Supplementary Data for:

The impact of Lewis acids variation on reactions with di-tert-butyl diazo diester

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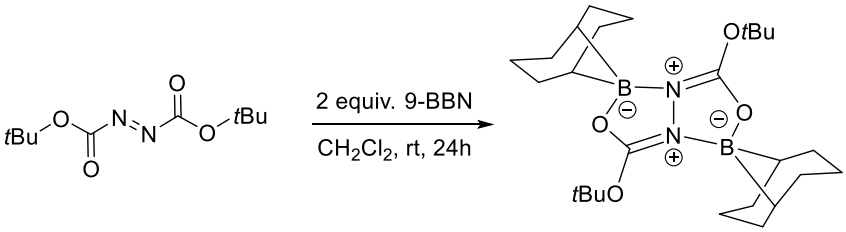
General information

Experiments were carried under inert conditions using standard Schlenk techniques or a glove box as appropriate. Dichloromethane (DCM, CH_2Cl_2), toluene ($PhCH_3$) and *n*-hexanes (C_6H_{14}) were dispensed from an MBRAUN Solvent Purification System, deoxygenated by bubbling nitrogen for 20 min, and stored over 3 Å molecular sieves prior to use. Chloroform-d ($CDCl_3$) and Acetonitrile-d_3 (CD_3CN) solvents were used as received without any purification and those were stored over 4 Å molecular sieves prior to use. Vials and stir bar for reactions were oven-dried overnight before experiments. ^1H (400 MHz), ^{19}F (377 MHz), ^{31}P (162 MHz), ^{11}B (128 MHz) and $^{13}C\{^1H\}$ (101 MHz) NMR spectra were run at 298 K on Bruker 400 spectrometer. The chemical shifts (δ, ppm) for ^1H and $^{13}C\{^1H\}$ NMR spectra are given relative to solvent signals whereas an external reference standards used for ^{19}F ($CFCl_3$), 31P (85% H_3PO_4) and ^{11}B ($BF_3.OEt_2$) NMR spectra. These NMR data are given as: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. The single-crystal *X*-ray data were collected on a Bruker Kappa Apex II diffractometer which was equipped with rotation anode using graphite-monochromated MoKα radiation (λ = 0.71073 Å) at 150 K. Structures were solved and refined using Full-matrix least-squares based on F^2 with a suite of programs SHELXS and SHELXL[1] compiled in OLEX2[2] High-resolution mass spectra (HRMS) were obtained on an AccuTOF Plus 4G (DART), Agilent 6538 UHD (ESI) or MALDI-TOF at AIMS Mass Spectrometry Laboratory whilst elemental (CHN) analysis was performed on Thermo Scientific Flash 2000 CHNS Analyzer at ANALEST Facility, University of Toronto. The reagent $[Et_3Si][B(C_6F_5)_4]$ [3] was prepared by following literature method or a slight variations thereof. All other reagents were purchased commercially and used as received.

Synthesis of (tBuOCO(BBN)CN)$_2$ 1



An open top PTFE (4 mL) vial was charged with di-(*t*butyl) azodicarboxylate (DBAD, 50 mg, 0.22 mmol, 1.0 equiv.) in CH_2Cl_2, and then 9-BBN (100 mg, 0.43 mmol, 2.0 equiv.) dissolved in CH_2Cl_2 (2.0 ml) was added slowly with stirring. The color of the solution slowly changed from yellow to white in 3 hours and there was white precipitation in the solution. After 24h, the solution was filtered and washed with cold CH_2Cl_2 and pentane. Colourless crystals suitable for single crystal X-ray diffraction were obtained by dissolving the reaction mixture in CH_2Cl_2 and layering it with *n*-hexane (1:5) at -30 °C for couple of days. After removal of oily liquid, crystals were washed with a minimum CH_2Cl_2 (1 x 0.3 mL) followed by drying afforded compound **1** (62 mg, 60%). δ_H 1H NMR S9 (400 MHz, $CDCl_3$):, 1.94 - 0.73 (m, 28 H, 9-BBN CH & CH_2), 1.57 (s, 18 H, -OC(CH_3)$_3$); 11B NMR (128 MHz, $CDCl_3$): δ_B 12.7 (br s, 2 B, 9- BBN); 13C NMR (101 MHz, $CDCl_3$): δ_C 160 (s, N=C(OtBu)O-), 88.8 (s, -OC(CH_3)$_3$), 34.2 (s, CH_2, 9-BBN), 30.3 (s, CH_2, 9-BBN), 27.9 (s, CH, 9-BBN), 24.8 (s, CH_2, 9-BBN), 24.5 (s, OC(CH_3)$_3$); HRMS (DART) m/z: 473.3727 for [M^++1] (calcd.: 473.3716).

