GGA density functional[3] with the BJ-damped DFT-D3 dispersion correction[4] and the def2-SVP basis set,[5] using the Conductor-like Screening Model (COSMO) continuum solvation model[6] for toluene solvent (dielectric constant ε = 2.38 and solvent radius R_{solv} = 3.48 Å). The density-fitting RI-J approach[5a, 7] is used to accelerate the geometry optimization and numerical harmonic frequency calculations[8] in solution. The optimized structures are characterized by frequency analysis to identify the nature of located stationary points (no imaginary frequency for true minima and only one imaginary frequency for transition state) and to provide thermal corrections (at 298.15 K and 1 atm) according to the modified ideal gas–rigid rotor–harmonic oscillator model.[9] This choice of dispersion-corrected meta-GGA functional makes the efficient exploration of all potential reaction paths possible.

The final solvation free energies in Toluene solution are computed with the COSMO-RS solvation model[10] (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm program package[[11] on the above TPSS-D3 optimized structures, and corrected by +1.89 kcal·mol^{-1} to account for higher reference solute concentration of 1 mol·L^{-1} usually used in solution. To check the effects of the chosen DFT functional on the reaction energies and barriers, single-point calculations at the meta-GGA TPSS-D3[3] and hybrid-meta-GGA PW6B95-D3[12] levels are performed using a larger def2-TZVP basis set.[5b, 13] The reaction energies from both DFT functionals are in good mutual agreement of -0.2 $\pm$ 2.2 kcal/mol (mean $\pm$ standard deviation), though as expected 2.5 $\pm$ 3.1 kcal/mol higher barriers are found at the PW6B95-D3 level. In our discussion, higher-level PW6B95-D3 Gibbs free energies (in kcal/mol, at 298.15 K and 1 mol/L concentration) are used unless specified otherwise. The applied DFT methods in combination with the large AO basis set provide usually accurate electronic energies leading to errors for chemical energies (including barriers) on the order of typically 1-2 kcal/mol. This has been tested thoroughly for the huge data base GMTKN55[14] which is the common standard in the field of DFT benchmarking.

References

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Table S1. TPSS-D3/def2-SVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in Toluene solution; TPSS-D3/def2-TZVP and PW6B95-D3/def2-TZVP single-point energies (TPSS-D3 and PW6B95-D3); the total PW6B95-D3 free energies G_P; the relative electronic energies (ΔE_T and ΔE_P) and Gibbs free energies (ΔG_T and ΔG_P) at the TPSS-D3 and PW6B95-D3 levels. See also main-text **Figures 3 and 6** for structures.

Reactions in Toluene	Im cm^{-1}	ZPE kcal /mol	Hc kcal /mol	Gc kcal /mol	Hsol kcal /mol	Gsol kcal /mol	TPSS-D3 E_h	PW6B95-D3 E_h	G_P E_h	ΔE_T kcal /mol	ΔE_P kcal /mol	ΔG_P kcal /mol	ΔG_T kcal /mol
*Unstable adduct of $B(C_6F_5)_3$ and reactant $(tBuO_2CN)_2$ (**R**) may lose CO_2 and alkene $CH_2{=}CMe_2$ (tBe) to form a new N-H bond*													
$B(C_6F_5)_3$ + **R**	0	268.93	300.30	207.32	-33.47	-23.82	-3012.26865	-3015.32754	-3015.02910	0.00	0.00	*0.00*	0.00
A	0	270.63	301.96	224.82	-26.95	-20.10	-3012.29353	-3015.35330	-3015.02404	-15.61	-16.17	*3.17*	3.73
*$(tBuO_2CN)_2$ (**R**) reacts easily with the $B(C_6F_5)_3$/TMP frustrated Lewis pair (FLP) via tBu group deprotonation*													
R + $B(C_6F_5)_3$ + TMP	0	435.84	474.78	352.59	-44.01	-30.76	-3421.67597	-3425.16327	-3424.64138	0.00	0.00	*0.00*	0.00
TS1	684i	432.86	473.21	378.00	-44.28	-34.78	-3421.68162	-3425.16448	-3424.61450	-3.55	-0.76	*16.87*	14.08
B$^{\boxplus}$ + $TMPH^+$ + tBe	0	435.63	475.17	353.58	-113.48	-98.50	-3421.59787	-3425.08892	-3424.67339	49.01	46.66	*-20.09*	-17.74
*..$TMPH^+$ cation is not bound to anion **B**$^{\boxplus}$ in solution*													
B$^{\boxplus}$ + $TMPH^+$	0	368.99	404.61	303.62	-108.58	-96.05	-3264.27809	-3267.60551	-3267.26870	0.00	0.00	*0.00*	0.00
B$^{\boxplus}$·$TMPH^+$	0	371.82	407.06	323.00	-36.74	-28.68	-3264.41225	-3267.73955	-3267.26752	-84.18	-84.12	*0.74*	0.67
*Further reaction with the $B(C_6F_5)_3$ / TMP FLP leads to the salt produc **3***													
B$^{\boxplus}$ + $B(C_6F_5)_3$	0	287.40	334.46	209.59	-72.74	-60.61	-5063.98669	-5069.13787	-5068.89444	0.00	0.00	*-20.09*	0.00
C$^{\boxplus}$	0	289.55	336.26	229.58	-59.98	-51.10	-5064.02193	-5069.17506	-5068.88762	-22.11	-23.33	*-15.81*	5.50
B$^{\boxplus}$ + $B(C_6F_5)_3$ + TMP	0	454.31	508.94	354.86	-83.27	-67.55	-5473.39400	-5478.97361	-5478.50672	0.00	0.00	*-20.09*	0.00
TS2$^{\boxplus}$	738i	452.46	508.02	383.17	-70.91	-60.34	-5473.41921	-5478.99567	-5478.47821	-15.82	-13.85	*-2.20*	15.92
D$^{\boxplus}$ + tBe	0	456.22	511.50	375.12	-70.77	-58.58	-5473.46101	-5479.04567	-5478.53520	-42.05	-45.22	*-37.96*	-14.70
*..now the $TMPH^+$ cation is 0.6 kcal/mol bound to the anion **D**$^{\boxplus}$*													
D$^{\boxplus}$ + $TMPH^+$	0	565.73	624.79	479.53	-118.48	-103.78	-5725.94307	-5731.78837	-5731.18356	0.00	0.00	*-37.96*	0.00
3	0	567.58	626.78	497.36	-50.93	-40.43	-5726.06959	-5731.91565	-5731.18448	-79.39	-79.87	*-38.54*	-0.10
$P(o\text{-Tol})_3/B(C_6F_5)_3$ is a true FLP													
$P(o\text{-Tol})_3$ + $B(C_6F_5)_3$	0	315.45	348.12	252.36	-38.96	-28.09	-3364.29595	-3367.69030	-3367.32688	0.00	0.00	*0.00*	0.00
$B(C_6F_5)_3$·$P(o\text{-Tol})_3$	0	317.44	350.07	270.83	-31.20	-23.93	-3364.32211	-3367.71600	-3367.31952	-16.42	-16.12	*4.62*	4.33
*Unstable adduct of $B(C_6F_5)_3$ and **R** may lose CO_2 and alkene tBe to form a new N-H bond*													
$B(C_6F_5)_3$ + **R**	0	268.93	300.30	207.32	-33.47	-23.82	-3012.26865	-3015.32754	-3015.02910	0.00	0.00	*0.00*	0.00

A	0	270.63	301.96	224.82	-26.95	-20.10	-3012.29353	-3015.35330	-3015.02404	-15.61	-16.17	*3.17*	3.73
TS3	806i	264.01	296.40	215.85	-34.94	-26.79	-3012.25049	-3015.30300	-3014.99869	11.40	15.40	*19.08*	15.08
E + CO_2 + tBe	0	267.19	299.09	196.55	-33.20	-21.75	-3012.29908	-3015.35736	-3015.06975	-19.09	-18.72	*-25.51*	-25.89
*..followed by trapping with weak base P(o-Tol)$_3$ to form the adduct **4***													
E + P(*o*-Tol)$_3$	0	414.25	453.50	344.45	-47.04	-34.37	-3821.06915	-3824.92223	-3824.42206	0.00	0.00	*-25.51*	0.00
TS4	0	414.68	454.66	360.87	-37.41	-28.61	-3821.08570	-3824.93210	-3824.39959	-10.39	-6.19	*-11.41*	9.91
4	0	416.30	455.37	364.43	-41.09	-32.33	-3821.12333	-3824.98638	-3824.45413	-34.00	-40.25	*-45.63*	-13.87
*..With Direct tBe elimination form ester group of **4** is kinetically slow over a sizeable barrier of 28.5 kcal/mol*													
4	0	416.30	455.37	364.43	-41.09	-32.33	-3821.12333	-3824.98638	-3824.45413	0.00	0.00	*0.00*	0.00
TS5a	432i	411.55	450.98	358.66	-41.61	-32.65	-3821.07759	-3824.93120	-3824.40865	28.70	34.63	*28.54*	22.61
F	0	413.65	453.14	347.87	-58.58	-38.68	-3821.09099	-3824.95569	-3824.45694	20.29	19.26	*-1.77*	-0.73
*B(C_6F_5)$_3$ catalyzed ester group decomposition of **4** is facile and exergonic to form carboxylic acid **F***													
4 + B(C_6F_5)$_3$	0	510.87	569.08	424.77	-57.85	-44.55	-6030.63377	-6036.74486	-6036.13293	0.00	0.00	*0.00*	0.00
4·Bf3	0	512.14	570.37	443.64	-49.89	-40.32	-6030.62853	-6036.74464	-6036.09890	3.29	0.14	*21.35*	24.50
TS5	53i	508.37	567.10	438.97	-56.24	-45.96	-6030.61075	-6036.72671	-6036.09741	14.45	11.39	*22.29*	25.34
TS5h	1188i	506.60	565.23	437.36	-52.82	-42.70	-6030.61805	-6036.73184	-6036.09991	9.86	8.17	*20.72*	22.41
F·B(C_6F_5)$_3$ + tBe	0	509.30	567.88	426.83	-58.05	-45.57	-6030.60927	-6036.72634	-6036.11275	15.37	11.62	*12.67*	16.42
F + tBe + B(C_6F_5)$_3$	0	508.22	566.86	408.20	-75.33	-50.90	-6030.60144	-6036.71417	-6036.13574	20.29	19.26	*-1.77*	-0.73
*..Further CO_2 release via intramolecular proton transfer is very facile to form **G***													
F	0	347.01	382.58	297.90	-53.68	-36.22	-3663.77121	-3667.47228	-3667.05224	0.00	0.00	*0.00*	0.00
TS6	1083i	344.82	380.02	295.91	-38.96	-30.45	-3663.77531	-3667.46997	-3667.04392	-2.57	1.45	*5.22*	1.20
G·CO_2	0	347.40	382.76	298.40	-39.51	-30.87	-3663.78201	-3667.47588	-3667.04653	-6.77	-2.26	*3.59*	-0.93
G + CO_2	0	346.05	382.16	285.15	-39.74	-28.64	-3663.78335	-3667.47700	-3667.06220	-7.62	-2.96	*-6.25*	-10.90
*..Intramolecular 1,2-H-shift is exergonic but kinetically unlikely due to very high barrier (**TS8**)*													
TS8 + CO_2	1731i	341.02	377.52	279.71	-40.51	-29.60	-3663.71151	-3667.40331	-3666.99872	37.46	43.28	*33.59*	27.77
5 + CO_2	0	345.28	381.51	284.25	-42.94	-31.50	-3663.78622	-3667.48267	-3667.07387	-9.41	-6.52	*-13.57*	-16.46
*..which however can be efficiently catalyzed by **F** via the carboxylic acid group (**TS7**)*													
G + **F**	0	685.89	755.31	588.88	-89.95	-64.07	-7138.85891	-7146.06574	-7145.22337	0.00	0.00	*0.00*	0.00
G.F	0	685.95	755.48	607.64	-59.59	-48.24	-7138.90038	-7146.10543	-7145.21095	-26.02	-24.91	*7.79*	6.67
TS7	1167i	683.93	753.25	605.92	-58.54	-47.27	-7138.89593	-7146.10025	-7145.20697	-23.23	-21.66	*10.29*	8.72
5 + **F**	0	685.12	754.66	587.98	-93.15	-66.93	-7138.86177	-7146.07141	-7145.23504	-1.80	-3.56	*-7.32*	-5.56

Table S2. TPSS-D3/def2-SVP + COSMO optimized Cartesian coordinates (in Å) in toluene solution. Each structure is labeled by a specific name (See also **Table S1** and main-text **Figures 3 and 6**), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list).

3 : salt product
136
Energy = -5719.553833172

N	0.3264325	-0.0652732	-0.0049500
N	-0.5472880	-0.8285769	0.4516872
C	1.5914208	0.0022133	0.6704332
O	2.5167430	-0.4821423	-0.0781463
O	1.7031181	0.6127435	1.7370952
C	-1.7448019	-0.7735284	-0.3839657
O	-2.8147517	-0.6333956	0.3176276
O	-1.6496179	-0.9094027	-1.6023581
B	4.0259556	-0.1703655	0.1541223
C	4.7949081	-0.9358802	-1.0737168
C	4.0383033	1.4696246	0.0358826
C	4.5532992	-0.8104689	1.5637385
C	4.4009935	-2.2263910	-1.4583322
C	5.8534464	-0.3934586	-1.8175889
C	3.6603312	2.0530010	-1.1848029
C	4.1670939	2.3764565	1.0954747
C	5.8461247	-0.4961512	2.0098061
C	3.8666352	-1.7389496	2.3580172
C	4.9484010	-2.9101613	-2.5514668
C	6.4527567	-1.0541452	-2.9000556
C	3.4194663	3.4184939	-1.3655184
C	3.9440718	3.7557402	0.9658824
C	6.4138175	-1.0038166	3.1836610
C	4.3948500	-2.2795623	3.5401755
C	5.9912646	-2.3215191	-3.2755954
C	3.5660594	4.2833503	-0.2734521
C	5.6740798	-1.9041666	3.9617499
F	3.4209872	-2.8716572	-0.7886310
F	6.3319952	0.8372365	-1.5412694
F	3.4757984	1.2737100	-2.2814658
F	4.4836696	1.9606977	2.3416595
F	6.6010368	0.3607343	1.2902812
F	2.6217366	-2.1659971	2.0328274
F	4.4723710	-4.1159166	-2.9114087
F	7.4537091	-0.4790342	-3.5859024
F	3.0349516	3.8987244	-2.5604357
F	4.0652491	4.5677387	2.0300879
F	7.6479068	-0.6437571	3.5680135
F	3.6751527	-3.1442112	4.2793023
F	6.5384236	-2.9613269	-4.3188281
F	3.3392282	5.5960125	-0.4122449
F	6.1884762	-2.4047531	5.0938492
B	-4.1662114	-0.3858023	-0.4265997
C	-5.2663999	-0.1983633	0.7719593
C	-4.1090926	1.0507993	-1.2253144
C	-4.3615884	-1.7109971	-1.3758282
C	-6.5359737	-0.7887223	0.8472686
C	-4.9632023	0.6752787	1.8253671
C	-3.1063371	2.0262974	-1.1491411
C	-5.2205524	1.4180577	-2.0006035
C	-4.5368783	-2.9691612	-0.7771892
C	-4.1572524	-1.7561005	-2.7613173
C	-7.4141029	-0.5834542	1.9231456
C	-5.7901990	0.8916191	2.9318312
C	-3.1642786	3.2544011	-1.8245571
C	-5.3303954	2.6306428	-2.6902603
C	-4.5438733	-4.1802461	-1.4834673
C	-4.1334769	-2.9389624	-3.5084213
C	-7.0369088	0.2568101	2.9784963
C	-4.2848828	3.5602401	-2.6024057
C	-4.3319114	-4.1662070	-2.8676530
F	-6.9789407	-1.6073297	-0.1270108
F	-3.8003230	1.3711833	1.8097666
F	-1.9716029	1.8277974	-0.4273749
F	-6.2535056	0.5558350	-2.1161117
F	-4.6810623	-3.0627304	0.5615214
F	-3.8854212	-0.6340193	-3.4760634
F	-8.6121916	-1.1868908	1.9513881
F	-5.3961451	1.7031168	3.9326482
F	-2.1356190	4.1167530	-1.7583933
F	-6.4142621	2.9108591	-3.4291012
F	-4.7277451	-5.3468401	-0.8473250
F	-3.8621118	-2.9000120	-4.8301064
F	-7.8597564	0.4512835	4.0175190
F	-4.3510173	4.7209506	-3.2689374
F	-4.3087648	-5.3089615	-3.5651216
N	0.6323917	1.3276952	4.1118887
C	1.4136998	0.5370689	5.1769706
C	-0.9005385	1.4438819	4.1768517
H	0.9188517	0.9852944	3.1527314
C	0.9136943	1.0134545	6.5537606
C	1.2292725	-0.9714651	4.9621877
C	2.8863265	0.9130985	4.9535599
C	-1.5590226	0.1175650	3.7748483
C	-1.2585018	2.5415425	3.1631119
C	-1.2662166	1.8714203	5.6107179
C	-0.6153522	0.9927646	6.6877057
H	1.2790814	2.0449238	6.7235028
H	1.3878067	0.3798087	7.3225339
H	0.2450004	-1.3334264	5.2905151
H	1.3755843	-1.2455329	3.9062070

H	1.9947542	-1.4997671	5.5515348
H	3.0398999	2.0048556	5.0326592
H	3.5037247	0.4277488	5.7264867
H	3.2356532	0.5828911	3.9630397
H	-1.1432128	-0.2765946	2.8335191
H	-1.4694123	-0.6532367	4.5528460
H	-2.6274681	0.3126947	3.6082108
H	-0.7340048	3.4853476	3.4003665
H	-1.0090934	2.2376997	2.1332398
H	-2.3416904	2.7294010	3.2034479
H	-0.9498498	2.9220523	5.7593490
H	-2.3664649	1.8574780	5.6947519
H	-0.9941793	-0.0429610	6.6215997
H	-0.9011822	1.3634506	7.6864555
H	0.9924120	2.2938322	4.1584209
N	-0.7296402	-0.5548007	-4.1172142
C	0.3644861	-1.6338564	-4.2576372
C	-0.4528432	0.9251246	-4.4499050
H	-1.0944937	-0.6132899	-3.1322366
C	1.0765620	-1.4174036	-5.6035867
C	1.3303180	-1.5612229	-3.0684042
C	-0.3961353	-2.9686475	-4.2214529
C	0.2835122	1.5868020	-3.2773326
C	-1.8410053	1.5583769	-4.6232448
C	0.3436556	0.9808870	-5.7669405
C	1.5460579	0.0300549	-5.7986787
H	0.3882846	-1.6921898	-6.4262956
H	1.9247470	-2.1217955	-5.6498495
H	2.0093073	-0.6988947	-3.1076968
H	0.7805607	-1.5177455	-2.1176621
H	1.9438280	-2.4754462	-3.0648903
H	-1.1542305	-3.0286030	-5.0224783
H	0.3166496	-3.7968032	-4.3623445
H	-0.8985046	-3.1054198	-3.2486119
H	-0.2322149	1.3982089	-2.3224601
H	1.3245348	1.2527413	-3.1804818
H	0.2992471	2.6754355	-3.4484155
H	-2.3934035	1.0910638	-5.4579636
H	-2.4398326	1.4556668	-3.7056480
H	-1.7267454	2.6313050	-4.8454988
H	-0.3358224	0.7269260	-6.6032904
H	0.6582377	2.0270882	-5.9211145
H	2.2818830	0.3077615	-5.0226731
H	2.0630015	0.1240921	-6.7683150
H	-1.5173117	-0.8503975	-4.7140278