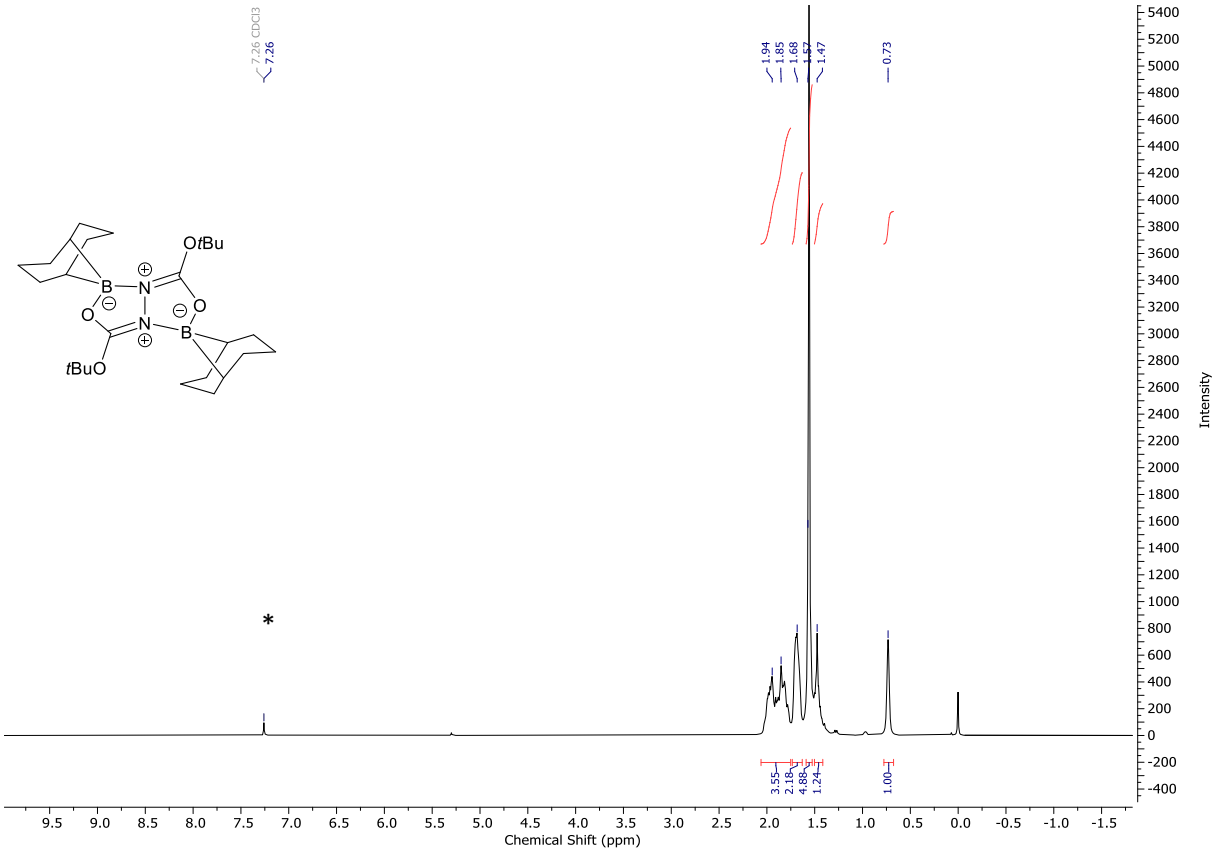


Figure S1. ^{1}H NMR (400 MHz) spectrum of the compound **1** in $CDCl_3$ (*= $CDCl_3$)