4·$B(C_6F_5)_3$: unstable adduct of **4** and $B(C_6F_5)_3$

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Energy = -6024.069176836

N	-1.1742299	-0.2275020	0.7101061
N	-0.7485522	-1.2889432	-0.0310110
H	-0.7436778	-0.1919265	1.6339813
C	0.5480946	-1.3199384	-0.5761300
O	1.3742819	-0.4278734	-0.3084662
O	0.6802945	-2.3878883	-1.3388049
C	1.6387514	-2.6619930	-2.4986256
C	1.5241555	-1.4969692	-3.4764665
C	3.0378452	-2.8931273	-1.9529977
C	1.0875870	-3.9504120	-3.1060481
H	0.5183064	-1.4459301	-3.9190846
H	1.7482610	-0.5361771	-2.9957477
H	2.2507195	-1.6509713	-4.2911949
H	3.6906022	-3.1921239	-2.7897516
H	3.4673665	-1.9909647	-1.5061876
H	3.0273074	-3.7019443	-1.2067604
H	1.2103072	-4.7957944	-2.4129641
H	0.0267129	-3.8468842	-3.3775382
H	1.6628739	-4.1678873	-4.0209964
B	-2.0525521	0.9892153	0.2459767
C	-3.3102953	1.2476633	1.3069193
C	-1.1928021	2.4122671	0.4361344
C	-2.5552511	0.7725421	-1.3215441
C	-3.5285704	0.5890248	2.5251224
C	-4.1917815	2.3161086	1.0685539
C	-0.7033682	2.6985575	1.7200099
C	-1.0469327	3.4649602	-0.4772088
C	-1.6052639	0.7386361	-2.3539558
C	-3.8759939	0.6819730	-1.7949009
C	-4.5874346	0.8918188	3.3935096
F	-2.7337887	-0.4250612	2.9456255
C	-5.2584423	2.6644502	1.9032271
F	-4.0448181	3.0613052	-0.0518968
C	-0.1387312	3.9190179	2.0991296
F	-0.8202223	1.7665054	2.7064721
C	-0.4258403	4.6845648	-0.1668572
F	-1.5111638	3.3706847	-1.7427466
C	-1.8949697	0.6569481	-3.7176052
F	-0.2903866	0.7800426	-2.0472123
C	-4.2285782	0.5766538	-3.1503008
F	-4.9349336	0.6665893	-0.9535210
C	-5.4616025	1.9367710	3.0833847
F	-4.7751291	0.1703021	4.5139641
F	-6.0784334	3.6825624	1.5935029
C	0.0393074	4.9137136	1.1308462
F	0.2253625	4.1520204	3.3737717
F	-0.2789446	5.6326819	-1.1060170
C	-3.2284870	0.5604597	-4.1243147
F	-0.9068472	0.5868966	-4.6296319
F	-5.5155249	0.4637553	-3.5095091
F	-6.4805941	2.2386959	3.9019834
F	0.6288809	6.0729061	1.4540307
F	-3.5331613	0.4073490	-5.4199608
P	-1.5854473	-2.9175456	0.0705156
C	-2.2585178	-3.3716705	-1.5603003

C	-3.0734502	-2.7160520	1.0897051
C	-0.4145213	-4.1483052	0.6858271
C	-2.0111666	-2.5135779	-2.6464617
C	-3.1272448	-4.4889222	-1.7071851
C	-3.4600172	-3.4519250	2.2485099
C	-3.9778370	-1.8043700	0.4989823
C	-0.1223226	-5.2634710	-0.1291746
C	0.2238516	-3.9731343	1.9403329
C	-2.5877981	-2.7517726	-3.8972001
H	-1.3632738	-1.6518927	-2.5000866
C	-3.6756170	-4.7173374	-2.9842922
C	-3.5299917	-5.3997716	-0.5719191
C	-4.7193199	-3.1466985	2.8028202
C	-2.6942952	-4.5699626	2.9186420
C	-5.2283406	-1.5486843	1.0608667
H	-3.6904840	-1.2955078	-0.4225347
C	0.8003013	-6.2216949	0.2943998
H	-0.6229011	-5.3724147	-1.0949939
C	1.1483646	-4.9557917	2.3387507
C	-0.0149118	-2.7842025	2.8350046
C	-3.4184569	-3.8669734	-4.0664216
H	-2.3886120	-2.0722892	-4.7306187
H	-4.3333627	-5.5823697	-3.1214319
H	-4.4202319	-4.9942485	-0.0575731
H	-3.7868988	-6.4005186	-0.9547942
H	-2.7398550	-5.5172041	0.1852657
C	-5.5886260	-2.2080162	2.2409657
H	-5.0297733	-3.6943890	3.6989200
H	-3.4100130	-5.2661053	3.3840178
H	-2.0619308	-5.1423590	2.2273563
H	-2.0463281	-4.1860273	3.7241664
H	-5.8957856	-0.8279061	0.5854389
C	1.4400772	-6.0613050	1.5338474
H	1.0212556	-7.0856768	-0.3393970
H	1.6624735	-4.8332555	3.2971288
H	-0.1159600	-3.1033798	3.8851190
H	0.8481179	-2.1054452	2.7866879
H	-0.9145359	-2.2056833	2.5689463
H	-3.8729711	-4.0731164	-5.0404585
H	-6.5550660	-2.0090791	2.7141480
H	2.1731420	-6.8001564	1.8724640
B	2.8293145	0.3122114	-0.1222275
C	3.1731243	0.8996483	-1.5980283
C	2.6488469	1.4379122	1.0503622
C	3.9150116	-0.7317078	0.5227115
C	2.3761469	1.9347454	-2.1197452
C	4.1682292	0.4340871	-2.4716822
C	2.1398473	1.0594905	2.3006175
C	3.2251799	2.7194645	1.0251628
C	3.6641329	-1.9921123	1.0724569
C	5.2279409	-0.2652553	0.7132699
C	2.4716398	2.4142279	-3.4297227
F	1.4593657	2.5242749	-1.3364563
C	4.3176944	0.8954323	-3.7873598
F	5.0368784	-0.5346223	-2.1015594
C	2.1966085	1.8425661	3.4554638
F	1.5811192	-0.1706401	2.4419699
C	3.2937316	3.5529673	2.1518698
F	3.7908573	3.2150137	-0.0923971
C	4.6292530	-2.7670663	1.7286896
F	2.4401135	-2.5627251	0.9603171
C	6.2294987	-0.9975821	1.3600939
F	5.5704296	0.9542115	0.2516355
C	3.4572816	1.8857464	-4.2738021
F	1.6591647	3.3829542	-3.8678692
F	5.2686115	0.3842383	-4.5844124
C	2.7964087	3.1053272	3.3797643
F	1.6841905	1.4049717	4.6132863
F	3.8480334	4.7702196	2.0614102
C	5.9248750	-2.2634425	1.8798489
F	4.3152250	-3.9824369	2.2110735
F	7.4658016	-0.4999535	1.4962939
F	3.5809671	2.3287260	-5.5293059
F	2.8637277	3.8867859	4.4610532
F	6.8641737	-2.9831032	2.5046429

4 : $B(C_6F_5)_3$ / P(*o*-Tol)$_3$ adduct of *t*BuO_2CNNH

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Energy = -3817.111237830

N	-0.0958316	0.0442704	0.8491552
N	1.1626211	0.4293044	0.4334333
H	-0.2159817	0.2238156	1.8456844
C	1.5338053	1.8024258	0.5100548
O	0.8613929	2.6491640	1.0571533
O	2.7159317	1.9528719	-0.1101589
C	3.3804004	3.2867769	-0.2157272
C	4.6549025	2.9603287	-0.9960768
C	2.4635261	4.2257538	-1.0056054
C	3.6974681	3.7982881	1.1917046
H	4.4082376	2.5246152	-1.9782535
H	5.2356924	3.8837771	-1.1561476
H	5.2783940	2.2441523	-0.4367965
H	2.9916062	5.1780325	-1.1836981
H	2.2022390	3.7792765	-1.9789576
H	1.5363938	4.4286380	-0.4494505
H	4.2799332	4.7322531	1.1150154
H	2.7726586	4.0029104	1.7515139
H	4.2990245	3.0554434	1.7415532
B	-1.3874051	0.1890802	-0.0051043
C	-2.4691978	-0.9451071	0.5400300
C	-2.1443695	1.6535513	0.2618907
C	-0.9572940	-0.0248413	-1.5894078
C	-2.3279460	-1.7648536	1.6699009
C	-3.6836198	-1.1117112	-0.1447489

C	-2.2479307	2.1324519	1.5764350
C	-2.7603481	2.4723195	-0.6954804
C	-0.2791328	0.9901836	-2.2804715
C	-1.1420781	-1.1903240	-2.3494353
C	-3.2735797	-2.7318033	2.0461622
F	-1.2492797	-1.6949887	2.4891110
C	-4.6626373	-2.0504201	0.1968636
F	-3.9310759	-0.3615438	-1.2428440
C	-2.8498064	3.3437274	1.9332220
F	-1.7564176	1.3993659	2.6138035
C	-3.3784523	3.6949594	-0.3933546
F	-2.7840098	2.1251259	-2.0032032
C	0.1773775	0.8885265	-3.5972485
F	-0.0013509	2.1641438	-1.6655565
C	-0.7006947	-1.3491327	-3.6732179
F	-1.7566439	-2.2804254	-1.8297261
C	-4.4523270	-2.8751753	1.3094895
F	-3.0490633	-3.5212140	3.1139016
F	-5.7907864	-2.1718270	-0.5236962
C	-3.4242001	4.1360333	0.9328287
F	-2.8965869	3.7434708	3.2170521
F	-3.9357336	4.4415142	-1.3641364
C	-0.0206780	-0.3023717	-4.3009752
F	0.8947523	1.8860091	-4.1531598
F	-0.8956623	-2.5077357	-4.3234138
F	-5.3689451	-3.7906351	1.6612931
F	-4.0129430	5.3022685	1.2434739
F	0.4632429	-0.4449450	-5.5435019
P	2.4519332	-0.7632462	0.5365366
C	1.6401861	-2.2879396	1.0744890
C	3.7054012	-0.1165768	1.6723702
C	3.1667338	-1.0986063	-1.1009039
C	0.6387274	-2.6864979	0.1597990
C	1.9049839	-3.0605773	2.2372805
C	3.3235813	0.3845873	2.9463469
C	5.0449962	-0.0591926	1.2392032
C	2.8432753	-0.2209294	-2.1529607
C	3.9711784	-2.2489051	-1.3368545
C	-0.1502055	-3.8113131	0.3989529
H	0.4821170	-2.1001587	-0.7481447
C	1.0792465	-4.1829469	2.4549956
C	3.0133812	-2.8074907	3.2346696
C	4.3430592	0.9060484	3.7637719
C	1.8943972	0.3981729	3.4403574
C	6.0349121	0.4670615	2.0748337
H	5.3050981	-0.4174458	0.2384132
C	3.2988426	-0.4660026	-3.4520601
H	2.2396174	0.6594620	-1.9400773
C	4.4246562	-2.4618017	-2.6521245
C	4.3357686	-3.2470790	-0.2630597
C	0.0574753	-4.5477859	1.5723836
H	-0.9265514	-4.0877184	-0.3177979
H	1.2614913	-4.7915560	3.3472388
H	2.7187884	-2.0639369	3.9948453
H	3.2456374	-3.7427658	3.7682562
H	3.9376431	-2.4417778	2.7627033
C	5.6791414	0.9475054	3.3432865
H	4.0756604	1.2904142	4.7538660
H	1.8705927	0.3962982	4.5415393
H	1.3688003	1.3096964	3.1008130
H	1.3117354	-0.4690282	3.0856200
H	7.0742230	0.5054504	1.7353176
C	4.0915270	-1.5934482	-3.7001437
H	3.0258147	0.2177830	-4.2606900
H	5.0501791	-3.3381543	-2.8537419
H	4.5533994	-2.7630037	0.7035542
H	3.5090421	-3.9595315	-0.0924260
H	5.2258021	-3.8232366	-0.5622104
H	-0.5656613	-5.4198145	1.7941190
H	6.4437247	1.3622245	4.0079211
H	4.4548530	-1.7995625	-4.7120046

5 : $B(C_6F_5)_3$ / P(*o*-Tol)$_3$ FLP adduct of HN=NH

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Energy = -3471.445256266

N	2.9141420	-1.0011085	-0.8438295
N	1.5804414	-1.5089567	-0.8153609
H	3.3157482	-1.1781724	-1.7697484
H	0.8526408	-0.9873032	-1.3296898
B	3.0275901	0.4961736	-0.4401290
C	4.5923016	0.9815017	-0.6126226
C	2.1608803	1.4744712	-1.4847882
C	2.4764328	0.5155953	1.1159087
C	5.6215306	0.2745943	-1.2497631
C	4.9580326	2.2582292	-0.1572345
C	2.2155649	1.2285178	-2.8655396
C	1.3972248	2.6010835	-1.1357178
C	1.1095781	0.4319433	1.4188670
C	3.3235286	0.3170277	2.2176284
C	6.9208714	0.7799468	-1.4142240
F	5.4225575	-0.9663825	-1.7611925
C	6.2394433	2.8039623	-0.2901930
F	4.0396777	3.0251644	0.4715475
C	1.5233748	1.9657267	-3.8342056
F	2.9912505	0.2189197	-3.3555662
C	0.6985073	3.3842517	-2.0667362
F	1.2865467	2.9939984	0.1489534
C	0.5992335	0.1656715	2.6949277
F	0.1726700	0.5836743	0.4447340
C	2.8611175	0.0487557	3.5145881
F	4.6658901	0.3019571	2.0698659
C	7.2338108	2.0538242	-0.9307213
F	7.8644056	0.0499262	-2.0352122
F	6.5239356	4.0289385	0.1829206

C	0.7552398	3.0620383	-3.4282401
F	1.6006107	1.6336628	-5.1363222
F	-0.0260479	4.4420352	-1.6666417
C	1.4868538	-0.0403579	3.7563222
F	-0.7271588	0.0649892	2.9001225
F	3.7293977	-0.1952215	4.5143740
F	8.4711035	2.5514483	-1.0780623
F	0.0860858	3.7954309	-4.3291922
F	1.0286902	-0.3280966	4.9829834
P	1.5649648	-3.1774464	-0.9582928
C	2.1509062	-3.8874524	0.6050013
C	2.6913989	-3.6448329	-2.3064336
C	-0.1356925	-3.7085068	-1.2801627
C	2.6575265	-2.9910480	1.5667985
C	2.0569744	-5.2788524	0.8763258
C	2.5206662	-3.1278251	-3.6219980
C	3.8702165	-4.3408994	-1.9580390
C	-0.3681223	-4.5525131	-2.3875524
C	-1.1923554	-3.3616032	-0.3929393
C	3.0811351	-3.4593195	2.8138071
H	2.7243469	-1.9318559	1.3139807
C	2.4968050	-5.7188134	2.1397665
C	1.4939971	-6.2807041	-0.1057074
C	3.5506292	-3.3687896	-4.5520294
C	1.3138395	-2.3397174	-4.0840324
C	4.8695400	-4.5693766	-2.9059631
H	4.0099321	-4.6836522	-0.9284005
C	-1.6491019	-5.0433082	-2.6505478
H	0.4666955	-4.8373573	-3.0350420
C	-2.4718197	-3.8729962	-0.6870091
C	-1.0082965	-2.4758125	0.8149740
C	3.0004798	-4.8295123	3.0984809
H	3.4773932	-2.7529539	3.5493494
H	2.4382164	-6.7880299	2.3709381
H	0.3900404	-6.2391499	-0.1231085
H	1.8439551	-6.0982882	-1.1358041
H	1.7894389	-7.3032681	0.1779680
C	4.7052859	-4.0803208	-4.2096053
H	3.4415068	-2.9719213	-5.5671812
H	0.6673500	-2.9619371	-4.7283687
H	0.6904410	-1.9784912	-3.2537044
H	1.6349494	-1.4656729	-4.6722671
H	5.7781188	-5.1087741	-2.6230994
C	-2.7050386	-4.6956466	-1.7956909
H	-1.8186607	-5.6971357	-3.5112157
H	-3.3010091	-3.6186845	-0.0181906
H	-1.8375280	-2.6177603	1.5253124
H	-0.0610682	-2.6809473	1.3393210
H	-0.9917298	-1.4115550	0.5290897
H	3.3328517	-5.2107902	4.0694352
H	5.4869144	-4.2391669	-4.9594101
H	-3.7143024	-5.0743098	-1.9869082

An : less stable $B(C_6F_5)_3$ adduct of **R** at N-atom 68

Energy = -3008.855897971

N	0.2327451	-0.7063493	-1.3609958
N	-0.6997089	-0.8792775	-2.1663926
C	1.4977417	-1.3799271	-1.8689486
O	2.4452767	-0.6905752	-2.1428718
O	1.2791777	-2.6607415	-1.9508971
C	-1.9941946	-0.2335549	-2.0614095
O	-2.3173879	0.5374971	-2.9392351
O	-2.6863117	-0.7915977	-1.0922852
C	2.3479558	-3.6102487	-2.4628869
C	2.5941867	-3.2756163	-3.9341981
C	3.6017046	-3.4749579	-1.5970900
C	1.6661831	-4.9635663	-2.2766696
H	1.6499884	-3.3129606	-4.5026536
H	3.0478393	-2.2783561	-4.0454138
H	3.2860266	-4.0225864	-4.3585017
H	3.3655330	-3.6345663	-0.5339608
H	4.3254086	-4.2438518	-1.9159117
H	4.0694798	-2.4860791	-1.7167849
H	2.3455771	-5.7658319	-2.6084152
H	1.4178102	-5.1228847	-1.2147199
H	0.7386411	-5.0153719	-2.8699377
C	-4.2028696	-0.8527870	-1.0871258
C	-4.7936069	0.5568530	-1.1119511
C	-4.6059383	-1.6858518	-2.3040206
C	-4.4766031	-1.5674657	0.2342235
H	-4.4454307	1.1451807	-0.2511204
H	-4.5369616	1.0825215	-2.0433125
H	-5.8914578	0.4695196	-1.0447874
H	-4.1162530	-2.6733923	-2.2757779
H	-5.6984352	-1.8362282	-2.2928469
H	-4.3389197	-1.1718477	-3.2418532
H	-5.5620383	-1.7205984	0.3514786
H	-3.9727403	-2.5473014	0.2587394
H	-4.1104321	-0.9590923	1.0767543
B	0.2130451	0.2173936	0.0400529
C	-0.5131307	-0.6664606	1.2127183
C	1.7552865	0.4649507	0.5228211
C	-0.5993052	1.5503519	-0.4339561
C	-0.9890085	-1.9810522	1.1433584
C	-0.6063045	-0.0644017	2.4784314
C	2.5509689	-0.6392627	0.8626542
C	2.3585753	1.7101740	0.7581001
C	-0.0899829	2.2859078	-1.5201103
C	-1.8079098	2.0352234	0.0896946
C	-1.5817479	-2.6378008	2.2304857
C	-1.1819785	-0.6833532	3.5928552
C	3.8644044	-0.5608806	1.3297109
C	3.6692058	1.8452951	1.2421843

C	-0.7087969	3.4133879	-2.0632510
C	-2.4620881	3.1660859	-0.4185460
C	-1.6800885	-1.9871103	3.4644624
C	4.4288367	0.7053363	1.5292737
C	-1.9185613	3.8522108	-1.5089304
F	-0.9026341	-2.6974860	0.0025322
F	-0.1536371	1.1963901	2.6460166
F	2.0444884	-1.8892341	0.6896092
F	1.6968818	2.8627999	0.5443995
F	1.0583547	1.8821903	-2.0997802
F	-2.4457828	1.4113865	1.1021339
F	-2.0649867	-3.8829240	2.0859096
F	-1.2606640	-0.0476503	4.7704661
F	4.5736170	-1.6709461	1.5855409
F	4.1947298	3.0613533	1.4443105
F	-0.1738526	4.0620042	-3.1047958
F	-3.6288115	3.5668883	0.1100510
F	-2.2417840	-2.6027433	4.5120010
F	5.6806674	0.8238002	1.9842743
F	-2.5425388	4.9206896	-2.0115251

A : $B(C_6F_5)_3$ adduct of **R** at an ester C=O

68

Energy = -3008.850882321

N	-1.7254194	-0.7755896	1.3602775
N	-2.6343084	-1.6207012	1.2310274
C	-0.5523988	-1.1612081	2.0458292
O	-0.2272727	-0.6270626	3.1344682
O	0.2044300	-1.9536455	1.3688164
C	-3.7366891	-1.1858116	0.3934125
O	-3.7277131	-1.4658161	-0.7856331
O	-4.6553662	-0.6207809	1.1466026
C	1.6406388	-2.3334499	1.7812724
C	2.4598575	-1.0530221	1.9357805
C	1.5423870	-3.1641089	3.0577532
C	2.0798241	-3.1594743	0.5762584
H	2.3659294	-0.4167142	1.0404581
H	2.1619172	-0.4758857	2.8225232
H	3.5193090	-1.3401444	2.0439532
H	0.8455922	-4.0066940	2.9186873
H	2.5424597	-3.5741515	3.2790380
H	1.2186024	-2.5557949	3.9134679
H	3.1060462	-3.5241192	0.7468421
H	1.4153786	-4.0275087	0.4374786
H	2.0704344	-2.5488375	-0.3412488
C	-6.0258947	-0.2735137	0.6015377
C	-5.8561833	0.8146598	-0.4609474
C	-6.6688939	-1.5499485	0.0554533
C	-6.7467164	0.2370248	1.8475401
H	-5.3573927	1.6987407	-0.0347655
H	-5.2784131	0.4419204	-1.3207264
H	-6.8541172	1.1229966	-0.8159545
H	-6.6852250	-2.3347772	0.8303754
H	-7.7106303	-1.3255346	-0.2296460
H	-6.1349553	-1.9244744	-0.8308719
H	-7.7708246	0.5429608	1.5763520
H	-6.8054136	-0.5569838	2.6102076
H	-6.2175627	1.1009678	2.2749807
B	-1.0343410	0.4364070	4.0272240
C	-2.0959263	-0.3810348	4.9544325
C	0.1596235	1.0362744	4.9691793
C	-1.6785078	1.5010573	2.9740812
C	-2.4209723	-1.7408649	4.8814916
C	-2.7126068	0.3211802	6.0024722
C	0.9545840	0.1475894	5.7107780
C	0.4576065	2.3943749	5.1540713
C	-0.8404619	2.0944573	2.0129464
C	-3.0280543	1.8756227	2.8915224
C	-3.3095177	-2.3691197	5.7670149
C	-3.6061094	-0.2577055	6.9086980
C	2.0099295	0.5484476	6.5387007
C	1.4986878	2.8450096	5.9793256
C	-1.2765037	2.9858773	1.0312816
C	-3.5056017	2.7885052	1.9406655
C	-3.9035915	-1.6223486	6.7898630
C	2.2798695	1.9159108	6.6765587
C	-2.6357354	3.3271495	0.9892097
F	-1.8814323	-2.5454196	3.9301629
F	-2.4655610	1.6417019	6.1439800
F	0.7135852	-1.1843159	5.6509168
F	-0.2612038	3.3544278	4.5387576
F	0.4764864	1.7786111	1.9992067
F	-3.9544403	1.3652161	3.7246269
F	-3.5846174	-3.6763811	5.6449825
F	-4.1740955	0.4697650	7.8810140
F	2.7425537	-0.3533109	7.2093262
F	1.7448452	4.1561498	6.1134870
F	-0.4260294	3.4989807	0.1317529
F	-4.8099948	3.1165027	1.9014876
F	-4.7534772	-2.2045828	7.6446456
F	3.2765175	2.3301646	7.4675076
F	-3.0985888	4.1607984	0.0520171

$B(C_6F_5)_3H^{\ominus}$: hydridoborate anion

35

Energy = -2207.662336754

B	0.1085098	0.1594407	0.8820058
C	0.2687701	1.6866356	0.3094850
C	1.2725568	-0.8875000	0.3927419
C	-1.3454941	-0.5226300	0.5230371
C	-0.6936856	2.6473845	0.6618224
C	1.3237180	2.1863464	-0.4658130
C	2.2401711	-1.3993377	1.2665643
C	1.3288131	-1.3915562	-0.9139788

C	-1.7901249	-1.6045968	1.2989286
C	-2.2050920	-0.1616621	-0.5234441
C	-0.6437121	3.9918300	0.2771740
C	1.4215337	3.5256829	-0.8774976
C	3.2006352	-2.3490053	0.8836522
C	2.2676305	-2.3357823	-1.3463814
C	-3.0025120	-2.2746082	1.0853018
C	-3.4301121	-0.7970531	-0.7756743
C	0.4291826	4.4367725	-0.5053043
C	3.2111436	-2.8225893	-0.4325940
C	-3.8306894	-1.8656524	0.0334384
F	-1.7563715	2.2818616	1.4177330
F	2.3397709	1.3849879	-0.8684494
F	2.2993262	-0.9851851	2.5517560
F	0.4547533	-0.9408505	-1.8441171
F	-1.0300189	-2.0589034	2.3219866
F	-1.8856056	0.8475191	-1.3660152
F	-1.6069680	4.8602263	0.6471148
F	2.4635783	3.9424091	-1.6256118
F	4.1113630	-2.8112295	1.7651680
F	2.2797859	-2.7805451	-2.6196192
F	-3.3774784	-3.3061507	1.8694842
F	-4.2194305	-0.4011835	-1.7952047
F	0.5053689	5.7257873	-0.8888366
F	4.1247174	-3.7330394	-0.8204785
F	-5.0003794	-2.4930533	-0.1957519
H	0.1663457	0.2452298	2.1009029

$B(C_6F_5)_3{\cdot}Po_3$: adduct of $B(C_6F_5)_3$ and P(*o*-Tol)$_3$
77
Energy = -3360.807287389

B	-0.0580131	0.3595555	-0.8975646
C	-1.3949496	-0.4394792	-1.2970526
C	-0.2821875	1.9630371	-0.7959502
C	1.3517411	-0.0881033	-1.5491845
C	-2.5893602	-0.2203093	-0.5849544
C	-1.5078400	-1.3574691	-2.3545094
C	0.5687203	2.8223046	-0.0803763
C	-1.3128395	2.6301541	-1.4876547
C	2.2400206	0.8098250	-2.1799913
C	1.8284523	-1.4113322	-1.4977632
C	-3.7905570	-0.8827554	-0.8343823
F	-2.6024100	0.6791989	0.4288740
C	-2.6904648	-2.0559621	-2.6397017
F	-0.4675363	-1.6044993	-3.1745368
C	0.3880987	4.2023507	0.0375023
F	1.6394279	2.3141064	0.5596185
C	-1.5301939	4.0139831	-1.4110903
F	-2.1555045	1.9669557	-2.3053574
C	3.5237626	0.4513479	-2.6168087
F	1.9005341	2.0930378	-2.4121500
C	3.1049454	-1.8130710	-1.8994766
F	1.0325247	-2.3956844	-1.0308330
C	-3.8364664	-1.8230073	-1.8710020
F	-4.8775291	-0.6524061	-0.0850105
F	-2.7347024	-2.9368221	-3.6503481
C	-0.6806296	4.8078250	-0.6337180
F	1.2201282	4.9407029	0.7862033
F	-2.5356745	4.5809914	-2.0927894
C	3.9685620	-0.8661409	-2.4611860
F	4.3212973	1.3600137	-3.1949946
F	3.5004254	-3.0842916	-1.7565654
F	-4.9665120	-2.4926472	-2.1243007
F	-0.8782282	6.1273622	-0.5437618
F	5.1941676	-1.2195918	-2.8615359
P	0.1354464	-0.5596504	1.4157210
C	-1.3425620	-1.6486640	1.6878048
C	0.2029617	0.7020402	2.7587151
C	1.5764979	-1.7120177	1.6496596
C	-1.4453172	-2.6956754	0.7384045
C	-2.3868414	-1.4822736	2.6416134
C	0.8815145	0.5640745	4.0034015
C	-0.5156014	1.8861306	2.4894136
C	1.3314115	-3.0652611	1.9676936
C	2.9227511	-1.2784664	1.4884879
C	-2.5317138	-3.5719687	0.7078333
H	-0.6529431	-2.8209034	0.0023358
C	-3.4816240	-2.3728782	2.5735671
C	-2.4423643	-0.4281385	3.7233022
C	0.8666468	1.6697971	4.8789244
C	1.5479097	-0.7028821	4.4901328
C	-0.5246506	2.9616543	3.3814438
H	-1.0919992	1.9545647	1.5668219
C	2.3689066	-3.9960903	2.0704813
H	0.3092060	-3.4028068	2.1467435
C	3.9495812	-2.2396875	1.5849576
C	3.3177866	0.1587813	1.2745307
C	-3.5706939	-3.3994617	1.6297416
H	-2.5681216	-4.3678959	-0.0423949
H	-4.2914047	-2.2420377	3.2995835
H	-3.3067957	-0.6205639	4.3783711
H	-1.5342520	-0.4146907	4.3448044
H	-2.5557599	0.5817658	3.2976683
C	0.1925174	2.8593074	4.5788688
H	1.3883118	1.5759402	5.8380122
H	0.9248700	-1.5900533	4.2941319
H	2.5199628	-0.8834373	4.0010342
H	1.7229678	-0.6331810	5.5757787
H	-1.0885354	3.8677390	3.1390824
C	3.6896809	-3.5863467	1.8550314
H	2.1384561	-5.0375489	2.3164215
H	4.9837941	-1.9044618	1.4492122
H	2.9832628	0.5266341	0.2944019
H	2.8676471	0.8219296	2.0318364

H	4.4125880	0.2660428	1.3260314
H	-4.4452584	-4.0577906	1.6168789
H	0.2110581	3.6915346	5.2900517
H	4.5141021	-4.3042703	1.9136565

$B(C_6F_5)_3$: Lewis acidic borane
34
Energy = -2206.936230233

B	-0.0000021	-0.0004756	0.0000377
C	-0.0000020	1.5681536	0.0000299
C	1.3582639	-0.7851840	-0.0016662
C	-1.3582803	-0.7851685	0.0017266
C	-0.9554778	2.3182402	0.7169109
C	0.9554694	2.3182388	-0.7168601
C	2.4865083	-0.3331648	0.7138881
C	1.5284814	-1.9881082	-0.7182019
C	-1.5285399	-1.9880616	0.7183047
C	-2.4864768	-0.3331859	-0.7139246
C	-0.9658199	3.7162818	0.7377981
C	0.9658601	3.7162818	-0.7376849
C	3.7019383	-1.0240415	0.7338430
C	2.7333805	-2.6971827	-0.7396925
C	-2.7334049	-2.6971972	0.7396567
C	-3.7018732	-1.0241188	-0.7340085
C	0.0000049	4.4166978	0.0000370
C	3.8239676	-2.2110933	-0.0034943
C	-3.8239586	-2.2111189	0.0034019
F	-1.8940047	1.6935201	1.4487747
F	1.8938980	1.6935196	-1.4488518
F	2.4161761	0.7923250	1.4453666
F	0.5170420	-2.4880894	-1.4488145
F	-0.5171979	-2.4879175	1.4491387
F	-2.4161344	0.7923346	-1.4453554
F	-1.8787444	4.3881010	1.4470523
F	1.8789053	4.3881019	-1.4467837
F	4.7413229	-0.5697040	1.4416181
F	2.8571024	-3.8244689	-1.4480576
F	-2.8571035	-3.8245748	1.4478808
F	-4.7411497	-0.5699200	-1.4420312
F	-0.0000524	5.7488613	-0.0000359
F	4.9772232	-2.8778568	-0.0043062
F	-4.9772527	-2.8778148	0.0042769

B$^{\boxtimes}$TMPH^{+} : unstable H-bonded contact ion pair
85
Energy = -3260.710420657

N	-2.5003634	-1.3801717	2.1844226
N	-3.4351358	-1.0237927	1.4337500
C	-1.2309202	-1.4139807	1.4709047
O	-0.2850619	-0.7733939	2.0451920
O	-1.1684790	-2.1346011	0.4663261
C	-4.7689904	-1.2707917	1.8985624
O	-5.3871179	-2.1530238	1.3089816
O	-5.1671860	-0.4413136	2.8272618
H	-2.5749978	-2.7480816	-0.1977042
C	-6.5941542	-0.4347248	3.3369981
C	-7.5265199	-0.1253098	2.1643619
C	-6.8751833	-1.7885129	3.9917022
C	-6.5620260	0.6999141	4.3586762
H	-7.2361125	0.8218142	1.6794380
H	-7.5151141	-0.9354439	1.4194367
H	-8.5549209	-0.0153887	2.5479301
H	-6.1231852	-2.0030998	4.7692960
H	-7.8681960	-1.7531481	4.4708340
H	-6.8719393	-2.5997509	3.2478514
H	-7.5590995	0.8084675	4.8166703
H	-5.8291203	0.4846538	5.1533170
H	-6.2905220	1.6514715	3.8730345
B	1.1481761	-0.8634021	1.4078843
C	1.1490963	-0.2341842	-0.1083406
C	2.0936190	0.1084986	2.3209214
C	1.4876801	-2.4692357	1.4881288
C	0.1051885	0.4475872	-0.7452915
C	2.3331738	-0.3187393	-0.8566202
C	1.6604237	1.4145419	2.6015609
C	3.3789628	-0.2044577	2.7865489
C	1.5988714	-3.0766171	2.7498150
C	1.4918728	-3.3639940	0.4078624
C	0.1876475	0.9388431	-2.0563038
C	2.4733356	0.1693606	-2.1602077
C	2.4143156	2.3431467	3.3309925
C	4.1723122	0.6946851	3.5143060
C	1.7358610	-4.4570792	2.9463564
C	1.6171372	-4.7524027	0.5549729
C	1.3828781	0.8041378	-2.7696124
C	3.6855524	1.9774984	3.7897123
C	1.7381890	-5.3063545	1.8331516
F	-1.0868609	0.6573596	-0.1291866
F	3.4076884	-0.9384507	-0.3206678
F	0.4628444	1.8405191	2.1450175
F	3.9286008	-1.4142068	2.5519193
F	1.5568929	-2.3192059	3.8665821
F	1.3164112	-2.9418094	-0.8637600
F	-0.8732856	1.5390319	-2.6271532
F	3.6301350	0.0367663	-2.8288649
F	1.9416073	3.5769529	3.5766430
F	5.3938017	0.3380081	3.9450469
F	1.8469809	-4.9718154	4.1818596
F	1.5686122	-5.5592134	-0.5231332
F	1.4842720	1.2759539	-4.0210352
F	4.4307051	2.8494198	4.4844504
F	1.8496345	-6.6333975	1.9904295
N	-3.3580549	-3.2550350	-0.7050606
C	-3.3005238	-2.7187676	-2.1424198

C	-3.1189044	-4.7423893	-0.4115285
H	-4.2328229	-2.9458022	-0.2351861
C	-1.9602182	-3.2016829	-2.7345567
C	-4.5172710	-3.1786510	-2.9576050
C	-3.3214234	-1.1868268	-2.0176213
C	-4.3128649	-5.5945565	-0.8633044
C	-2.9694677	-4.8417976	1.1165784
C	-1.7995865	-5.1274645	-1.1094868
C	-1.7420962	-4.7139996	-2.5857670
H	-1.1393315	-2.6684705	-2.2216596
H	-1.9311648	-2.9006851	-3.7958550
H	-4.4685497	-4.2366881	-3.2511577
H	-5.4555858	-3.0091126	-2.4016633
H	-4.5593944	-2.5774021	-3.8803482
H	-2.5137272	-0.8190776	-1.3685662
H	-3.1898251	-0.7448028	-3.0186473
H	-4.2842106	-0.8350596	-1.6080835
H	-5.2649144	-5.1674996	-0.5034440
H	-4.3695028	-5.7129531	-1.9544256
H	-4.2060849	-6.5995431	-0.4235530
H	-2.1260710	-4.2274463	1.4695442
H	-3.8914052	-4.5192591	1.6302162
H	-2.7694160	-5.8903891	1.3897909
H	-0.9686236	-4.6378062	-0.5747805
H	-1.6564929	-6.2155693	-0.9962720
H	-2.4856152	-5.2767022	-3.1798662
H	-0.7510154	-4.9793807	-2.9905331

B[2] : anion *t*$BuO_2CN{=}NCO_2B(C_6F_5)_3$[2]
55
Energy = -2851.201773315

N	-2.0137619	-1.1446743	1.3403686
N	-2.5822151	-0.1272312	0.8872191
C	-0.5934020	-0.9861637	1.5999681
O	-0.3876695	-0.5509904	2.8097728
O	0.1996678	-1.3599569	0.7535174
C	-3.9590859	-0.3127548	0.5230138
O	-4.2952905	-0.4654667	-0.6356641
O	-4.7298960	-0.1596513	1.5995161
C	-6.2150748	-0.1279568	1.4890686
C	-6.6314934	1.0500804	0.6012878
C	-6.7072906	-1.4767169	0.9519529
C	-6.6463953	0.0861394	2.9415473
H	-6.2042279	1.9902556	0.9895841
H	-6.2928931	0.9014431	-0.4351439
H	-7.7317040	1.1388072	0.6080700
H	-6.3232667	-2.2986569	1.5796257
H	-7.8104476	-1.5003792	0.9826048
H	-6.3751617	-1.6314342	-0.0856295
H	-7.7472544	0.1250246	3.0035820
H	-6.2828982	-0.7397392	3.5751912
H	-6.2342131	1.0325233	3.3290442
B	1.0200240	-0.5127765	3.4084560
C	1.9595423	0.6416226	2.7060477
C	0.8019924	0.0062007	4.9610982
C	1.5937452	-2.0482107	3.2877451
C	1.5495431	1.5827244	1.7515708
C	3.2718426	0.8102454	3.1727954
C	0.0148448	1.1476069	5.1892084
C	1.3992704	-0.5353605	6.1082854
C	0.9163188	-3.0751273	3.9634757
C	2.6410685	-2.4794755	2.4632372
C	2.3913475	2.5965733	1.2645098
C	4.1472928	1.8009171	2.7173681
C	-0.2126207	1.6943994	6.4597411
C	1.2052955	-0.0180915	7.3981114
C	1.2608589	-4.4290120	3.8770058
C	3.0262221	-3.8236611	2.3464657
C	3.6969449	2.7086872	1.7508804
C	0.3921051	1.1054685	7.5756803
C	2.3296360	-4.8064966	3.0561578
F	0.3014111	1.5762829	1.2399231
F	3.7537707	-0.0345187	4.1147635
F	-0.5581133	1.7973905	4.1559181
F	2.2115540	-1.6119593	6.0349939
F	-0.1317017	-2.7773161	4.7649748
F	3.3460941	-1.6103985	1.7099386
F	1.9477670	3.4713308	0.3415659
F	5.4020850	1.8982092	3.1972369
F	-0.9852106	2.7864888	6.6161534
F	1.7977140	-0.5882837	8.4650730
F	0.5795658	-5.3658328	4.5647620
F	4.0461642	-4.1795790	1.5416892
F	4.5125646	3.6767160	1.2958346
F	0.1950281	1.6153578	8.8044399
F	2.6823704	-6.1000246	2.9516441

CO_2 : carbon dioxide molecule
3
Energy = -188.4745630662

C	-0.0001336	-0.0000149	0.0000029
O	1.1719348	0.0000507	0.0000316
O	-1.1722048	-0.0000826	-0.0000260

C[2] : adduct of anion **B**[2] and $B(C_6F_5)_3$ at C=O
89
Energy = -5058.186414170

N	0.0358860	-0.4273785	1.2612125
N	-0.9120668	0.3794807	1.1406078
C	1.1251986	-0.1600569	0.3100798
O	2.2522298	-0.2862559	0.9380077
O	0.8885683	0.0404028	-0.8667303
C	-1.9968806	0.2403318	2.0269220
O	-3.1851821	0.2498450	1.6101212

O	-1.6807437	0.2644358	3.2795967
C	-2.7012786	0.3053791	4.4152549
C	-3.4708168	1.6215581	4.3189405
C	-3.5904539	-0.9351202	4.3153570
C	-1.7837481	0.2570852	5.6350555
H	-2.7741633	2.4746917	4.2762450
H	-4.1294819	1.6435357	3.4400296
H	-4.0910091	1.7244655	5.2257305
H	-2.9764070	-1.8474557	4.2383780
H	-4.1949142	-0.9996245	5.2359313
H	-4.2681370	-0.8845061	3.4514676
H	-2.3972296	0.2811435	6.5507678
H	-1.1842356	-0.6677371	5.6330827
H	-1.1026214	1.1234061	5.6415822
B	3.5808378	-0.2248847	0.1555016
C	3.8747509	1.2848303	-0.4202745
C	4.7461937	-0.5047995	1.2835044
C	3.4281509	-1.3966922	-0.9831356
C	3.1204004	2.4384984	-0.1684526
C	5.0553421	1.4991497	-1.1472049
C	4.7276674	0.2319675	2.4790545
C	5.8389333	-1.3716170	1.1403781
C	3.2460775	-2.7235050	-0.5614787
C	3.2824936	-1.1920742	-2.3618142
C	3.4862509	3.7114128	-0.6353369
C	5.4617886	2.7453274	-1.6338416
C	5.6895013	0.0990763	3.4896803
C	6.8285495	-1.5325532	2.1220000
C	2.9686936	-3.7870272	-1.4267781
C	3.0077708	-2.2266675	-3.2677701
C	4.6651620	3.8668685	-1.3705354
C	6.7529943	-0.7919782	3.3061153
C	2.8432347	-3.5318280	-2.7968578
F	1.9805767	2.3968454	0.5565680
F	5.8628843	0.4482482	-1.4210364
F	3.7557724	1.1420736	2.7007015
F	6.0002851	-2.1160549	0.0263791
F	3.3278623	-3.0288979	0.7544831
F	3.3724260	0.0401034	-2.9008932
F	2.7201542	4.7851517	-0.3694888
F	6.6014240	2.8812481	-2.3371758
F	5.6137779	0.8277807	4.6193394
F	7.8509847	-2.3877820	1.9345034
F	2.8041247	-5.0379556	-0.9593146
F	2.8664286	-1.9688892	-4.5807635
F	5.0311059	5.0797025	-1.8201239
F	7.6923291	-0.9333720	4.2569971
F	2.5590262	-4.5305734	-3.6483609
B	-3.6257818	0.1254532	0.0771061
C	-3.5364807	1.6002320	-0.6118910
C	-2.6606726	-1.0305231	-0.5440826
C	-5.2051250	-0.2912317	0.2121210
C	-3.0685413	2.7849421	-0.0294748
C	-4.0654597	1.7411635	-1.9040886
C	-1.8165328	-0.9062074	-1.6599597
C	-2.5855953	-2.2655500	0.1247786
C	-6.0574851	0.4895951	1.0082835
C	-5.8280164	-1.3569540	-0.4537445
C	-3.0902671	4.0235133	-0.6888574
C	-4.1063656	2.9512882	-2.6026246
C	-0.9609541	-1.9345524	-2.0878789
C	-1.7349486	-3.3060079	-0.2494523
C	-7.4203365	0.2230718	1.1880737
C	-7.1910726	-1.6581825	-0.3118574
C	-3.6142009	4.1074087	-1.9827749
C	-0.9181804	-3.1365433	-1.3780577
C	-7.9926520	-0.8628419	0.5146240
F	-2.5712729	2.8076371	1.2302877
F	-4.5525460	0.6510438	-2.5385129
F	-1.7667456	0.2266943	-2.3747518
F	-3.3623411	-2.4795049	1.2184169
F	-5.5741087	1.5798330	1.6512508
F	-5.1348277	-2.1597548	-1.2843235
F	-2.6274654	5.1284800	-0.0825815
F	-4.6142665	3.0195853	-3.8439887
F	-0.1691269	-1.7611331	-3.1523352
F	-1.7028550	-4.4599643	0.4348520
F	-8.1805577	1.0026786	1.9751218
F	-7.7349031	-2.6959154	-0.9679998
F	-3.6464025	5.2841890	-2.6249042
F	-0.1040541	-4.1271583	-1.7655034
F	-9.2969199	-1.1373251	0.6603606