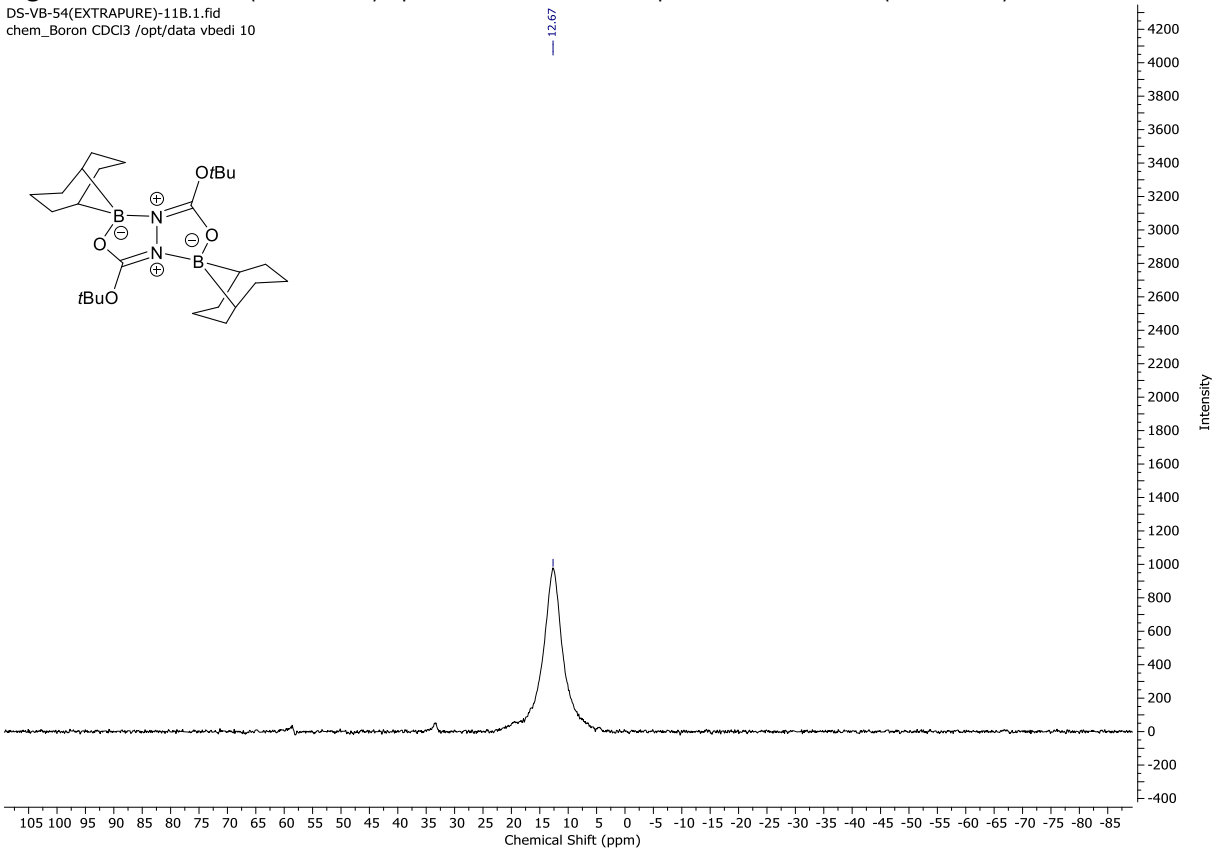


Figure S2. ^{11}B NMR (128 MHz) spectrum of the compound **1** in $CDCl_3$

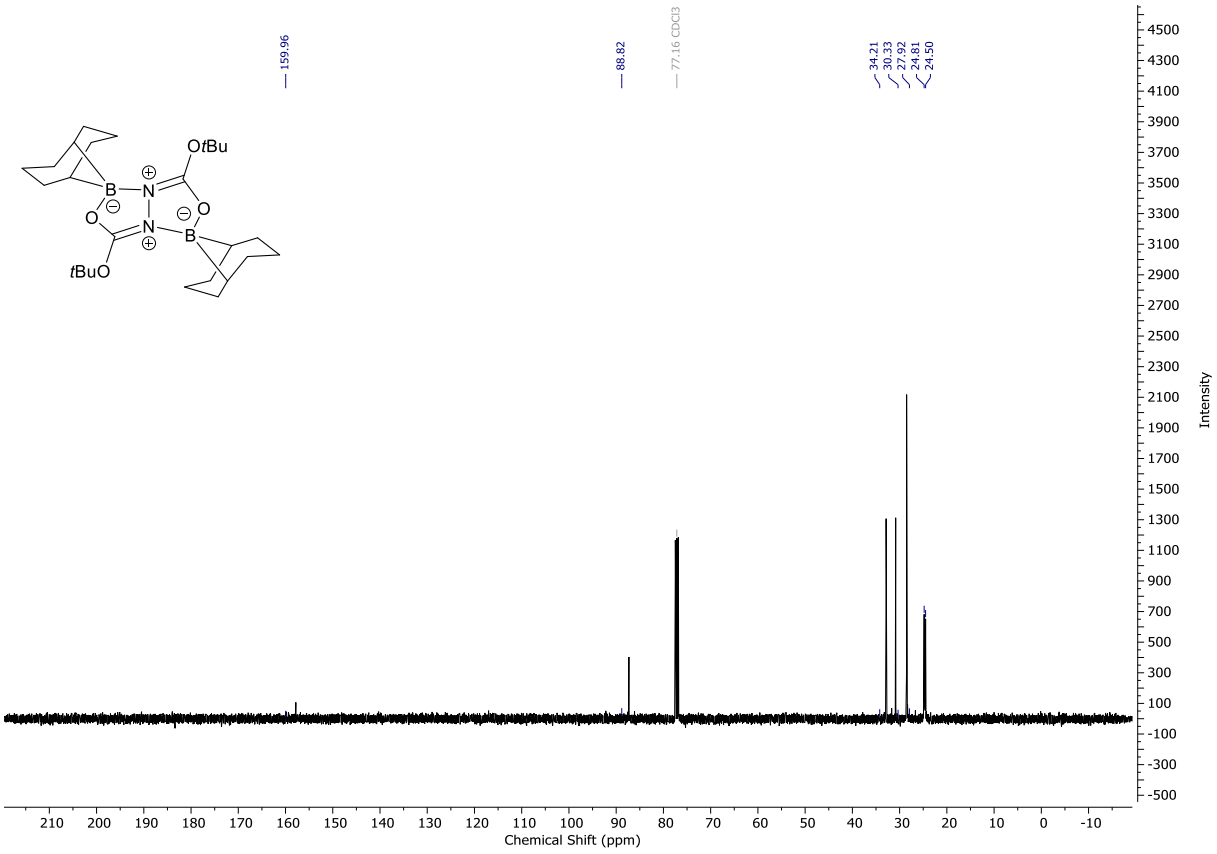