D[2] : H-bonded $TMPH^+$ and dianion

106

Energy = -5310.048504751

N	0.2957005	0.2028756	-0.6401881
N	-0.5630567	-0.6313009	-0.2867758
C	1.5122169	0.1439931	0.1331494
O	2.5828151	0.1602807	-0.5900608
O	1.4564783	0.2320466	1.3637483
C	-1.8648512	-0.5050621	-0.9189182
O	-2.6285098	0.2042973	-0.1339983
O	-2.1238991	-1.1127910	-1.9389341
B	3.9340490	0.4526779	0.1075578
C	5.0738588	0.3686784	-1.0669191
C	3.6919838	1.9558863	0.7405787
C	4.3329647	-0.7120445	1.1998961
C	5.1033079	-0.7555884	-1.9076132
C	6.1131301	1.2879281	-1.2678797
C	3.4339897	3.0269589	-0.1332374
C	3.4752772	2.2541716	2.0894767
C	5.4942025	-0.5332874	1.9673822
C	3.6846405	-1.9398702	1.3977581

C	6.0608650	-0.9495476	-2.9121510
C	7.0963038	1.1329726	-2.2560847
C	3.0104337	4.2967099	0.2852195
C	3.0313521	3.4966806	2.5563329
C	5.9732600	-1.4626604	2.8976334
C	4.1211119	-2.9002255	2.3245491
C	7.0689795	0.0061936	-3.0850073
C	2.7897168	4.5313091	1.6489786
C	5.2734317	-2.6623823	3.0798424
F	4.1857993	-1.7336828	-1.7575370
F	6.2226208	2.3947929	-0.5024491
F	3.5711438	2.8568997	-1.4620319
F	3.6264695	1.3147294	3.0596536
F	6.2030680	0.6103374	1.8346517
F	2.5675762	-2.2732608	0.7142857
F	6.0344236	-2.0437921	-3.6925340
F	8.0656221	2.0525623	-2.4113663
F	2.7918271	5.2769165	-0.6027607
F	2.7658656	3.6684000	3.8725973
F	7.0840332	-1.2184978	3.6150209
F	3.4232281	-4.0357198	2.5093489
F	8.0031167	-0.1584730	-4.0350731
F	2.3508298	5.7226916	2.0758648
F	5.6961821	-3.5663038	3.9787895
B	-4.1538193	0.2584087	-0.2618241
C	-4.6241093	1.0262646	1.1264824
C	-4.6373450	1.2252278	-1.4946184
C	-4.6437229	-1.3063048	-0.3565730
C	-5.6303392	0.6081061	2.0087520
C	-3.9738431	2.2159824	1.4957103
C	-3.8070111	1.9601097	-2.3514264
C	-6.0117311	1.4461201	-1.6663298
C	-4.3408901	-2.1780002	0.7007622
C	-5.2369961	-1.9185174	-1.4682297
C	-5.9313978	1.2704572	3.2092410
C	-4.2438703	2.9099162	2.6828606
C	-4.3048145	2.8348273	-3.3318258
C	-6.5544000	2.3028004	-2.6286138
C	-4.6295861	-3.5467112	0.6973211
C	-5.5494632	-3.2855503	-1.5192987
C	-5.2201666	2.4228419	3.5583757
C	-5.6852274	3.0087127	-3.4702616
C	-5.2407241	-4.1068346	-0.4305226
F	-6.3715620	-0.4894619	1.7550798
F	-3.0134021	2.7450214	0.7094171
F	-2.4637587	1.8745129	-2.2788905
F	-6.8903377	0.7877797	-0.8729529
F	-3.7421065	-1.7008387	1.8198189
F	-5.5346818	-1.2155479	-2.5800068
F	-6.8903964	0.8048393	4.0296477
F	-3.5528074	4.0233902	3.0067433
F	-3.4651637	3.5148158	-4.1332050
F	-7.8855246	2.4614786	-2.7512741
F	-4.3253999	-4.3243416	1.7532476
F	-6.1237807	-3.8178785	-2.6135799
F	-5.4783849	3.0622879	4.7113893
F	-6.1747050	3.8440028	-4.4025854
F	-5.5287913	-5.4186129	-0.4649009
N	0.8284467	0.4781950	3.9455498
C	1.1373971	-0.7432263	4.8223157
C	-0.6011508	1.0515958	3.8707541
H	1.1288455	0.2915785	2.9517120
C	0.4931158	-0.5058543	6.2034554
C	0.6468373	-2.0227853	4.1255499
C	2.6673563	-0.7934663	4.9504555
C	-1.5013804	0.1159248	3.0567501
C	-0.4506226	2.3957092	3.1417917
C	-1.0988204	1.2360705	5.3141506
C	-0.9698473	-0.0467460	6.1462669
H	1.0871514	0.2641344	6.7332023
H	0.5942604	-1.4377004	6.7860298
H	-0.4464011	-2.1310560	4.1444665
H	0.9843008	-2.0542367	3.0765284
H	1.0837837	-2.8893283	4.6477633
H	3.0646127	0.1345554	5.3968851
H	2.9450432	-1.6362961	5.6039115
H	3.1428672	-0.9398146	3.9694029
H	-1.0221531	-0.1840829	2.1129128
H	-1.7968100	-0.7878114	3.6069358
H	-2.4234295	0.6562535	2.8013428
H	0.2688283	3.0557237	3.6585358
H	-0.1141772	2.2384748	2.1043105
H	-1.4233788	2.9071561	3.1106952
H	-0.5193383	2.0477571	5.7965193
H	-2.1468907	1.5792957	5.2684807
H	-1.6092317	-0.8425756	5.7245600
H	-1.3348007	0.1351983	7.1714682
H	1.4432413	1.2418489	4.2672158

E : adduct *t*$BuO_2CN{=}NHB(C_6F_5)_3$

53

Energy = -2663.211798749

N	-1.0623655	-0.4615563	-0.5082495
N	-2.1688369	0.0810173	-0.3600462
C	-3.1768626	-0.5437754	-1.2619322
O	-4.3271247	0.0172168	-1.0013299
O	-2.8684425	-1.4106505	-2.0560472
B	0.2894597	-0.0415869	0.2250433
C	-5.5878595	-0.3967939	-1.7335480
C	0.8402688	-1.3650152	1.0128575
C	1.3130111	0.2251035	-1.0496919
C	-0.0622419	1.2483081	1.1433187
C	-5.8490695	-1.8759998	-1.4420753
C	-6.6377152	0.5095588	-1.0945944

C	-5.3978962	-0.0985397	-3.2222056
C	0.1286811	-2.5515692	1.2107214
C	2.1470243	-1.3488098	1.5236823
C	1.4460985	-0.7315962	-2.0681533
C	2.1729596	1.3303177	-1.1587888
C	-0.5405969	2.4197787	0.5331960
C	0.0184291	1.2968880	2.5422413
H	-5.0705673	-2.5180742	-1.8815068
H	-5.9009651	-2.0523641	-0.3547360
H	-6.8206716	-2.1540835	-1.8836632
H	-6.3873554	1.5701576	-1.2598639
H	-7.6210079	0.3038292	-1.5483989
H	-6.7030592	0.3233765	-0.0101694
H	-5.1355785	0.9618003	-3.3738199
H	-4.6182982	-0.7366125	-3.6654751
H	-6.3493765	-0.2968275	-3.7435168
C	0.6581128	-3.6660757	1.8751208
F	-1.1452403	-2.6684373	0.7510533
C	2.7176508	-2.4321631	2.2003931
F	2.8938780	-0.2328187	1.4021138
C	2.3393959	-0.6230801	-3.1393030
F	0.6833613	-1.8618398	-2.0355636
C	3.0850366	1.4832155	-2.2134483
F	2.1875768	2.2969656	-0.2256338
C	-0.8985074	3.5751689	1.2321387
F	-0.6677715	2.4576507	-0.8134018
C	-0.3242451	2.4357845	3.2884714
F	0.4280431	0.2302120	3.2586980
C	1.9659171	-3.6037048	2.3708096
F	-0.0691396	-4.7798953	2.0365737
F	3.9652951	-2.3634321	2.6826280
C	3.1670103	0.5044298	-3.2116623
F	2.4100664	-1.5741586	-4.0790251
F	3.8868792	2.5540025	-2.2663356
C	-0.7856465	3.5800193	2.6295828
F	-1.3458843	4.6635365	0.5910497
F	-0.2239752	2.4292711	4.6257295
F	2.4934704	-4.6534124	3.0097845
F	4.0319310	0.6415919	-4.2207168
F	-1.1216463	4.6710105	3.3276087
H	-1.0373896	-1.2346542	-1.2240596

F·$B(C_6F_5)_3$: adduct of **F** and $B(C_6F_5)_3$ at C=O

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Energy = -5866.886937035

N	-1.5578037	-0.1717364	0.8554973
N	-0.8791034	-1.1424868	0.1672940
H	-1.1905873	-0.0706755	1.8023857
C	0.4883928	-1.0366989	-0.0256946
O	1.1331124	-0.0944569	0.4810839
O	1.1245885	-1.9712377	-0.7144737
H	0.5387060	-2.4753666	-1.3236252
B	-2.3166073	1.0800214	0.2833250
C	-3.6579725	1.3515929	1.2208148
C	-1.4022211	2.4544831	0.5233000
C	-2.6847214	0.8330935	-1.3102209
C	-4.0426917	0.6551636	2.3756075
C	-4.4893044	2.4384343	0.9013117
C	-0.8981759	2.6782786	1.8138891
C	-1.1891960	3.5167928	-0.3676529
C	-1.6474766	0.7791161	-2.2497397
C	-3.9593902	0.6978959	-1.8861383
C	-5.2036093	0.9499012	3.1067850
F	-3.3257503	-0.3855931	2.8671768
C	-5.6480876	2.7826561	1.6041773
F	-4.2029166	3.1920656	-0.1850346
C	-0.1998350	3.8247916	2.2046756
F	-1.1249077	1.7599944	2.7923968
C	-0.5360158	4.7068483	-0.0149937
F	-1.6381049	3.4627929	-1.6441410
C	-1.8153105	0.6247569	-3.6276573
F	-0.3632803	0.8633280	-1.8219801
C	-4.1898466	0.5275709	-3.2609622
F	-5.0820886	0.6983452	-1.1316733
C	-6.0119444	2.0236190	2.7243250
F	-5.5444277	0.1969221	4.1688292
F	-6.4101712	3.8191828	1.2205291
C	-0.0200472	4.8555034	1.2759815
F	0.2794065	3.9507901	3.4541732
F	-0.3873437	5.6964215	-0.9079490
C	-3.1066134	0.4780710	-4.1428499
F	-0.7518160	0.5293139	-4.4471398
F	-5.4385409	0.3822156	-3.7260288
F	-7.1220526	2.3203579	3.4155566
F	0.6392810	5.9698235	1.6197216
F	-3.2957227	0.2738888	-5.4510877
P	-1.5614541	-2.8387070	0.1697948
C	-1.7842413	-3.2878831	-1.5751403
C	-3.1739441	-2.7663603	0.9536182
C	-0.3268041	-3.8959843	0.9417566
C	-1.2709870	-2.4277591	-2.5706689
C	-2.4873915	-4.4723537	-1.9363727
C	-3.6155352	-3.5333830	2.0710014
C	-4.0568067	-1.8905763	0.2812517
C	0.2091085	-4.9765509	0.2043829
C	0.1549558	-3.5762507	2.2403143
C	-1.4157646	-2.7343157	-3.9283696
H	-0.7921891	-1.4865103	-2.2936188
C	-2.6148159	-4.7531077	-3.3088039
C	-3.1230439	-5.3933846	-0.9231493
C	-4.9360614	-3.3070589	2.5032504
C	-2.8176261	-4.5885954	2.8009856
C	-5.3637461	-1.7062429	0.7320225
H	-3.7061078	-1.3515782	-0.6017245

C	1.2072123	-5.7754886	0.7649516
H	-0.1521797	-5.1851023	-0.8077166
C	1.1541213	-4.4072717	2.7751033
C	-0.3215170	-2.3774304	3.0242369
C	-2.0887726	-3.9055329	-4.2942161
H	-1.0183245	-2.0495113	-4.6822873
H	-3.1480053	-5.6614668	-3.6081321
H	-4.0818291	-4.9739078	-0.5689726
H	-3.3261617	-6.3785376	-1.3708812
H	-2.4857930	-5.5473114	-0.0363872
C	-5.7936838	-2.4025564	1.8680408
H	-5.3005078	-3.8783365	3.3632551
H	-3.5073843	-5.2595356	3.3360644
H	-2.1964374	-5.1990572	2.1283137
H	-2.1464012	-4.1436816	3.5545037
H	-6.0232385	-1.0141220	0.2056968
C	1.6746828	-5.4896147	2.0563549
H	1.6206316	-6.6122454	0.1949412
H	1.5480830	-4.1800954	3.7702786
H	-0.3247464	-2.5985208	4.1036369
H	0.3697194	-1.5292706	2.8775793
H	-1.3346854	-2.0431990	2.7439315
H	-2.2126150	-4.1603366	-5.3510962
H	-6.8082617	-2.2578232	2.2514177
H	2.4638005	-6.1029968	2.5006549
B	2.6572959	0.3855094	0.1774027
C	2.4850353	1.1462221	-1.2549372
C	3.0410620	1.3272666	1.4548613
C	3.7024664	-0.8745538	0.2084969
C	2.1625232	2.5102544	-1.3443028
C	2.4799688	0.4687403	-2.4868867
C	2.4120494	1.3492344	2.7078008
C	4.1822854	2.1400189	1.3559306
C	3.6042930	-1.8578045	1.2029347
C	4.8405926	-0.9829383	-0.6083217
C	1.8616239	3.1637654	-2.5467685
F	2.1085846	3.2796540	-0.2377250
C	2.1875724	1.0779157	-3.7113472
F	2.7316223	-0.8597472	-2.5540177
C	2.8473725	2.1514986	3.7741908
F	1.3291514	0.5841153	2.9764822
C	4.6510959	2.9597791	2.3869258
F	4.8762598	2.1641837	0.1964367
C	4.5089517	-2.9116448	1.3645017
F	2.5806200	-1.8039666	2.0909612
C	5.7793628	-2.0187807	-0.4833314
F	5.1017878	-0.0753390	-1.5660738
C	1.8602452	2.4367797	-3.7411703
F	1.5562212	4.4678169	-2.5577011
F	2.1789184	0.3592919	-4.8455434
C	3.9728282	2.9644536	3.6128874
F	2.1987314	2.1314982	4.9472844
F	5.7375636	3.7283295	2.2176815
C	5.6102221	-2.9952517	0.5047144
F	4.3410000	-3.8280185	2.3356578
F	6.8403708	-2.0782782	-1.3014247
F	1.5521503	3.0333963	-4.8982753
F	4.4029469	3.7347052	4.6207528
F	6.4963763	-3.9911853	0.6346170

F : $B(C_6F_5)_3$ / P(*o*-Tol)$_3$ adduct of $HN{=}NCO_2H$

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Energy = -3659.918363293

N	-0.0268489	0.0297486	0.9124867
N	1.2569044	0.3512993	0.5481538
H	-0.1593936	0.1173383	1.9193506
C	1.7853905	1.6460759	0.6273268
O	0.9271198	2.5165092	1.1760558
O	2.9251930	1.9031925	0.2634926
H	1.3471371	3.3994264	1.1214004
B	-1.2996794	0.1979534	0.0326721
C	-2.4077759	-0.9321339	0.5300421
C	-2.0521511	1.6618299	0.3262511
C	-0.8474314	0.0273425	-1.5496467
C	-2.2951729	-1.7932763	1.6317986
C	-3.6225231	-1.0434239	-0.1657421
C	-2.2015376	2.0873722	1.6548365
C	-2.6336706	2.5192583	-0.6188104
C	-0.1166574	1.0406965	-2.1877092
C	-1.0820891	-1.0901590	-2.3668815
C	-3.2672726	-2.7475805	1.9701754
F	-1.2182297	-1.7809636	2.4570862
C	-4.6269715	-1.9680381	0.1376851
F	-3.8442894	-0.2492800	-1.2380916
C	-2.8208941	3.2815779	2.0400373
F	-1.7384588	1.3143829	2.6761382
C	-3.2675360	3.7269760	-0.2881827
F	-2.6106972	2.2264149	-1.9387549
C	0.3394774	0.9825507	-3.5073743
F	0.2029435	2.1755593	-1.5185788
C	-0.6348971	-1.2081688	-3.6925021
F	-1.7554376	-2.1718559	-1.9061170
C	-4.4445397	-2.8353556	1.2225923
F	-3.0688428	-3.5787424	3.0103858
F	-5.7527422	-2.0356449	-0.5926700
C	-3.3630660	4.1127875	1.0526756
F	-2.9136917	3.6283856	3.3365820
F	-3.7919155	4.5113960	-1.2461803
C	0.0972532	-0.1656673	-4.2660344
F	1.0832313	1.9809761	-4.0198189
F	-0.8778359	-2.3248607	-4.3970669
F	-5.3857473	-3.7385290	1.5373902
F	-3.9666144	5.2632854	1.3895548
F	0.5799143	-0.2700251	-5.5117673

P	2.5159621	-0.9036587	0.5528904
C	1.6287248	-2.4131533	1.0028313
C	3.8041140	-0.4031409	1.7164323
C	3.1905505	-1.1394485	-1.1158216
C	0.6082927	-2.7136429	0.0729176
C	1.8676333	-3.2692084	2.1129793
C	3.4641346	0.0351714	3.0241763
C	5.1416788	-0.4088563	1.2740492
C	2.9882552	-0.1127658	-2.0597342
C	3.8642927	-2.3401650	-1.4789786
C	-0.2235631	-3.8203949	0.2451618
H	0.4753101	-2.0678896	-0.7974706
C	0.9970231	-4.3670497	2.2664109
C	2.9965149	-3.1327609	3.1102083
C	4.5202974	0.4216354	3.8679233
C	2.0392300	0.1158162	3.5267371
C	6.1697447	-0.0208436	2.1381719
H	5.3701757	-0.7097677	0.2470056
C	3.4191184	-0.2698745	-3.3810373
H	2.5063541	0.8147604	-1.7507174
C	4.2903579	-2.4631115	-2.8143025
C	4.1379341	-3.4718349	-0.5153376
C	-0.0417482	-4.6358572	1.3687721
H	-1.0102861	-4.0222297	-0.4846930
H	1.1585411	-5.0377229	3.1171515
H	2.7609135	-2.4022749	3.9026427
H	3.1669504	-4.1030604	3.6027316
H	3.9406039	-2.8122797	2.6436634
C	5.8547209	0.3913033	3.4406589
H	4.2853426	0.7534708	4.8850720
H	2.0151580	0.0390236	4.6253775
H	1.5771918	1.0836413	3.2583839
H	1.3954931	-0.6815348	3.1168068
H	7.2080631	-0.0337458	1.7934530
C	4.0636838	-1.4538418	-3.7591748
H	3.2394239	0.5275384	-4.1071920
H	4.8124718	-3.3781865	-3.1140820
H	4.4115216	-3.1076935	0.4891413
H	3.2506482	-4.1190143	-0.3992615
H	4.9670440	-4.0946377	-0.8873421
H	-0.6970408	-5.4958867	1.5386473
H	6.6503660	0.6978462	4.1272467
H	4.4005345	-1.5913674	-4.7916165

G·CO_2 : unstable CO_2 adduct of **G**

84

Energy = -3659.927660924

N	0.0311815	0.4061315	0.9704876
N	1.3644722	0.4435016	0.4296563
H	-0.0369418	-0.2655767	1.7486877
C	1.9911780	1.8439924	0.6511707
O	1.2265638	2.6037144	1.2731968
O	3.1324351	1.9087408	0.1876930
H	0.0555192	1.3853552	1.3974631
B	-1.3185903	0.3010607	-0.0032003
C	-2.2888305	-0.9076984	0.5527257
C	-2.1642883	1.6879879	0.2755163
C	-0.8044569	0.1376793	-1.5457415
C	-2.1321283	-1.7062870	1.6911797
C	-3.4991629	-1.1238761	-0.1311515
C	-2.3917935	2.0920050	1.5999196
C	-2.7999152	2.4800895	-0.6934104
C	-0.0785773	1.1863076	-2.1350501
C	-0.9924813	-0.9700874	-2.3869647
C	-3.0373436	-2.6970798	2.0922682
F	-1.0334753	-1.5865762	2.4993524
C	-4.4433691	-2.0913815	0.2271230
F	-3.7786370	-0.3852495	-1.2243879
C	-3.1483850	3.2073778	1.9714642
F	-1.8464763	1.3651111	2.6163231
C	-3.5716040	3.6075197	-0.3744393
F	-2.7048265	2.1909892	-2.0058707
C	0.4354318	1.1544904	-3.4335708
F	0.1590724	2.3107436	-1.4302487
C	-0.4923678	-1.0542677	-3.6953960
F	-1.6658552	-2.0686049	-1.9677311
C	-4.2080579	-2.8915192	1.3539111
F	-2.7782806	-3.4606852	3.1651620
F	-5.5649409	-2.2565628	-0.4871131
C	-3.7491653	3.9734850	0.9648065
F	-3.3117929	3.5372215	3.2605346
F	-4.1490769	4.3326969	-1.3432389
C	0.2417689	0.0129922	-4.2182265
F	1.1797666	2.1686938	-3.9025883
F	-0.6863244	-2.1612979	-4.4274372
F	-5.0911349	-3.8294224	1.7164279
F	-4.4844648	5.0460929	1.2804319
F	0.7755706	-0.0622699	-5.4431657
P	2.4907008	-0.8397554	0.5434160
C	1.5500568	-2.3279182	1.0185550
C	3.8187341	-0.4162167	1.6966838
C	3.1556985	-1.1556660	-1.1184989
C	0.5655134	-2.6511340	0.0574159
C	1.7667595	-3.1852005	2.1351903
C	3.5345152	0.0563216	3.0047900
C	5.1451164	-0.5411896	1.2402352
C	3.0372525	-0.1184604	-2.0648901
C	3.7498909	-2.4004103	-1.4684001
C	-0.2580605	-3.7680973	0.2038162
H	0.4593008	-2.0134849	-0.8230702
C	0.9004271	-4.2899258	2.2651185
C	2.8706568	-3.0513238	3.1593438
C	4.6281919	0.3568562	3.8339711
C	2.1287175	0.2624821	3.5207833

C	6.2128644	-0.2386241	2.0911197
H	5.3380012	-0.8600822	0.2115044
C	3.4668417	-0.3113142	-3.3817009
H	2.6347278	0.8442601	-1.7465517
C	4.1718491	-2.5601773	-2.8015227
C	3.9529160	-3.5408105	-0.4966784
C	-0.1028376	-4.5790200	1.3345500
H	-1.0141724	-3.9845175	-0.5540671
H	1.0416044	-4.9551607	3.1234665
H	2.6386248	-2.2892379	3.9218170
H	2.9967013	-4.0108849	3.6845012
H	3.8355244	-2.7747085	2.7076439
C	5.9504787	0.2084277	3.3928265
H	4.4334356	0.7177437	4.8495347
H	2.1189398	0.2745624	4.6218877
H	1.7228141	1.2286497	3.1722517
H	1.4419850	-0.5395494	3.1949665
H	7.2417121	-0.3409303	1.7336560
C	4.0236600	-1.5416648	-3.7521090
H	3.3587126	0.4968970	-4.1104377
H	4.6314168	-3.5106426	-3.0936438
H	4.2381201	-3.1875755	0.5082467
H	3.0334576	-4.1429105	-0.3868114
H	4.7517689	-4.2074648	-0.8588037
H	-0.7485695	-5.4497070	1.4844867
H	6.7772837	0.4523176	4.0675088
H	4.3574791	-1.7075564	-4.7814094

G : adduct $(C_6F_5)_3BNH_2NP(o\text{-Tol})_3$

81

Energy = -3471.438877650

N	-0.0010534	-0.7790333	0.4726479
N	0.9670622	0.2635509	0.6663825
H	0.3636492	-1.5374843	-0.1360261
H	-0.2261417	-1.2369723	1.3680991
B	-1.3932599	-0.2761697	-0.2102759
C	-2.3694387	-1.6020468	-0.3376569
C	-2.1543638	0.7659833	0.8017928
C	-0.9038601	0.3329721	-1.6471139
C	-2.1225853	-2.8925569	0.1464590
C	-3.6232742	-1.4466816	-0.9515560
C	-2.1964698	0.5227631	2.1816266
C	-2.9081777	1.8793143	0.3915382
C	-0.3698222	1.6278664	-1.7747573
C	-0.7951798	-0.4593882	-2.8005526
C	-3.0300782	-3.9563406	0.0489018
F	-0.9339898	-3.2001339	0.7474087
C	-4.5646759	-2.4742587	-1.0808757
F	-3.9620531	-0.2503398	-1.4736444
C	-2.8614410	1.3262105	3.1138725
F	-1.5772860	-0.5810203	2.6987161
C	-3.5982080	2.7141764	1.2827528
F	-3.0122477	2.2110745	-0.9089876
C	0.2189420	2.1106382	-2.9508731
F	-0.4084140	2.4987029	-0.7491856
C	-0.2128023	-0.0189883	-3.9975058
F	-1.1947215	-1.7528482	-2.7954113
C	-4.2658773	-3.7442735	-0.5706661
F	-2.7211478	-5.1671366	0.5377220
F	-5.7415034	-2.2568727	-1.6852329
C	-3.5733058	2.4401680	2.6547594
F	-2.8378733	1.0299981	4.4226100
F	-4.2884089	3.7712753	0.8287815
C	0.3114053	1.2751366	-4.0708572
F	0.7011693	3.3614439	-3.0136550
F	-0.1015886	-0.8509268	-5.0494775
F	-5.1504186	-4.7434736	-0.6790094
F	-4.2277702	3.2288199	3.5168093
F	0.8814806	1.7144363	-5.1994861
P	2.5498201	-0.1517780	0.5935194
C	2.7476812	-1.6554599	-0.4412263
C	3.4100057	-0.2770019	2.2097484
C	3.3721181	1.2106323	-0.3034979
C	2.1419761	-1.4561109	-1.7058853
C	3.3341072	-2.9097389	-0.1245776
C	2.8320381	-1.0049494	3.2834006
C	4.6194033	0.4210837	2.4062257
C	2.6591300	2.4246221	-0.3437369
C	4.6289545	1.0830144	-0.9523839
C	2.0668109	-2.4839522	-2.6497951
H	1.7271424	-0.4684344	-1.9372666
C	3.2497675	-3.9261340	-1.0995315
C	4.0745460	-3.2095941	1.1588873
C	3.5227769	-1.0471043	4.5066900
C	1.4940544	-1.6931037	3.1630574
C	5.2883635	0.3688182	3.6354268
H	5.0358941	1.0222058	1.5930884
C	3.1777896	3.5294138	-1.0271879
H	1.6839467	2.4740781	0.1467359
C	5.1229636	2.2116427	-1.6356912
C	5.4381684	-0.1951023	-0.9684836
C	2.6204897	-3.7322222	-2.3352335
H	1.5791696	-2.3096233	-3.6128981
H	3.7024246	-4.8982459	-0.8752744
H	3.3886614	-3.3193890	2.0155623
H	4.6314868	-4.1542920	1.0570703
H	4.7875806	-2.4112254	1.4211986
C	4.7412394	-0.3773057	4.6865288
H	3.0887684	-1.6146131	5.3374516
H	1.3239485	-2.3738478	4.0119980
H	0.6844133	-0.9431703	3.1602241
H	1.4097123	-2.2900560	2.2369348
H	6.2283268	0.9134689	3.7685836
C	4.4140067	3.4191743	-1.6772358

H	2.6096187	4.4635388	-1.0611736
H	6.0883262	2.1332382	-2.1483426
H	5.3938546	-0.7319577	-0.0067213
H	5.0674026	-0.8887144	-1.7443149
H	6.4957972	0.0240402	-1.1878157
H	2.5735533	-4.5543084	-3.0564890
H	5.2537471	-0.4293739	5.6526607
H	4.8300803	4.2738440	-2.2209130

G.F : H-bonded complex of **G** and **F**

165

Energy = -7131.423334674

N	-2.6507869	0.4109983	0.7435666
N	-2.2031562	-0.9468057	0.8752594
H	-3.0459765	0.7186378	1.6431170
H	-1.6793759	0.8958588	0.7445564
B	-3.5845095	1.1294684	-0.4747615
C	-2.9355171	2.6401229	-0.5368190
C	-3.3866707	0.2645073	-1.8380461
C	-5.1298068	1.1566103	0.0814112
C	-2.6885303	3.3748595	0.6327165
C	-2.6335724	3.3219731	-1.7252716
C	-2.0786880	-0.0203796	-2.2527781
C	-4.3925800	-0.2583304	-2.6628510
C	-5.7780282	-0.0658333	0.2817524
C	-5.9164285	2.2775308	0.3928644
C	-2.1883867	4.6777644	0.6558274
F	-3.0041950	2.8307278	1.8442875
C	-2.1246266	4.6289404	-1.7536090
F	-2.8390340	2.7521689	-2.9289555
C	-1.7554160	-0.8066934	-3.3619107
F	-1.0655202	0.5023194	-1.5346438
C	-4.1243882	-1.0757864	-3.7692549
F	-5.7004139	-0.0071477	-2.4308800
C	-7.0687531	-0.2311590	0.7812292
F	-5.1039540	-1.1971999	-0.0532514
C	-7.2242222	2.1760726	0.9005479
F	-5.4693565	3.5338054	0.2068163
C	-1.8945487	5.3107886	-0.5561057
F	-1.9854285	5.3304248	1.8153712
F	-1.8238366	5.2169898	-2.9215137
C	-2.7998400	-1.3505948	-4.1183475
F	-0.4896218	-1.1087409	-3.6761210
F	-5.1289581	-1.6080367	-4.4836596
C	-7.8020453	0.9177383	1.1059870
F	-7.5951912	-1.4514171	0.9651531
F	-7.9243923	3.2812271	1.1891564
F	-1.3962177	6.5522879	-0.5668055
F	-2.5290515	-2.1612109	-5.1494988
F	-9.0401388	0.8133348	1.6000149
P	-2.8796872	-2.4583377	1.0525788
C	-4.2600570	-2.5350580	2.2436743
C	-1.5212813	-3.3400214	1.8985621
C	-3.0687147	-3.2580649	-0.5823687
C	-4.7395234	-1.3335782	2.8039796
C	-4.7529221	-3.7844329	2.7070569
C	-0.9875876	-2.8408803	3.1221855
C	-1.0803266	-4.5779100	1.3855834
C	-1.8260568	-3.2283767	-1.2719189
C	-4.1959047	-3.8862407	-1.1705646
C	-5.7343090	-1.3412950	3.7847485
H	-4.3426894	-0.3747923	2.4693518
C	-5.7635617	-3.7622168	3.6875095
C	-4.2289377	-5.1196315	2.2346112
C	-0.0134033	-3.6243015	3.7687935
C	-1.3771633	-1.5277438	3.7577585
C	-0.1177716	-5.3338633	2.0572008
H	-1.4938609	-4.9591531	0.4491698
C	-1.6648396	-3.8767578	-2.4955469
H	-0.9688037	-2.7009742	-0.8360441
C	-4.0037809	-4.5089843	-2.4247997
C	-5.5924497	-3.9252577	-0.5921423
C	-6.2570657	-2.5656069	4.2194994
H	-6.1006031	-0.3964361	4.1966517
H	-6.1668617	-4.7173419	4.0407171
H	-3.3746859	-5.4358315	2.8601836
H	-5.0127575	-5.8893724	2.3157842
H	-3.8757165	-5.0985397	1.1926187
C	0.4206066	-4.8508032	3.2556937
H	0.4151582	-3.2494847	4.7045496
H	-2.4697090	-1.4101689	3.8352926
H	-0.9592891	-1.4680789	4.7744101
H	-0.9887465	-0.6727618	3.1802921
H	0.2240670	-6.2800270	1.6305203
C	-2.7661513	-4.5285155	-3.0716893
H	-0.6931954	-3.8559780	-2.9950585
H	-4.8655781	-4.9927470	-2.8973496
H	-5.9578579	-4.9656080	-0.5466742
H	-5.6720795	-3.4765256	0.4032340
H	-6.2733525	-3.3642477	-1.2557849
H	-7.0454381	-2.5906165	4.9782077
H	1.1874004	-5.4229962	3.7853465
H	-2.6629715	-5.0337745	-4.0366059
N	3.1298696	-0.1430453	0.9486582
N	2.0474016	0.7014549	0.9460564
H	3.1492250	-0.7155569	1.7921856
C	0.6907238	0.2475657	0.9343154
O	0.4450531	-0.9805653	0.9107300
O	-0.1435651	1.2124610	0.9936599
H	-1.1156435	-0.9962662	0.8822079
B	3.8086611	-0.7799743	-0.2961141
C	5.4044979	-1.0607438	0.0596842
C	3.1764703	-2.3108589	-0.5698564
C	3.6335066	0.2404899	-1.5831134

C	6.0561831	-0.8188607	1.2774221
C	6.2212692	-1.6260952	-0.9321071
C	3.1482359	-3.1982951	0.5165526
C	2.7005054	-2.8626797	-1.7679804
C	2.3635633	0.4051682	-2.1536134
C	4.6227347	1.0484031	-2.1646294
C	7.4286052	-1.0393655	1.4737991
F	5.4060465	-0.3411393	2.3660198
C	7.5887428	-1.8771171	-0.7825874
F	5.6892185	-1.9061553	-2.1457288
C	2.6992532	-4.5205287	0.4498164
F	3.6193795	-2.8050797	1.7312955
C	2.1659141	-4.1567110	-1.8677622
F	2.7432117	-2.1749053	-2.9298173
C	2.0689298	1.2868602	-3.1984246
F	1.3350797	-0.3174816	-1.6735260
C	4.3819682	1.9563318	-3.2081869
F	5.9054727	1.0266702	-1.7274873
C	8.2013309	-1.5771974	0.4409498
F	8.0034412	-0.7410924	2.6547501
F	8.3165282	-2.3941007	-1.7883454
C	2.1560887	-4.9939990	-0.7487602
F	2.7817792	-5.3357400	1.5203445
F	1.6626278	-4.6023383	-3.0390915
C	3.0884534	2.0888692	-3.7193882
F	0.8100499	1.4398592	-3.6518519
F	5.3778259	2.7167579	-3.6940734
F	9.5137887	-1.8008581	0.6177382
F	1.6527131	-6.2399118	-0.8251585
F	2.8202046	2.9826152	-4.6825282
P	2.1573335	2.2981249	1.6794278
C	3.9171691	2.4990046	2.0796280
C	1.0718313	2.3706908	3.1318467
C	1.7678501	3.6010893	0.4680459
C	4.7280318	2.3771207	0.9294310
C	4.5074904	2.7642127	3.3456311
C	1.0945024	1.3298219	4.0960728
C	0.1345236	3.4161309	3.2170807
C	1.1871411	3.1997622	-0.7504318
C	2.1320551	4.9589607	0.6838578
C	6.1187778	2.4619998	1.0085002
H	4.2503235	2.2148180	-0.0396885
C	5.9153277	2.8297617	3.3936076
C	3.7604377	3.0177872	4.6364291
C	0.1841545	1.4210703	5.1649557
C	2.0116618	0.1311545	3.9944234
C	-0.7722431	3.4703355	4.2796019
H	0.0987721	4.1755508	2.4321221
C	0.9825171	4.1247883	-1.7785800
H	0.8825445	2.1625604	-0.8797514
C	1.8859305	5.8712081	-0.3595305
C	2.7827494	5.4550832	1.9538536
C	6.7154878	2.6658044	2.2585564
H	6.7186210	2.3512569	0.1028881
H	6.3895029	3.0285915	4.3609585
H	3.4352996	2.0784963	5.1152910
H	4.4246704	3.5343116	5.3475233
H	2.8601157	3.6347472	4.4938210
C	-0.7377725	2.4722900	5.2632943
H	0.1983604	0.6408891	5.9340990
H	2.1648381	-0.3227167	4.9868637
H	1.5705999	-0.6439197	3.3397962
H	3.0017819	0.3832311	3.5773143
H	-1.5053939	4.2801297	4.3251294
C	1.3346913	5.4655607	-1.5812614
H	0.5429650	3.7947819	-2.7231376
H	2.1426726	6.9247799	-0.2049550
H	2.3810172	4.9581888	2.8523494
H	3.8713743	5.2679798	1.9357609
H	2.6254667	6.5398952	2.0667613
H	7.8053246	2.7147572	2.3496115
H	-1.4357515	2.5052363	6.1063704
H	1.1618992	6.2014601	-2.3724696

P(*o*-Tol)$_3$: weak phosphine base

43

Energy = -1153.830714853

P	0.2592736	-0.6024812	1.4688497
C	-1.3326246	-1.5331136	1.6418880
C	0.1646163	0.7186898	2.7707408
C	1.5448019	-1.8292308	1.9522336
C	-1.8722495	-1.9414713	0.4017901
C	-2.0287607	-1.8508019	2.8415472
C	0.8923318	0.8776135	3.9834327
C	-0.7802554	1.7067371	2.4043640
C	1.2225434	-3.1157096	2.4280149
C	2.9047926	-1.4941797	1.6988211
C	-3.0711976	-2.6604602	0.3226898
H	-1.3313065	-1.6809118	-0.5154984
C	-3.2411599	-2.5622015	2.7381149
C	-1.5245326	-1.4653845	4.2108170
C	0.6293664	2.0235566	4.7656302
C	1.9060245	-0.1117479	4.5135523
C	-1.0426512	2.8184527	3.2099373
H	-1.3251421	1.5866383	1.4594877
C	2.2258520	-4.0552185	2.7004189
H	0.1724097	-3.3824023	2.5860742
C	3.8965166	-2.4490067	1.9860816
C	3.2828109	-0.1439207	1.1344304
C	-3.7624229	-2.9667838	1.5019901
H	-3.4637204	-2.9703146	-0.6515352
H	-3.7827168	-2.8108447	3.6583720
H	-2.0556750	-2.0327144	4.9925956
H	-0.4449434	-1.6624105	4.3095070

H -1.6729236 -0.3883661 4.4050956
C -0.3223935 2.9823828 4.4014396
H 1.1853576 2.1487049 5.7022863
H 1.5298317 -1.1468550 4.4876921
H 2.8392297 -0.1076577 3.9247790
H 2.1653408 0.1388785 5.5550251
H -1.7928296 3.5546806 2.9024744
C 3.5694836 -3.7170011 2.4884156
H 1.9566706 -5.0475565 3.0778849
H 4.9464677 -2.1926225 1.8022034
H 2.7191818 0.0602105 0.2051180
H 3.0361068 0.6776178 1.8330270
H 4.3618158 -0.0926842 0.9158115
H -4.7061757 -3.5215499 1.4633948
H -0.4996832 3.8506269 5.0450373
H 4.3626589 -4.4419592 2.7004556