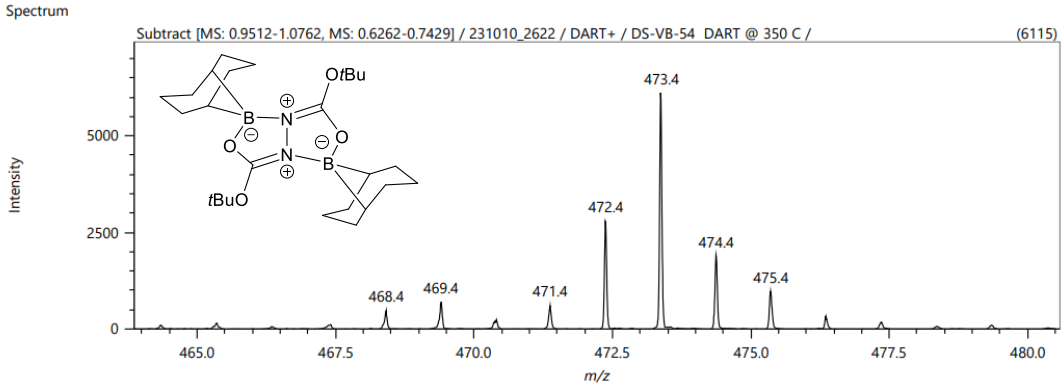


Figure S3. ^{13}C NMR (126 MHz) spectrum of the compound **3** in $CDCl_3$ (*= $CDCl_3$)