R : (tBuO$_2$CN)$_2$ diazo reactant
34
Energy = -801.8728949798
N 0.3242872 0.4256936 -0.3648209
N -0.3166581 -0.3815757 0.3445181
C 1.6620137 -0.0110872 -0.6987326
O 1.9130245 -0.3660522 -1.8320749
O 2.4685025 0.1491665 0.3397149
C -1.6539227 0.0535748 0.6805333
O -1.8982559 0.4329547 1.8074170
O -2.4679790 -0.1392801 -0.3464265
C 3.9453112 -0.0969652 0.2247605
C 4.1722632 -1.5706538 -0.1249205
C 4.5301031 0.8608714 -0.8171842
C 4.4391204 0.2309850 1.6340156
H 3.6669997 -2.2201475 0.6097157
H 3.7944092 -1.8018610 -1.1322517
H 5.2540042 -1.7857235 -0.0930887
H 4.2838977 1.9049364 -0.5598373
H 5.6284486 0.7557388 -0.8249957
H 4.1468779 0.6356954 -1.8238695
H 5.5307277 0.0831973 1.6881143
H 4.2109619 1.2790533 1.8890354
H 3.9553442 -0.4266624 2.3750227
C -3.9467819 0.0909020 -0.2226474
C -4.5088597 -0.8482712 0.8483970
C -4.1893118 1.5697589 0.0930313
C -4.4501250 -0.2782786 -1.6182407
H -4.2510563 -1.8950938 0.6146442
H -4.1193620 -0.5930530 1.8454473
H -5.6084076 -0.7575411 0.8641087
H -3.6999385 2.2073665 -0.6624717
H -5.2740186 1.7702325 0.0672293
H -3.8043121 1.8304311 1.0904168
H -5.5439709 -0.1452894 -1.6649864
H -3.9819645 0.3665128 -2.3802389
H -4.2113722 -1.3295347 -1.8493345

tBe : alkene CH_2=CMe_2
12
Energy = -157.1529051957
C -0.0447611 -0.0266577 -0.1021160
C -1.2918400 -0.5013708 -0.2854987
C 1.1579313 -0.9379208 -0.0264754
C 0.2389673 1.4503869 0.0408385
H -2.1582677 0.1694255 -0.3389055
H -1.4864933 -1.5761435 -0.3879940
H 1.8921625 -0.6847244 -0.8156537
H 1.6829962 -0.8147869 0.9405132
H 0.8781054 -1.9983855 -0.1383359
H 0.7304777 1.6632401 1.0098883
H 0.9378768 1.7933921 -0.7464249
H -0.6812817 2.0540889 -0.0231284

tBu$^+$: CMe_3^+ carbocation
13
Energy = -157.5226596561
C 0.0022371 -0.0019212 -0.0132734
C -1.3725251 -0.5100299 -0.0113428
C 1.1397128 -0.9259267 0.0113972
C 0.2413120 1.4419515 0.0029942
H -2.0983858 0.2133233 -0.4168201
H -1.4761900 -1.5155199 -0.4451828
H -1.6189225 -0.5988062 1.0759002
H 2.0670273 -0.4762191 -0.3789672
H 1.3249352 -1.0864472 1.1025600
H 0.9216430 -1.9124478 -0.4235769
H 1.2175359 1.7242478 0.4273601
H 0.2931309 1.6931378 -1.0866802
H -0.5989719 2.0255384 0.4106046

TMPH$^+$: *N*-protonated TMP base
30
Energy = -409.4121063455
N 0.8829134 0.3844648 -0.0000723
C 0.2150871 0.0241036 1.3544395
C 0.2148481 0.0241037 -1.3544762
H 1.8435650 0.0058581 -0.0001662
C -1.2577770 0.4644521 1.2607591
C 0.3792312 -1.4747467 1.6340709
C 0.9799796 0.8441694 2.4030381
C 0.3789954 -1.4747253 -1.6342222
C 0.9794860 0.8442772 -2.4031745
C -1.2580294 0.4643720 -1.2605121
C -1.9692868 -0.0431274 0.0002110
H -1.2999162 1.5702386 1.2824516
H -1.7666271 0.1123777 2.1737196

H	-0.2614243	-2.1039258	1.0008625
H	1.4281541	-1.7952288	1.5094744
H	0.0963435	-1.6581349	2.6827329
H	0.9265683	1.9260233	2.1858948
H	0.5242103	0.6767469	3.3918215
H	2.0398490	0.5398965	2.4612939
H	1.4279192	-1.7952383	-1.5097022
H	-0.2616414	-2.1039224	-1.0010125
H	0.0959613	-1.6580215	-2.6828558
H	0.9260131	1.9261085	-2.1859158
H	2.0393786	0.5401134	-2.4616159
H	0.5234883	0.6768818	-3.3918571
H	-1.3002256	1.5701508	-1.2823375
H	-1.7671378	0.1122056	-2.1733003
H	-2.0248613	-1.1462251	0.0002425
H	-3.0106026	0.3182467	0.0002971
H	0.9969401	1.4107824	-0.0000888

TMP : bulky tetramethylpiperidine base
29
Energy = -408.9798401783

N	0.8649460	0.4036311	0.0000008
C	0.2502816	0.0257485	1.2904480
C	0.2503208	0.0257428	-1.2904610
H	1.8555511	0.1377890	0.0000052
C	-1.2313534	0.4639018	1.2555219
C	0.3681540	-1.4787706	1.6500503
C	0.9970300	0.8349619	2.3678985
C	0.3682085	-1.4787939	-1.6500133
C	0.9969955	0.8350411	-2.3679372
C	-1.2313130	0.4638858	-1.2555355
C	-1.9596259	-0.0309848	-0.0000179
H	-1.2625643	1.5698223	1.2697322
H	-1.7365163	0.1097658	2.1726933
H	-0.2568869	-2.1164783	1.0053416
H	1.4157136	-1.8147163	1.5466061
H	0.0561439	-1.6518981	2.6960294
H	0.9520790	1.9104340	2.1281352
H	0.5561391	0.6672457	3.3665248
H	2.0609045	0.5351632	2.4119251
H	1.4157417	-1.8147782	-1.5464432
H	-0.2569175	-2.1164504	-1.0053368
H	0.0562812	-1.6519749	-2.6960038
H	0.9517732	1.9104832	-2.1281093
H	2.0608958	0.5353529	-2.4120339
H	0.5560113	0.6673043	-3.3665202
H	-1.2624724	1.5698002	-1.2697240
H	-1.7364914	0.1097825	-2.1727118
H	-2.0174535	-1.1359339	-0.0000220
H	-3.0029665	0.3333928	-0.0000422

TS1 : activated **R** *t*Bu deprotonation with TMP
97
Energy = -3417.815896361

N	-2.9090536	-0.7270709	0.5946510
N	-3.7294453	0.1648074	0.2863963
C	-1.5273799	-0.2731333	0.4808982
O	-0.8521068	-0.5792401	1.5401691
O	-1.1214669	0.2381047	-0.5586541
C	-5.1007073	-0.2689750	0.1914092
O	-5.5550790	-0.5398970	-0.9081510
O	-5.7050109	-0.1917914	1.3630476
C	-1.7535759	0.3080216	-2.9321988
C	-2.6874032	-0.8583076	-2.9831365
C	-2.3638394	1.6574339	-2.7398474
C	-0.4068779	0.1576318	-3.2952514
H	-2.1725521	-1.8117646	-2.7900858
H	-3.5344054	-0.7362013	-2.2907236
H	-3.1214844	-0.9032028	-4.0028674
H	-1.6132436	2.4602009	-2.7036597
H	-3.0858715	1.8591614	-3.5562602
H	-2.9372421	1.6478834	-1.7955331
H	-0.3892666	0.2507852	-4.6051148
H	0.2708930	0.9675307	-2.9971156
H	0.0199680	-0.8434654	-3.1508872
C	-7.1853844	-0.4299204	1.5047802
C	-7.9346640	0.6077487	0.6639395
C	-7.4919195	-1.8702450	1.0885384
C	-7.4057795	-0.2134364	3.0023912
H	-7.6303102	1.6279716	0.9521373
H	-7.7455530	0.4618770	-0.4114382
H	-9.0177518	0.5047919	0.8493048
H	-6.8705609	-2.5757439	1.6647193
H	-8.5530238	-2.0868031	1.3025546
H	-7.3091630	-2.0206494	0.0131101
H	-8.4714235	-0.3638595	3.2446282
H	-6.8047167	-0.9283893	3.5886273
H	-7.1184333	0.8105858	3.2916907
B	0.6465474	-0.2210133	1.6269772
C	0.8716126	1.4052189	1.7253433
C	1.1285666	-0.8301121	3.0769239
C	1.3574091	-0.9312881	0.3212503
C	-0.1203573	2.3926799	1.7931850
C	2.1836168	1.8822861	1.8623632
C	0.3755104	-0.5202662	4.2223354
C	2.2870749	-1.5811017	3.3178031
C	1.2809646	-2.3280571	0.1901459
C	1.9516308	-0.2733664	-0.7663417
C	0.1641322	3.7584454	1.9454963
C	2.5174506	3.2309455	2.0162137
C	0.7066762	-0.9546242	5.5119502
C	2.6609076	-2.0325601	4.5921367
C	1.7737804	-3.0448389	-0.9100839
C	2.4821903	-0.9491738	-1.8765088

C	1.4899921	4.1827153	2.0615578
C	1.8643411	-1.7174396	5.6978509
C	2.3805134	-2.3418691	-1.9590156
F	-1.4334452	2.0849071	1.7155243
F	3.2133374	1.0043994	1.8224119
F	-0.7259907	0.2527540	4.1206405
F	3.1246036	-1.9184656	2.3117054
F	0.7015413	-3.0600587	1.1656482
F	2.0126388	1.0774512	-0.8295831
F	-0.8303931	4.6636776	1.9939265
F	3.7994167	3.6215370	2.1240570
F	-0.0583004	-0.6296210	6.5697240
F	3.7806509	-2.7581181	4.7611075
F	1.6680520	-4.3827225	-0.9726068
F	3.0149559	-0.2610982	-2.9106311
F	1.7768370	5.4873289	2.2094797
F	2.2077501	-2.1407151	6.9245762
F	2.8440116	-2.9923487	-3.0411353
N	-0.1709698	0.3160423	-6.0695701
C	0.6783163	1.5362822	-6.3445086
C	0.2955328	-1.0483487	-6.5217520
H	-1.1212905	0.4816164	-6.4305475
C	2.0968538	1.2433011	-5.8097120
C	0.6986814	1.9190786	-7.8405558
C	0.0385174	2.7055492	-5.5711565
C	0.2414282	-1.2170663	-8.0565213
C	-0.6719958	-2.0766382	-5.9082694
C	1.7253845	-1.2489239	-5.9735483
C	2.6669658	-0.0886674	-6.3155434
H	2.0646735	1.2204869	-4.7063813
H	2.7544484	2.0830715	-6.0909009
H	1.3143560	1.2427932	-8.4504550
H	-0.3233932	1.9334155	-8.2590227
H	1.1196264	2.9336477	-7.9409978
H	0.0377746	2.5238244	-4.4866643
H	0.6107776	3.6281892	-5.7590457
H	-1.0020194	2.8786093	-5.9014887
H	-0.7306977	-0.8779529	-8.4574895
H	1.0413517	-0.6740140	-8.5778013
H	0.3532508	-2.2862531	-8.3003172
H	-0.6578281	-2.0467266	-4.8087044
H	-1.7082000	-1.9031818	-6.2540087
H	-0.3766635	-3.0915701	-6.2227256
H	1.6776633	-1.3516599	-4.8764667
H	2.1197691	-2.2038705	-6.3623709
H	2.8443616	-0.0438090	-7.4056294
H	3.6492964	-0.2679204	-5.8462074

TS2[P] : activated **B**[P] *t*Bu deprotonation with TMP

118

Energy = -5467.166210782

N	-0.1273769	-1.7155251	0.4042308
N	0.4400600	-1.5194326	-0.6949708
C	-1.4852799	-2.2249995	0.2816686
O	-2.2936739	-1.1950101	0.1711279
O	-1.7376154	-3.4081490	0.3736016
C	1.7079328	-0.8234911	-0.5883161
O	2.6615540	-1.4823414	-0.0180357
O	1.7419188	0.3006915	-1.0885655
C	-0.0652617	1.9733369	-0.6029568
C	-0.9596698	1.4313836	-1.6647832
C	-0.2968286	1.5246881	0.8013469
C	0.7508123	3.0896561	-0.8442387
H	-1.0518785	0.3391532	-1.5739838
H	-1.9803737	1.8352547	-1.5110468
H	-0.6169044	1.6978446	-2.6748355
H	0.5818377	1.6734624	1.4426776
H	-1.1235204	2.1338458	1.2144570
H	-0.6357435	0.4821080	0.8583164
H	-0.0909251	4.0536785	-0.5275917
H	1.5586720	3.2681546	-0.1236366
H	1.0301743	3.2902176	-1.8867900
B	-3.8094279	-1.3071246	-0.0125288
C	-4.5923493	-1.7272356	1.3651863
C	-4.2356338	0.2710557	-0.3084427
C	-4.0331760	-2.3303328	-1.2768609
C	-4.0120251	-1.9701061	2.6164842
C	-5.9943902	-1.7510230	1.3456109
C	-3.7946241	1.2515937	0.5960431
C	-4.9664676	0.7630246	-1.3988488
C	-3.4748406	-2.0130564	-2.5248040
C	-4.6192303	-3.6018611	-1.2069929
C	-4.7675554	-2.2529074	3.7664063
C	-6.7893002	-2.0298814	2.4613097
C	-3.9567970	2.6265012	0.3848663
C	-5.1674432	2.1328552	-1.6411287
C	-3.5144193	-2.8543198	-3.6417842
C	-4.6876787	-4.4806983	-2.2986735
C	-6.1635031	-2.2816481	3.6890842
C	-4.6481850	3.0716515	-0.7451982
C	-4.1287593	-4.1064325	-3.5244521
F	-2.6757408	-1.9329203	2.7926532
F	-6.6415768	-1.5083340	0.1803150
F	-3.1539860	0.8987554	1.7296219
F	-5.5141720	-0.0682350	-2.3041358
F	-2.8579795	-0.8198401	-2.7053675
F	-5.1492899	-4.0690153	-0.0578450
F	-4.1616755	-2.4825895	4.9452366
F	-8.1322905	-2.0519391	2.3745231
F	-3.4239863	3.5366065	1.2412470
F	-5.8454843	2.5509770	-2.7224266
F	-2.9722291	-2.4790089	-4.8137867
F	-5.2690046	-5.6873617	-2.1718444
F	-6.8989698	-2.5477417	4.7818723

F	-4.8014239	4.3914788	-0.9714240
F	-4.1827570	-4.9370774	-4.5781815
B	4.0799652	-0.9108818	0.1500617
C	4.9571164	-1.1133814	-1.2246564
C	3.9435140	0.6566380	0.6434456
C	4.7570749	-1.9009488	1.2815786
C	4.4959341	-1.6314529	-2.4417511
C	6.3322464	-0.8369241	-1.1843651
C	4.4126834	1.7881873	-0.0381960
C	3.2267035	0.9364650	1.8168583
C	4.6734003	-3.2909081	1.0918000
C	5.4782529	-1.5029333	2.4153533
C	5.3332695	-1.8518440	-3.5479496
C	7.2051502	-1.0362725	-2.2581432
C	4.2259788	3.1005809	0.4235486
C	3.0061866	2.2270465	2.3123646
C	5.2181733	-4.2300246	1.9782162
C	6.0435655	-2.4059937	3.3277406
C	6.6965371	-1.5565211	-3.4550056
C	3.5243605	3.3211577	1.6117060
C	5.9123765	-3.7807635	3.1073996
F	3.1982253	-1.9526064	-2.6270330
F	6.8704189	-0.3156520	-0.0564750
F	5.0561023	1.6852307	-1.2189459
F	2.6805660	-0.0738367	2.5254127
F	4.0598094	-3.7923119	0.0007838
F	5.6782858	-0.1955326	2.6955925
F	4.8362373	-2.3500370	-4.6944500
F	8.5137186	-0.7381038	-2.1575791
F	4.6723051	4.1555175	-0.2858381
F	2.2683582	2.4315330	3.4214304
F	5.1007019	-5.5496834	1.7465606
F	6.7185663	-1.9630855	4.4048577
F	7.5098818	-1.7623156	-4.5047243
F	3.3156274	4.5770409	2.0537770
F	6.4499525	-4.6603817	3.9684170
N	-0.9478747	5.2223341	-0.1638220
C	-0.2995068	5.9227473	1.0069087
C	-1.2158894	5.9798785	-1.4404275
H	-1.8222121	4.7845758	0.1594129
C	1.0061571	6.5626811	0.4892788
C	-1.2279625	6.9676341	1.6650410
C	-0.0014349	4.8461120	2.0652048
C	-2.3406198	7.0282868	-1.2913898
C	-1.6814912	4.9505226	-2.4877637
C	0.1181788	6.6238506	-1.8742446
C	0.7844856	7.4338966	-0.7542564
H	1.7274637	5.7604902	0.2502293
H	1.4559099	7.1504272	1.3081932
H	-1.3330301	7.8887922	1.0748166
H	-2.2333360	6.5444325	1.8339866
H	-0.8083705	7.2460031	2.6464102
H	0.6564928	4.0589048	1.6762941
H	0.5071150	5.3045628	2.9279340
H	-0.9362385	4.3812489	2.4245238
H	-3.2226617	6.5842168	-0.8002424
H	-2.0317989	7.9165506	-0.7228386
H	-2.6475474	7.3651077	-2.2960742
H	-0.9272315	4.1687171	-2.6576822
H	-2.6270068	4.4749880	-2.1778656
H	-1.8629996	5.4618338	-3.4472510
H	0.8063491	5.8193379	-2.1942310
H	-0.0690278	7.2550223	-2.7605292
H	0.1663641	8.3149544	-0.5003878
H	1.7529248	7.8278497	-1.1084764

TS3 : activated **R** *t*Bu proton transfer to N-atom 68

Energy = -3008.804885032

N	-2.4233044	0.3838435	-1.3979749
N	-3.2036490	0.6704927	-0.4800968
C	-0.9676922	0.5611043	-1.1696585
O	-0.5677954	0.0073749	-0.0963582
O	-0.4162821	1.1692715	-2.0734537
C	-4.6319941	0.5732623	-0.8880877
O	-4.9948853	0.1700933	-1.9734214
O	-5.3286333	0.9827624	0.1465497
C	-1.6654179	0.1830385	-4.5963046
C	-1.4406875	1.5796123	-5.0752667
C	-0.5130386	-0.7653737	-4.6550155
C	-2.8941267	-0.2060142	-4.0771994
H	-2.2882654	2.2426967	-4.8449224
H	-0.5129812	1.9909039	-4.6438622
H	-1.3063308	1.5539529	-6.1750802
H	-0.6531532	-1.6410166	-4.0038884
H	-0.4233332	-1.1325729	-5.6973289
H	0.4322442	-0.2586153	-4.4062801
H	-3.7730203	0.4259148	-4.2552184
H	-3.0941280	-1.2765992	-3.9285252
H	-2.6829970	0.1194274	-2.7782627
C	-6.8371796	1.0017259	0.1202484
C	-7.2939443	1.9518430	-0.9899073
C	-7.3361802	-0.4325040	-0.0730024
C	-7.1746203	1.5426226	1.5087869
H	-6.8503536	2.9517329	-0.8487862
H	-7.0234755	1.5681277	-1.9853485
H	-8.3912576	2.0507485	-0.9393881
H	-6.9239614	-1.0932962	0.7076474
H	-8.4356049	-0.4379362	0.0147304
H	-7.0626153	-0.8235710	-1.0647990
H	-8.2695188	1.6057646	1.6206435
H	-6.7767544	0.8764185	2.2916654
H	-6.7461122	2.5487517	1.6474045
B	0.9203002	-0.0817992	0.3726230

C	1.2894627	1.2740370	1.2127980
C	0.8838359	-1.3408936	1.4260302
C	1.8310882	-0.3596911	-0.9605505
C	0.5145355	2.4366383	1.3092841
C	2.4592761	1.2769857	1.9891686
C	-0.0867335	-1.3450961	2.4422043
C	1.7755205	-2.4221944	1.4502598
C	1.4972476	-1.4327562	-1.8010889
C	2.9401556	0.3875914	-1.3807841
C	0.8642329	3.5294336	2.1177586
C	2.8523555	2.3415977	2.8063392
C	-0.2032096	-2.3635019	3.3975259
C	1.6987122	-3.4616618	2.3890198
C	2.2104601	-1.7833692	-2.9500282
C	3.6898744	0.0753643	-2.5264014
C	2.0391593	3.4805453	2.8742428
C	0.7016048	-3.4316339	3.3702064
C	3.3199986	-1.0143815	-3.3216130
F	-0.6381531	2.5794629	0.6124850
F	3.2899005	0.2116927	1.9398522
F	-0.9664755	-0.3269360	2.5437775
F	2.7827156	-2.5157265	0.5558552
F	0.4093051	-2.1939362	-1.5167050
F	3.3552181	1.4727217	-0.6986286
F	0.0794649	4.6189715	2.1698223
F	3.9896453	2.2864926	3.5175113
F	-1.1580593	-2.3182028	4.3419396
F	2.5765996	-4.4780406	2.3599397
F	1.8147400	-2.8117925	-3.7232007
F	4.7462530	0.8257081	-2.8758266
F	2.3890453	4.5165925	3.6496491
F	0.6133376	-4.4158094	4.2762157
F	4.0130108	-1.3159531	-4.4282499