Elemental Composition

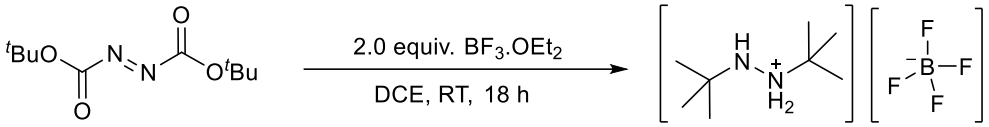
Parameters		Elements Set 1:					
Tolerance:	±10.00 mDa	Symbol	C	H	O	N	B
Electron:	Even	Min	0	0	0	0	2
Charge:	+1	Max	100	200	20	10	2
DBE:	-1.5 - 100.0						

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
473.37278	6115.45	C27 H43 B2 N6	473.37298	-0.20	-0.43	10.5
		C26 H47 B2 N2 O4	473.37165	1.14	2.40	5.5
		C31 H47 B2 O2	473.37567	-2.89	-6.10	9.5
		C22 H43 B2 N8 O2	473.36896	3.82	8.07	6.5
		C21 H47 B2 N4 O6	473.36762	5.16	10.90	1.5
		C20 H47 B2 N6 O5	473.37886	-6.07	-12.83	1.5

Figure S4. HRMS (DART) spectrum of the compound

Synthesis of [*t*BuNHNH$_2$*t*Bu][BF$_4$] 2



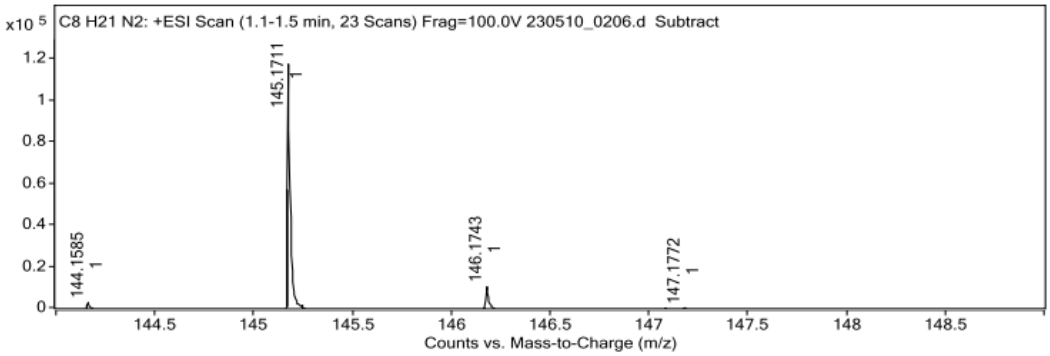
An open top PTFE (4 mL) vial was charged with $BF_3.OEt_2$ (142 mg (123 uL), 1.0 mmol, 2.0 equiv.) in CH_2Cl_2 (1.0 mL). Then a solution of di-(*t*-butyl) azodicarboxylate (DBAD) (115 mg, 0.50 mmol, 1.0 equiv.) in CH_2Cl_2 (1.0 mL) was added drop wise gently, immediate effervescence with color change from yellow to colorless was noted. The reaction mixture was allowed to stand at room temperature for additional 18 hours without stirring. Colourless crystals suitable for single crystal X-ray diffraction were directly obtained from the reaction mixture. The crystals were filtered, washed with cold CH_2Cl_2 (kept at -30°C) and hexane, followed by drying under reduced pressure afforded compound **2** in 35% (41.0 mg) yield. HRMS (DART) m/z: 145.1711 for [M$^+$+1] (calcd.: 145.1699). **Note:** Compound 2 was insoluble in all coordinating organic solvents with which it does not react.

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	145.1711	C8 H21 N2

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
145.1711	C8 H21 N2	145.1699	1.2	8.3	-0.5	80.38

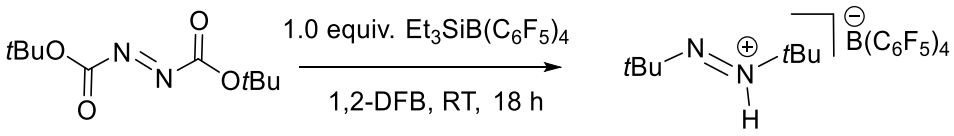


Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	145.1711	145.1699	1.2	100.0	100.0	0.0
2	146.1743	146.1729	1.4	9.3	9.6	0.3

Figure S5. HRMS (ESI) spectrum of the compound 2

Synthesis of [*t*BuN(H)N*t*Bu][B(C$_6$F$_5$)$_4$] 3



Into a 4 mL vial equipped with a stir bar, [Et$_3$Si][B(C$_6$F$_5$)$_4$] (79.0 mg, 0.10 mmol, 1.0 equiv.) was taken in 1,2-DFB (0.5 mL). A solution of di-*tert*-butyl azodicarboxylate (23.0 mg, 0.10 mmol, 1.0 equiv.) in 1,2-DFB (0.5 mL) was transferred to the vial. At addition a gentle bubble observed. The reaction

mixture was allowed to stir at RT for 18 h. After removal of all volatiles, the residue was washed with *n*-hexane (3 x 1 mL) and crystallized with a mixture of solvent of CH_2Cl_2:*n*-hexane (1:5) at -30 °C for a week. After removal of oily liquid, crystals were washed with a minimum $CHCl_3$ (1 x 0.3 mL) followed by drying afforded compound **1** (34 mg, 41%). **1**: ^{1}H NMR (400 MHz, $CDCl_3/CH_2Cl_2$): δ_H 12.42 (br s, 1 H, -N*H*$^+$), 1.64 (s, 9 H, C*H*$_3$ of *t*Bu), 1.54 (s, 9 H, C*H*$_3$ of *t*Bu); ^{19}F NMR (377 MHz, $CDCl_3/CH_2Cl_2$): δ_F -132.8 (m, 8 F, *o*-C$_6$*F*$_5$ of -B(C$_6$*F*$_5$)$_4$), -162.8 (m, 4 F, *p*-C$_6$*F*$_5$ of -B(C$_6$*F*$_5$)$_4$), -166.8 (m, 8 F, *m*-C$_6$*F*$_5$ of -B(C$_6$*F*$_5$)$_4$); ^{11}B NMR (128 MHz, $CDCl_3/CH_2Cl_2$): δ_B 16.7 (br s, 1 B, -*B*(C$_6$F$_5$)$_4$); ^{13}C NMR (126 MHz, CD_2Cl_2): δ_C 149.4 (br m, -*C*$_6$F$_5$), 146.8 (br m, -*C*$_6$F$_5$), 139.9 (br m, -*C*$_6$F$_5$), 137.6 (br m, -*C*$_6$F$_5$), 134.9 (br m, -*C*$_6$F$_5$), 63.9 (s, -*C*Me$_3$), 61.5 (s, -*C*Me$_3$), 26.0 (s, -*C*H$_3$ of *t*Bu), 25.0 (s, -*C*H$_3$ of *t*Bu).

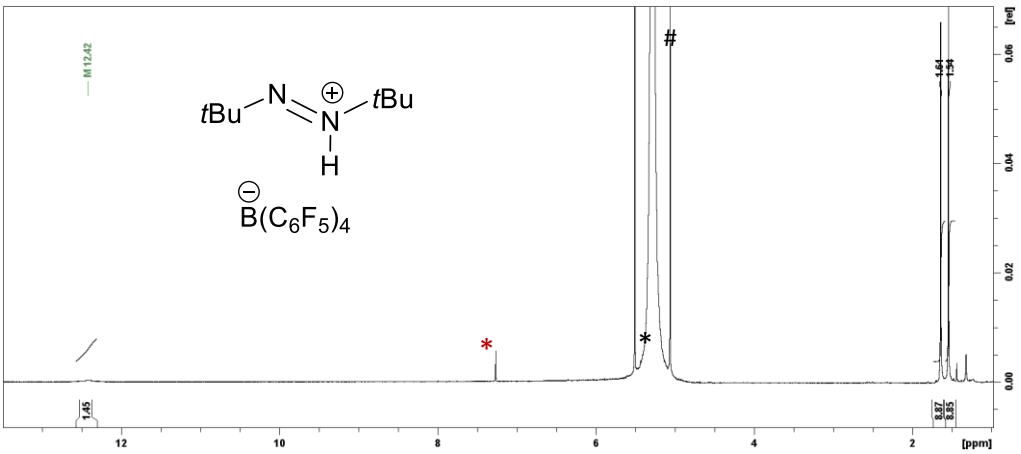


Figure S6. ^{1}H NMR (400 MHz) spectrum of the compound **3** in $CDCl_3/CH_2Cl_2$ (1:5) (*= $CDCl_3$, #= CH_2Cl_2).