TS4 : phosphine addition to $B(C_6F_5)_3$ adduct **E**

96

Energy = -3817.074134533

N	-0.7209038	-0.9449272	-0.2930887
N	0.3977699	-1.4355242	0.0690171
H	-1.0052935	-1.1261750	-1.2708903
C	0.9472813	-2.4339784	-0.8438935
O	1.9979106	-2.9906881	-0.5981191
O	0.1091024	-2.6839676	-1.8461375
C	0.1995605	-3.9203405	-2.6984784
C	1.5126978	-3.9045935	-3.4781585
C	0.0660527	-5.1306742	-1.7716851
C	-1.0108680	-3.7638660	-3.6181629
H	1.5998792	-2.9758913	-4.0625451
H	2.3770601	-3.9831445	-2.8031612
H	1.5224249	-4.7608286	-4.1741131
H	-0.8697554	-5.0710844	-1.1905867
H	0.0380700	-6.0491521	-2.3816835
H	0.9213051	-5.1959516	-1.0811202
H	-1.0696938	-4.6289638	-4.2990994
H	-1.9417091	-3.7058277	-3.0316973
H	-0.9181414	-2.8453727	-4.2210568
B	-1.6861346	-0.1192879	0.6548530
C	-1.2063671	1.4590661	0.6058556
C	-3.2007947	-0.1245787	-0.0001032
C	-1.5835424	-0.8829809	2.1000209
C	-0.8426057	2.0095384	-0.6296392
C	-1.2208642	2.3713105	1.6725503
C	-3.6086287	-0.6351183	-1.2378206
C	-4.2215982	0.5135378	0.7249809
C	-2.4712751	-1.8942537	2.4980308
C	-0.4940169	-0.6903019	2.9612222
C	-0.4633669	3.3399598	-0.8271282
F	-0.8683413	1.2247639	-1.7446870
C	-0.8772413	3.7220759	1.5199439
F	-1.5638640	1.9873974	2.9157686
C	-4.9153182	-0.5355100	-1.7363579
F	-2.7319262	-1.2880645	-2.0567413
C	-5.5422011	0.6353141	0.2791844
F	-3.9439671	1.0351494	1.9379520
C	-2.3224050	-2.6313752	3.6829708
F	-3.5291718	-2.2335281	1.7288924
C	-0.2957358	-1.4036086	4.1476397
F	0.4459487	0.2293113	2.6551437
C	-0.4932190	4.2105331	0.2661245
F	-0.0723680	3.7739193	-2.0364130
F	-0.8665120	4.5457781	2.5802259
C	-5.8927473	0.1067571	-0.9700651
F	-5.2302365	-1.0518118	-2.9341595
F	-6.4679410	1.2498233	1.0293330
C	-1.2214023	-2.3888985	4.5117542
F	-3.2113085	-3.5812956	4.0130400
F	0.7786690	-1.1719449	4.9211028
F	-0.1340578	5.4924388	0.1231019
F	-7.1479960	0.2133967	-1.4232587
F	-1.0545987	-3.0912086	5.6395675
P	2.6744546	0.0354438	-0.3541394
C	2.6929659	1.8752472	-0.1566592
C	2.9294091	-0.3852462	-2.1205675
C	4.1774319	-0.3603467	0.6415501
C	2.3177560	2.2248470	1.1638303
C	3.1180674	2.8937386	-1.0548721
C	3.9131680	-1.2491568	-2.6796018
C	1.9307022	0.1689310	-2.9586701
C	5.3576580	0.3506447	0.3215642
C	4.1592179	-1.2574723	1.7357053
C	2.3336486	3.5476425	1.6072111
H	2.0322948	1.4304396	1.8571884
C	3.0954183	4.2256199	-0.5846427
C	3.6397522	2.6707993	-2.4566440

C	3.9193754	-1.4035961	-4.0817942
C	4.9265326	-2.0274179	-1.8722168
C	1.9487408	-0.0225986	-4.3419035
H	1.1483375	0.7941232	-2.5183760
C	6.5382535	0.1402257	1.0353636
H	5.3436686	1.0764719	-0.4981558
C	5.3673592	-1.4487576	2.4443863
C	2.9244262	-1.9931414	2.1956994
C	2.7129958	4.5616782	0.7169227
H	2.0355818	3.7844608	2.6332078
H	3.4166569	5.0181265	-1.2699099
H	4.3003502	3.5060291	-2.7410466
H	4.2013682	1.7297903	-2.5552714
H	2.8166255	2.6321620	-3.1917227
C	2.9717094	-0.7932697	-4.9120271
H	4.6868443	-2.0473383	-4.5262895
H	5.7390180	-1.3853977	-1.4924847
H	4.4534363	-2.5090516	-1.0030501
H	5.3786248	-2.8103262	-2.5028203
H	1.1744843	0.4340391	-4.9665696
C	6.5421775	-0.7757130	2.1007959
H	7.4456389	0.6924549	0.7702552
H	5.3689459	-2.1392387	3.2955454
H	2.0136659	-1.5966014	1.7277022
H	2.9910569	-3.0635256	1.9340750
H	2.8239289	-1.9158725	3.2915672
H	2.7150550	5.6087362	1.0346401
H	3.0155159	-0.9448757	-5.9955260
H	7.4585769	-0.9484151	2.6751610

TS5a : direct ester tBu deprotonation of **4**

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Energy = -3817.063242761

N	-0.0537304	-0.0797023	0.8994610
N	1.2224385	0.2814047	0.5264394
H	-0.1820601	0.0300187	1.9051125
C	1.7067411	1.6241067	0.6606336
O	0.9360150	2.4616145	1.2162341
O	2.8682906	1.8277995	0.2128406
C	3.1749915	4.1020989	-0.3470205
C	4.4132757	4.1053609	0.4885795
C	3.2898825	3.7029991	-1.7817770
C	1.9769329	4.6806677	0.1466377
H	5.0398684	3.2249783	0.2826733
H	4.9909286	5.0146389	0.2221145
H	4.1784635	4.1561295	1.5628332
H	3.6631849	4.5904542	-2.3343376
H	4.0115397	2.8848601	-1.9233556
H	2.3147500	3.4296780	-2.2105290
H	1.2329950	4.9855929	-0.6026983
H	1.4593769	3.6976893	0.6933406
H	2.0881838	5.3660557	1.0003106
B	-1.3207457	0.1712743	0.0407123
C	-2.4643003	-0.9401645	0.5024872
C	-2.0186259	1.6534421	0.3761467
C	-0.8759647	0.0270739	-1.5493308
C	-2.3789848	-1.8276156	1.5860614
C	-3.6720234	-1.0141639	-0.2093847
C	-2.1143894	2.0673593	1.7132275
C	-2.5785331	2.5533317	-0.5415319
C	-0.1635772	1.0503660	-2.1928781
C	-1.0891438	-1.0981590	-2.3612823
C	-3.3742011	-2.7688344	1.8939227
F	-1.3127839	-1.8529820	2.4231378
C	-4.6977162	-1.9251016	0.0634039
F	-3.8660553	-0.1944691	-1.2683905
C	-2.6499951	3.2916093	2.1269938
F	-1.6770897	1.2568968	2.7149746
C	-3.1279818	3.7934477	-0.1822530
F	-2.6084403	2.2769147	-1.8665627
C	0.2872454	0.9932765	-3.5141185
F	0.1477299	2.1918212	-1.5303018
C	-0.6447738	-1.2143718	-3.6884524
F	-1.7407075	-2.1903186	-1.8938333
C	-4.5445772	-2.8176859	1.1319920
F	-3.2068732	-3.6230529	2.9214992
F	-5.8165579	-1.9564475	-0.6814850
C	-3.1648136	4.1675584	1.1644735
F	-2.6899305	3.6268623	3.4299873
F	-3.6304705	4.6203472	-1.1184401
C	0.0649194	-0.1608836	-4.2692432
F	1.0181731	2.0022129	-4.0355741
F	-0.8687161	-2.3389502	-4.3875301
F	-5.5078479	-3.7081553	1.4184573
F	-3.6895449	5.3491175	1.5303060
F	0.5461335	-0.2592175	-5.5169454
P	2.4925245	-0.9249564	0.5466718
C	1.6478746	-2.4621388	0.9989542
C	3.7738715	-0.3866559	1.7071480
C	3.1933438	-1.1760009	-1.1132648
C	0.6219266	-2.7758237	0.0792338
C	1.8960569	-3.3051722	2.1149267
C	3.4144955	0.0656802	3.0047785
C	5.1103728	-0.3424616	1.2658057
C	2.9349024	-0.1815765	-2.0754029
C	3.9273730	-2.3451666	-1.4560478
C	-0.2025251	-3.8855178	0.2664375
H	0.4769341	-2.1364559	-0.7938517
C	1.0341372	-4.4085650	2.2843316
C	3.0250195	-3.1417688	3.1083477
C	4.4517579	0.5221180	3.8379735
C	1.9870489	0.0997504	3.5041441
C	6.1194632	0.1160797	2.1180438
H	5.3533646	-0.6550840	0.2455043

C	3.3766349	-0.3335430	-3.3936741
H	2.3957867	0.7139585	-1.7687248
C	4.3665176	-2.4657419	-2.7881056
C	4.2427459	-3.4487037	-0.4733422
C	-0.0089442	-4.6907052	1.3958827
H	-0.9953341	-4.0963200	-0.4547374
H	1.2046822	-5.0699039	3.1408291
H	2.7670789	-2.4273977	3.9090246
H	3.2321454	-4.1105197	3.5903749
H	3.9543748	-2.7823872	2.6412220
C	5.7858385	0.5470248	3.4100735
H	4.2005460	0.8666391	4.8471582
H	1.9649945	0.0607261	4.6049835
H	1.4842938	1.0349023	3.1945931
H	1.3810769	-0.7394770	3.1213458
H	7.1578116	0.1410309	1.7734799
C	4.0906538	-1.4846957	-3.7498767
H	3.1518798	0.4386221	-4.1349653
H	4.9362956	-3.3571360	-3.0725851
H	4.5070778	-3.0554277	0.5226312
H	3.3752385	-4.1190617	-0.3397343
H	5.0889616	-4.0538050	-0.8362298
H	-0.6597388	-5.5518164	1.5781004
H	6.5661376	0.9085910	4.0877818
H	4.4395385	-1.6202290	-4.7787371

TS5h : CMe_3^+ deprotonation of activated **4**

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Energy = -6024.059443449

N	-1.5142530	-0.0846616	0.8510289
N	-0.8450574	-1.1963784	0.4154905
H	-1.1701570	0.2312932	1.7581301
C	0.5329617	-1.1737093	0.1095159
O	1.1432111	-0.0864553	0.3408786
O	0.9701209	-2.2848139	-0.3383397
C	2.8560668	-3.4069209	-2.7673514
C	1.6473074	-3.6702707	-3.6037889
C	4.0119445	-2.7643704	-3.4595138
C	2.8716149	-3.7100563	-1.4115760
H	0.8896070	-4.2708351	-3.0824414
H	1.2074640	-2.6957448	-3.8902395
H	1.9380460	-4.1688920	-4.5454423
H	4.4335321	-3.5202350	-4.1518909
H	3.6802595	-1.9172525	-4.0823854
H	4.8057493	-2.4427546	-2.7746489
H	3.8118761	-3.6098562	-0.8582131
H	2.0491976	-2.7317020	-0.9213055
H	2.1776335	-4.4822589	-1.0503384
B	-2.2615353	0.9779565	-0.0248591
C	-3.5834461	1.5235738	0.8145120
C	-1.3232656	2.3498354	-0.2126199
C	-2.6614273	0.3115773	-1.4885076
C	-3.9501686	1.1867936	2.1259676
C	-4.4174958	2.4779084	0.2094417
C	-0.7889984	2.9303444	0.9485980
C	-1.0612348	3.0762289	-1.3821696
C	-1.6402841	0.0212327	-2.4012962
C	-3.9433243	0.0211901	-1.9840455
C	-5.1001415	1.6843456	2.7578259
F	-3.2250638	0.3280022	2.8821640
C	-5.5662252	3.0139503	0.8003454
F	-4.1444192	2.8913436	-1.0504681
C	0.0083920	4.0792545	0.9695695
F	-1.0695937	2.3832569	2.1582957
C	-0.2967200	4.2517805	-1.4125284
F	-1.5571728	2.6930829	-2.5826404
C	-1.8290292	-0.4820457	-3.6888406
F	-0.3526689	0.2339404	-2.0436858
C	-4.1953396	-0.4999493	-3.2637901
F	-5.0526303	0.2113897	-1.2326055
C	-5.9140401	2.6070748	2.0950334
F	-5.4270350	1.2698852	3.9961403
F	-6.3338790	3.9027533	0.1473622
C	0.2530954	4.7565287	-0.2308017
F	0.5252630	4.5393274	2.1227004
F	-0.0841787	4.8896022	-2.5778909
C	-3.1262927	-0.7643446	-4.1239432
F	-0.7730866	-0.7897060	-4.4700596
F	-5.4501098	-0.7733323	-3.6524788
F	-7.0146846	3.0939440	2.6887206
F	1.0050426	5.8638336	-0.2474796
F	-3.3332382	-1.3135771	-5.3287300
P	-1.4935715	-2.8332208	0.7874325
C	-1.9320574	-3.6944337	-0.7546315
C	-3.0623407	-2.5583477	1.6489787
C	-0.2612292	-3.7754249	1.7127621
C	-1.4735556	-3.1588082	-1.9718877
C	-2.7861778	-4.8343833	-0.7407295
C	-3.4605014	-3.0437045	2.9274954
C	-3.9758594	-1.8413241	0.8443309
C	0.2004200	-4.9937764	1.1697568
C	0.2970344	-3.2431164	2.9022977
C	-1.8720119	-3.7176964	-3.1915249
H	-0.7975127	-2.3046573	-1.9549429
C	-3.1561089	-5.3822180	-1.9830550
C	-3.3173852	-5.4690006	0.5227095
C	-4.7532288	-2.6911376	3.3644095
C	-2.6566008	-3.9464772	3.8357375
C	-5.2571637	-1.5303299	1.3003034
H	-3.6699195	-1.5294012	-0.1558039
C	1.2125594	-5.7090408	1.8133529
H	-0.2332460	-5.3680280	0.2369601
C	1.3155659	-3.9871065	3.5261996
C	-0.1232637	-1.9166591	3.4843642

C	-2.7216017	-4.8301544	-3.1947916
H	-1.5248561	-3.2794901	-4.1311079
H	-3.8087807	-6.2617885	-1.9922398
H	-4.2127604	-4.9336469	0.8852136
H	-3.6014868	-6.5161643	0.3317837
H	-2.5768360	-5.4605179	1.3389644
C	-5.6347396	-1.9344216	2.5860010
H	-5.0773362	-3.0470798	4.3481992
H	-3.3427027	-4.4941375	4.5009363
H	-2.0526609	-4.6818906	3.2843291
H	-1.9696219	-3.3728689	4.4795009
H	-5.9352514	-0.9649889	0.6583320
C	1.7733516	-5.1974192	2.9946166
H	1.5660797	-6.6560785	1.3943223
H	1.7699551	-3.5913611	4.4400481
H	-0.1125102	-1.9554642	4.5859776
H	0.5832754	-1.1280603	3.1849248
H	-1.1289468	-1.5971533	3.1641854
H	-3.0444070	-5.2739266	-4.1418624
H	-6.6253585	-1.6820291	2.9766976
H	2.5770552	-5.7412409	3.5003060
B	2.5992098	0.4485383	0.1710444
C	2.5562553	1.2767221	-1.2410866
C	2.9441775	1.3797323	1.4755466
C	3.7041781	-0.7731026	0.2466458
C	2.6765749	2.6631812	-1.4173001
C	2.3189788	0.5736190	-2.4256653
C	2.1743824	1.5486826	2.6312848
C	4.1903076	2.0280583	1.5044067
C	3.6774649	-1.6383108	1.3519460
C	4.8238921	-0.9269357	-0.5825739
C	2.5881356	3.2927641	-2.6692140
F	2.8831324	3.4951913	-0.3764211
C	2.2133880	1.1426582	-3.6934565
F	2.1619652	-0.7770050	-2.3641655
C	2.5642913	2.3548486	3.7116257
F	0.9905503	0.9153028	2.7872734
C	4.6272194	2.8410901	2.5537721
F	5.0242284	1.9024676	0.4458249
C	4.6461911	-2.6109437	1.6230571
F	2.6738055	-1.5284322	2.2508480
C	5.8272978	-1.8813131	-0.3519459
F	5.0010991	-0.1555705	-1.6731955
C	2.3439097	2.5313600	-3.8174973
F	2.7278759	4.6200808	-2.7653972
F	1.9963507	0.3725190	-4.7759011
C	3.8005784	3.0058982	3.6733504
F	1.7713860	2.4826545	4.7854062
F	5.8199667	3.4534999	2.5038225
C	5.7359352	-2.7389473	0.7510393
F	4.5458918	-3.4101565	2.6969961
F	6.8521158	-2.0068877	-1.2117685
F	2.2460612	3.1189563	-5.0149809
F	4.1947002	3.7749997	4.6968994
F	6.6783604	-3.6620203	0.9737233

TS5 : CMe_3^+ elimination of borane-activated **4**

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Energy = -6024.051084024

N	-1.4255091	-0.1157557	0.8300094
N	-0.7933022	-1.1892745	0.2552515
H	-1.0275041	0.1090566	1.7411667
C	0.6125324	-1.1836566	-0.0617869
O	1.2426381	-0.1430501	0.3668731
O	1.0654050	-2.1681513	-0.6712429
C	2.4851209	-3.9290689	-2.3755981
C	2.3782632	-3.0078860	-3.5189015
C	3.6668515	-3.9099741	-1.5022344
C	1.3641570	-4.7915910	-2.0461764
H	1.7804697	-3.4298236	-4.3414127
H	1.8039722	-2.1397786	-3.1179635
H	3.3449519	-2.6138647	-3.8591388
H	4.5174565	-4.3006336	-2.1017246
H	3.9399741	-2.8689013	-1.2571862
H	3.5450067	-4.5162244	-0.5943441
H	1.6350332	-5.6576152	-1.4268187
H	0.8158055	-4.0670433	-1.3751856
H	0.6916731	-5.0317405	-2.8811234
B	-2.2492145	1.0151743	0.1356601
C	-3.5872909	1.3620255	1.0640292
C	-1.4076236	2.4580029	0.1591312
C	-2.6184386	0.5660651	-1.4175235
C	-3.9077956	0.8113885	2.3136954
C	-4.4777647	2.3625664	0.6375839
C	-0.7803829	2.8602291	1.3476025
C	-1.3463433	3.4059369	-0.8723029
C	-1.5700447	0.3725032	-2.3253991
C	-3.8839502	0.3677310	-1.9944126
C	-5.0605232	1.1485591	3.0395623
F	-3.1316277	-0.1224291	2.9154821
C	-5.6341852	2.7423828	1.3261686
F	-4.2560698	2.9921306	-0.5387353
C	-0.1300416	4.0858241	1.5198051
F	-0.8140349	2.0531857	2.4459326
C	-0.6975834	4.6433232	-0.7554866
F	-1.9089812	3.1670452	-2.0795929
C	-1.7155062	0.0200429	-3.6681170
F	-0.2917403	0.5143115	-1.9091495
C	-4.0935108	0.0043028	-3.3351182
F	-5.0200254	0.4865768	-1.2699987
C	-5.9309330	2.1237360	2.5473043
F	-5.3345220	0.5296602	4.2030176
F	-6.4545731	3.6871239	0.8360594
C	-0.0722190	4.9828920	0.4473901

F	0.4265425	4.4165895	2.7005716
F	-0.6469120	5.4899499	-1.7974896
C	-2.9976725	-0.1857808	-4.1819524
F	-0.6286116	-0.2179978	-4.4330086
F	-5.3376716	-0.1934353	-3.7976813
F	-7.0358078	2.4597816	3.2308585
F	0.5700859	6.1532314	0.5786193
F	-3.1680617	-0.5877788	-5.4489508
P	-1.4672913	-2.8124415	0.4894463
C	-1.8157949	-3.5572116	-1.1402649
C	-3.0986293	-2.6276587	1.2665426
C	-0.3465918	-3.8420184	1.4656307
C	-1.3543766	-2.8708796	-2.2812082
C	-2.6133330	-4.7278901	-1.2776603
C	-3.5632131	-3.2083712	2.4829023
C	-3.9870335	-1.8961904	0.4484132
C	0.0167494	-5.1217272	1.0001198
C	0.1401264	-3.3516659	2.7050732
C	-1.6503175	-3.3338499	-3.5670335
H	-0.7501712	-1.9752998	-2.1457588
C	-2.8682045	-5.1884831	-2.5844487
C	-3.2395976	-5.4604083	-0.1143536
C	-4.9005477	-2.9442502	2.8415372
C	-2.7863457	-4.1133165	3.4120364
C	-5.3114339	-1.6712998	0.8263571
H	-3.6248456	-1.5040378	-0.5041070
C	0.8798271	-5.9268595	1.7485560
H	-0.3889838	-5.4899042	0.0540229
C	0.9995685	-4.1876200	3.4394958
C	-0.1992596	-1.9781810	3.2252563
C	-2.4031272	-4.5060487	-3.7164317
H	-1.3013693	-2.7747673	-4.4401578
H	-3.4665262	-6.0973155	-2.7101625
H	-4.2060169	-4.9946113	0.1505992
H	-3.4313067	-6.5124284	-0.3801913
H	-2.6133563	-5.4427050	0.7907015
C	-5.7629164	-2.1826925	2.0476298
H	-5.2730813	-3.3711744	3.7785979
H	-3.4888002	-4.6168740	4.0942204
H	-2.2134190	-4.8869957	2.8778925
H	-2.0726202	-3.5501174	4.0345335
H	-5.9669675	-1.0895498	0.1761221
C	1.3756858	-5.4514168	2.9718909
H	1.1564687	-6.9210020	1.3839647
H	1.3927249	-3.8239746	4.3943942
H	-0.0737413	-1.9370612	4.3187982
H	0.4837280	-1.2281953	2.7936141
H	-1.2310388	-1.6689980	2.9861951
H	-2.6399206	-4.8864265	-4.7152100
H	-6.7913455	-2.0046970	2.3768793
H	2.0574152	-6.0688630	3.5650100
B	2.7141406	0.3131234	0.1072462
C	2.7628195	0.7322243	-1.4833965
C	2.9282793	1.5764910	1.1422564
C	3.8596672	-0.7865022	0.5422933
C	2.0112804	1.8360015	-1.9134404
C	3.4006262	0.0496244	-2.5245334
C	2.5593079	1.4306720	2.4881277
C	3.5327991	2.8062138	0.8367179
C	3.6707916	-1.9594514	1.2813379
C	5.2078330	-0.4874727	0.2731305
C	1.8333491	2.2093650	-3.2495059
F	1.3741913	2.5894473	-1.0047517
C	3.2634126	0.3794575	-3.8808894
F	4.2185243	-1.0136162	-2.2839634
C	2.7008811	2.4301675	3.4568779
F	2.0516102	0.2533683	2.9278467
C	3.6974011	3.8389275	1.7713522
F	3.9892769	3.0723327	-0.4055246
C	4.7117164	-2.8196176	1.6652961
F	2.4404956	-2.3491331	1.6671667
C	6.2826632	-1.3065366	0.6377206
F	5.5164702	0.6452645	-0.3903080
C	2.4568974	1.4596561	-4.2529138
F	1.0502036	3.2483015	-3.5685771
F	3.8861144	-0.3564644	-4.8246254
C	3.2848595	3.6478290	3.0937899
F	2.3023567	2.2245194	4.7223306
F	4.2600071	5.0029216	1.4092607
C	6.0307500	-2.4940541	1.3399248
F	4.4391861	-3.9609808	2.3269385
F	7.5436710	-0.9691361	0.3280553
F	2.2942002	1.7720202	-5.5439816
F	3.4329766	4.6241854	3.9981183
F	7.0404790	-3.3013893	1.6939424

TS6 : CO_2 release via 1,4-H-shift within **F** 84

Energy = -3659.922293344

N	0.0012623	1.1480150	0.3576331
N	1.2707729	1.1558651	-0.2935475
H	0.1150933	1.2089643	1.3744621
C	1.4510403	2.4498047	-0.9984797
O	0.4263189	3.2003773	-0.7957395
O	2.4880719	2.6238406	-1.6233006
H	-0.1563288	2.3766399	-0.1134077
B	-1.2300382	0.1821325	-0.0763814
C	-1.7755849	-0.6760323	1.2243056
C	-2.4860424	1.2032613	-0.4371967
C	-0.7582006	-0.7264659	-1.3600373
C	-1.3487499	-0.5968183	2.5554178
C	-2.8808619	-1.5244619	1.0317423
C	-2.7988254	2.2273050	0.4702036
C	-3.3613732	1.1059295	-1.5292316

C	-0.4095567	-0.0803356	-2.5570075
C	-0.6450684	-2.1243834	-1.4196818
C	-1.8980329	-1.3457370	3.6046726
F	-0.3178159	0.2181728	2.9289393
C	-3.4730918	-2.2903122	2.0410703
F	-3.4076391	-1.6514540	-0.2043687
C	-3.8626351	3.1229317	0.3186216
F	-2.0370202	2.3860041	1.5870769
C	-4.4425604	1.9778387	-1.7278514
F	-3.2090031	0.1476072	-2.4663190
C	0.0248771	-0.7340161	-3.7124652
F	-0.4834656	1.2661696	-2.6345826
C	-0.2060434	-2.8303878	-2.5505796
F	-0.9367628	-2.9042505	-0.3502649
C	-2.9720692	-2.2017865	3.3470778
F	-1.3878035	-1.2558861	4.8441319
F	-4.5106861	-3.0975034	1.7761741
C	-4.6971081	2.9919969	-0.7979764
F	-4.0946656	4.0843484	1.2255955
F	-5.2405784	1.8418013	-2.7980337
C	0.1471423	-2.1269185	-3.7042759
F	0.4062569	-0.0354988	-4.7949023
F	-0.0921560	-4.1666962	-2.5158560
F	-3.5141347	-2.9277897	4.3334831
F	-5.7268226	3.8299709	-0.9750519
F	0.6213610	-2.7701570	-4.7785548
P	2.7214340	0.4067472	0.2470774
C	2.2753901	-0.6976587	1.6185978
C	3.9186292	1.6904141	0.6827872
C	3.3666841	-0.6341294	-1.0942746
C	1.3885100	-1.7150176	1.2032542
C	2.7888316	-0.6907875	2.9471662
C	3.5654473	2.7584556	1.5489034
C	5.2021195	1.6129607	0.1078676
C	2.9187902	-0.3494911	-2.3997063
C	4.2775991	-1.7001569	-0.8501753
C	0.9423602	-2.6972534	2.0884221
H	1.0554247	-1.7326978	0.1638746
C	2.2985926	-1.6829313	3.8198057
C	3.8458190	0.2439595	3.4894706
C	4.5569526	3.7122034	1.8341297
C	2.1876053	2.9134759	2.1513672
C	6.1689241	2.5751601	0.4152367
H	5.4363610	0.8058490	-0.5927947
C	3.3325475	-1.1391690	-3.4771923
H	2.2630706	0.5061331	-2.5657036
C	4.6722189	-2.4751233	-1.9563687
C	4.8380724	-2.0331868	0.5139200
C	1.3852208	-2.6625612	3.4158358
H	0.2481237	-3.4640356	1.7380979
H	2.6701442	-1.6899882	4.8498206
H	3.4354847	1.2379108	3.7328012
H	4.2586154	-0.1759019	4.4198581
H	4.6758100	0.3992575	2.7829202
C	5.8430062	3.6255670	1.2834961
H	4.3098442	4.5421255	2.5047496
H	2.2326782	3.5285418	3.0637922
H	1.5030788	3.4196969	1.4480291
H	1.7378393	1.9433388	2.4277547
H	7.1658174	2.5090903	-0.0302689
C	4.2014697	-2.2132832	-3.2499086
H	2.9668455	-0.9168953	-4.4834565
H	5.3708320	-3.3026232	-1.7920838
H	5.0605054	-1.1296635	1.1057317
H	4.1298143	-2.6451329	1.1001509
H	5.7730655	-2.6060651	0.4080603
H	1.0361024	-3.4092550	4.1356219
H	6.5897697	4.3873317	1.5291310
H	4.5258387	-2.8445849	-4.0832769

TS8 : unlikely 1,2-H-shift within **G**

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Energy = -3471.368356407

N	-0.0747817	1.1162662	0.2846770
N	1.2258477	1.0847289	-0.5565309
H	0.1431196	1.2428422	1.2745173
H	0.4583692	2.0029496	-0.4454138
B	-1.2549018	0.0969672	-0.0495784
C	-1.6105476	-0.8513543	1.2564065
C	-2.6062533	1.0250964	-0.2762254
C	-0.7926551	-0.7230351	-1.3934022
C	-1.0771005	-0.7671758	2.5479522
C	-2.6310686	-1.8085864	1.1203883
C	-2.9005014	2.0193305	0.6681724
C	-3.5535203	0.8874470	-1.3004665
C	-0.5377163	0.0137778	-2.5611082
C	-0.4863921	-2.0853334	-1.4965681
C	-1.4485325	-1.6074813	3.6066372
F	-0.1164870	0.1474335	2.8676329
C	-3.0450725	-2.6692957	2.1420855
F	-3.2469328	-1.9513145	-0.0726350
C	-4.0264900	2.8485881	0.6117951
F	-2.0715479	2.2058166	1.7294622
C	-4.6982727	1.6930089	-1.4014714
F	-3.4083261	-0.0451007	-2.2649005
C	-0.0160951	-0.5315502	-3.7355685
F	-0.7643415	1.3480497	-2.5733915
C	0.0364678	-2.6847494	-2.6548607
F	-0.6385161	-2.9276724	-0.4443200
C	-2.4422564	-2.5686218	3.4034055
F	-0.8468993	-1.5019457	4.8041759
F	-4.0084181	-3.5800683	1.9327772
C	-4.9366086	2.6805942	-0.4392234
F	-4.2462512	3.7863848	1.5489220

F	-5.5681718	1.5237383	-2.4108021
C	0.2865892	-1.8974665	-3.7803726
F	0.2793376	0.2515413	-4.7901869
F	0.3294648	-3.9953766	-2.6710451
F	-2.8139859	-3.3833015	4.4010105
F	-6.0256019	3.4586002	-0.5215320
F	0.8334710	-2.4312839	-4.8823969
P	2.7205531	0.7647116	0.0984169
C	2.5547759	-0.4333797	1.4581961
C	3.6459330	2.2769183	0.5259001
C	3.5934236	-0.0506027	-1.2835665
C	1.7629966	-1.5327862	1.0573256
C	3.1046250	-0.3791485	2.7672498
C	3.1014762	3.2488501	1.4085491
C	4.8922032	2.4987357	-0.0962297
C	3.0159736	0.1140930	-2.5593171
C	4.7453793	-0.8620341	-1.1077735
C	1.4719132	-2.5729537	1.9418084
H	1.3702942	-1.5571800	0.0373103
C	2.7771724	-1.4357596	3.6402865
C	4.0225860	0.7069142	3.2804689
C	3.8610261	4.4043413	1.6614303
C	1.7494123	3.0929144	2.0636721
C	5.6265642	3.6601205	0.1709326
H	5.2845659	1.7588842	-0.8003831
C	3.5551213	-0.5367914	-3.6733598
H	2.1275534	0.7416928	-2.6586073
C	5.2675031	-1.5025132	-2.2484124
C	5.4075476	-1.0793042	0.2329662
C	1.9700895	-2.5106170	3.2493823
H	0.8471943	-3.4055582	1.6092524
H	3.1822950	-1.4118458	4.6577694
H	3.4600760	1.6042183	3.5919914
H	4.5708366	0.3424948	4.1635899
H	4.7568078	1.0321266	2.5273793
C	5.1093339	4.6125311	1.0580673
H	3.4601599	5.1574044	2.3487325
H	1.6661310	3.7491847	2.9440731
H	0.9325903	3.3697060	1.3730114
H	1.5658644	2.0581532	2.4027825
H	6.5942030	3.8179553	-0.3149111
C	4.6822944	-1.3538356	-3.5127529
H	3.0821827	-0.4167857	-4.6525625
H	6.1528563	-2.1375985	-2.1333856
H	5.4526507	-0.1516905	0.8283293
H	4.8551543	-1.8252944	0.8318709
H	6.4375832	-1.4464554	0.0986573
H	1.7384268	-3.3037321	3.9670965
H	5.6736707	5.5243787	1.2784170
H	5.1106739	-1.8773877	-4.3736184

TS7 : carboxylic acid **F** catalyzed **G** to **5**

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Energy = -7131.419023839

N	-2.6792106	0.4137970	0.7417345
N	-2.1662788	-0.9248596	0.8813915
H	-3.0944252	0.7067248	1.6373695
H	-1.7560094	0.9440609	0.7368504
B	-3.6296746	1.1191133	-0.4763066
C	-2.9874827	2.6347777	-0.5557766
C	-3.4218898	0.2492665	-1.8343901
C	-5.1698358	1.1390811	0.0882120
C	-2.7229968	3.3793595	0.6042198
C	-2.6845953	3.3007459	-1.7533285
C	-2.1098103	-0.0140113	-2.2495452
C	-4.4195804	-0.2989560	-2.6518760
C	-5.8104746	-0.0853061	0.2997816
C	-5.9573010	2.2577985	0.4035739
C	-2.2010137	4.6740688	0.6093116
F	-3.0316747	2.8516539	1.8239665
C	-2.1501183	4.5970052	-1.7994079
F	-2.9140942	2.7252054	-2.9499583
C	-1.7746511	-0.7990641	-3.3556276
F	-1.1036598	0.5358155	-1.5387296
C	-4.1388335	-1.1174622	-3.7542911
F	-5.7311729	-0.0712307	-2.4172436
C	-7.0962030	-0.2525616	0.8119368
F	-5.1360675	-1.2132372	-0.0364411
C	-7.2588353	2.1538068	0.9257286
F	-5.5153129	3.5149095	0.2099375
C	-1.9016629	5.2880303	-0.6109111
F	-1.9792993	5.3370080	1.7600807
F	-1.8452305	5.1663489	-2.9759134
C	-2.8103827	-1.3668312	-4.1065934
F	-0.5039751	-1.0780343	-3.6732203
F	-5.1348711	-1.6742758	-4.4620298
C	-7.8298772	0.8944319	1.1410708
F	-7.6177129	-1.4732575	1.0030776
F	-7.9596504	3.2574030	1.2191384
F	-1.3805149	6.5202508	-0.6375230
F	-2.5263788	-2.1745215	-5.1363828
F	-9.0627622	0.7874625	1.6482160
P	-2.8471865	-2.4161760	1.0445554
C	-4.2326305	-2.5562619	2.2358884
C	-1.4948478	-3.3149939	1.8953286
C	-3.0412799	-3.2426802	-0.5860104
C	-4.7342224	-1.3705966	2.8101379
C	-4.7057048	-3.8171817	2.6881724
C	-0.9716600	-2.8259798	3.1279577
C	-1.0397743	-4.5441544	1.3762992
C	-1.8031590	-3.2132034	-1.2823596
C	-4.1641065	-3.8837661	-1.1701813
C	-5.7295655	-1.4030435	3.7900515
H	-4.3517749	-0.4022795	2.4857400

C	-5.7164655	-3.8219919	3.6689939
C	-4.1641910	-5.1405402	2.2025951
C	0.0092735	-3.6044665	3.7712707
C	-1.3910475	-1.5328033	3.7863579
C	-0.0729380	-5.2980973	2.0451067
H	-1.4464694	-4.9227352	0.4358174
C	-1.6372756	-3.8723583	-2.4998881
H	-0.9504752	-2.6740038	-0.8539632
C	-3.9699715	-4.5184406	-2.4186568
C	-5.5634155	-3.9254140	-0.5974531
C	-6.2313307	-2.6399591	4.2129236
H	-6.1124118	-0.4685997	4.2106244
H	-6.1037314	-4.7874912	4.0118204
H	-3.2998379	-5.4475065	2.8188521
H	-4.9350567	-5.9231184	2.2851204
H	-3.8197227	-5.1052445	1.1584056
C	0.4588958	-4.8212274	3.2486479
H	0.4280984	-3.2353903	4.7138820
H	-2.4852256	-1.4606101	3.8911123
H	-0.9504938	-1.4679651	4.7934019
H	-1.0590626	-0.6561454	3.2080295
H	0.2757813	-6.2387868	1.6126817
C	-2.7339608	-4.5378081	-3.0683088
H	-0.6667594	-3.8488320	-3.0014205
H	-4.8299421	-5.0120669	-2.8845014
H	-5.9390511	-4.9627159	-0.5846846
H	-5.6432069	-3.5053868	0.4101922
H	-6.2356853	-3.3375213	-1.2463948
H	-7.0195963	-2.6861903	4.9705567
H	1.2301914	-5.3902548	3.7753238
H	-2.6292258	-5.0525682	-4.0280519
N	3.0729145	-0.1457472	0.9522535
N	2.0179339	0.7295338	0.9581831
H	3.0898333	-0.7135434	1.7990708
C	0.6563200	0.3489041	0.9322513
O	0.3637827	-0.8941350	0.8985420
O	-0.1576779	1.3095761	0.9909102
H	-0.8750372	-0.9488922	0.8766716
B	3.7562258	-0.7815146	-0.2945592
C	5.3478523	-1.0753616	0.0687361
C	3.1233593	-2.3084358	-0.5766352
C	3.5920214	0.2462697	-1.5762160
C	5.9915120	-0.8556898	1.2947592
C	6.1670877	-1.6377532	-0.9221743
C	3.1078127	-3.2057101	0.5022600
C	2.6648261	-2.8587993	-1.7823690
C	2.3228042	0.4217641	-2.1442210
C	4.5873131	1.0460267	-2.1587427
C	7.3588357	-1.0934268	1.5018393
F	5.3365768	-0.3840820	2.3826613
C	7.5297850	-1.9060720	-0.7624104
F	5.6429025	-1.8987311	-2.1431541
C	2.6955150	-4.5388945	0.4194892
F	3.5599767	-2.8103572	1.7236498
C	2.1654408	-4.1656164	-1.8978391
F	2.6925262	-2.1569993	-2.9356777
C	2.0321010	1.3061406	-3.1877891
F	1.2910343	-0.2930836	-1.6579159
C	4.3517201	1.9557173	-3.2019559
F	5.8704454	1.0122776	-1.7243899
C	8.1345923	-1.6274151	0.4700862
F	7.9255894	-0.8132538	2.6908105
F	8.2598943	-2.4200223	-1.7663910
C	2.1728399	-5.0143677	-0.7874379
F	2.7963756	-5.3627498	1.4804577
F	1.6808276	-4.6116224	-3.0756109
C	3.0581351	2.0992476	-3.7102498
F	0.7736823	1.4737273	-3.6349721
F	5.3524193	2.7076359	-3.6900271
F	9.4419932	-1.8678693	0.6563269
F	1.7043619	-6.2716328	-0.8786525
F	2.7958066	2.9969991	-4.6707562
P	2.1802490	2.3397470	1.6883333
C	3.9408432	2.4815974	2.0940075
C	1.0828877	2.4321541	3.1287294
C	1.8230929	3.6412419	0.4681378
C	4.7534781	2.3403286	0.9473432
C	4.5302911	2.7297267	3.3645030
C	1.0729364	1.3886657	4.0908447
C	0.1627757	3.4943572	3.2010888
C	1.2208616	3.2558189	-0.7452478
C	2.2162896	4.9911596	0.6846403
C	6.1453844	2.3877676	1.0345969
H	4.2768373	2.1936853	-0.0247106
C	5.9385930	2.7569411	3.4196205
C	3.7831390	3.0052182	4.6504558
C	0.1485011	1.4943012	5.1461408
C	1.9691821	0.1732872	4.0024207
C	-0.7580921	3.5620506	4.2503865
H	0.1500046	4.2546504	2.4161046
C	1.0196682	4.1891163	-1.7666053
H	0.8944574	2.2263305	-0.8797377
C	1.9748097	5.9118188	-0.3521803
C	2.8874444	5.4687798	1.9509391
C	6.7399479	2.5731840	2.2884261
H	6.7470886	2.2633412	0.1322393
H	6.4130562	2.9422220	4.3894145
H	3.4373335	2.0750458	5.1332724
H	4.4552876	3.5122224	5.3614722
H	2.8963794	3.6399895	4.5004639
C	-0.7556318	2.5616608	5.2323274
H	0.1362767	0.7121095	5.9130349
H	2.1157034	-0.2709535	5.0001391
H	1.5127101	-0.6042606	3.3614165

H	2.9630232	0.4017886	3.5811318
H	-1.4785151	4.3834832	4.2864984
C	1.3988011	5.5221206	-1.5677880
H	0.5628849	3.8712980	-2.7071056
H	2.2541777	6.9594494	-0.1970615
H	2.4812046	4.9786493	2.8504985
H	3.9708851	5.2584501	1.9249113
H	2.7547315	6.5552788	2.0684450
H	7.8300296	2.5925912	2.3856857
H	-1.4661782	2.6050116	6.0642678
H	1.2290260	6.2646912	-2.3534664