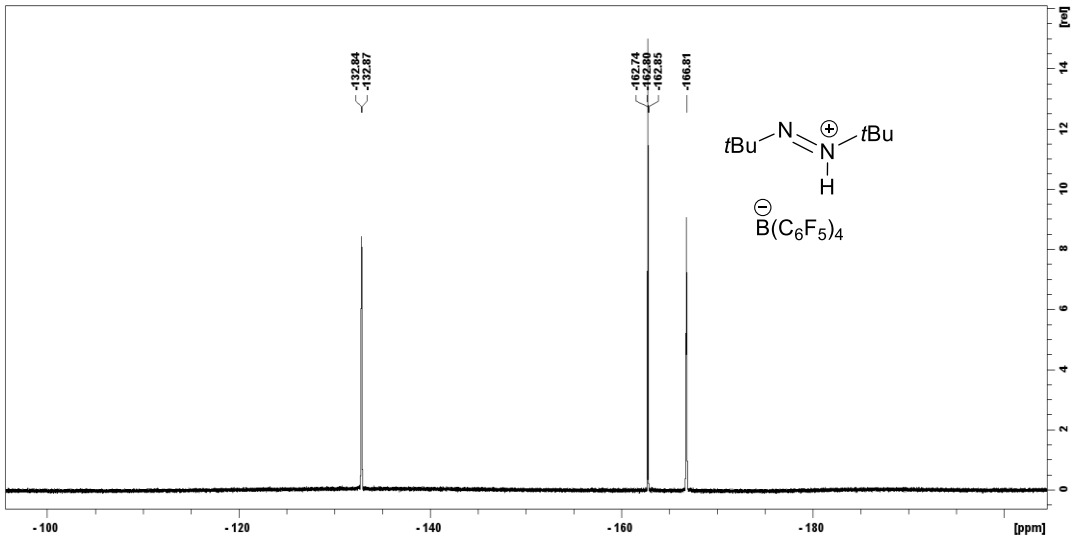


Figure S7. ^{19}F NMR (377 MHz) spectrum of the compound 3 in $CDCl_3/CH_2Cl_2$ (1:5).

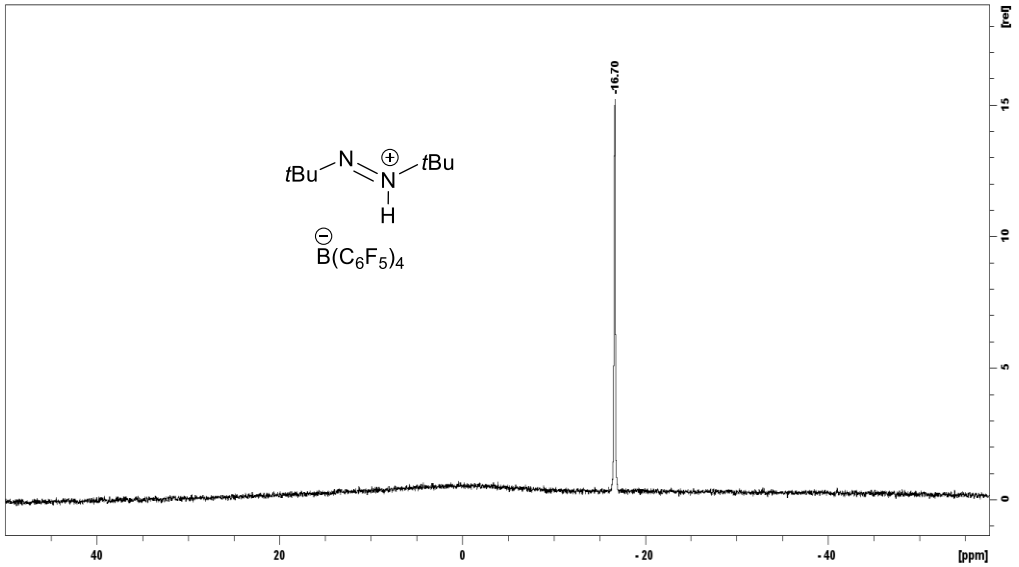


Figure S8. ^{11}B NMR (128 MHz) spectrum of the compound 3 in $CDCl_3/CH_2Cl_2$ (1:5).

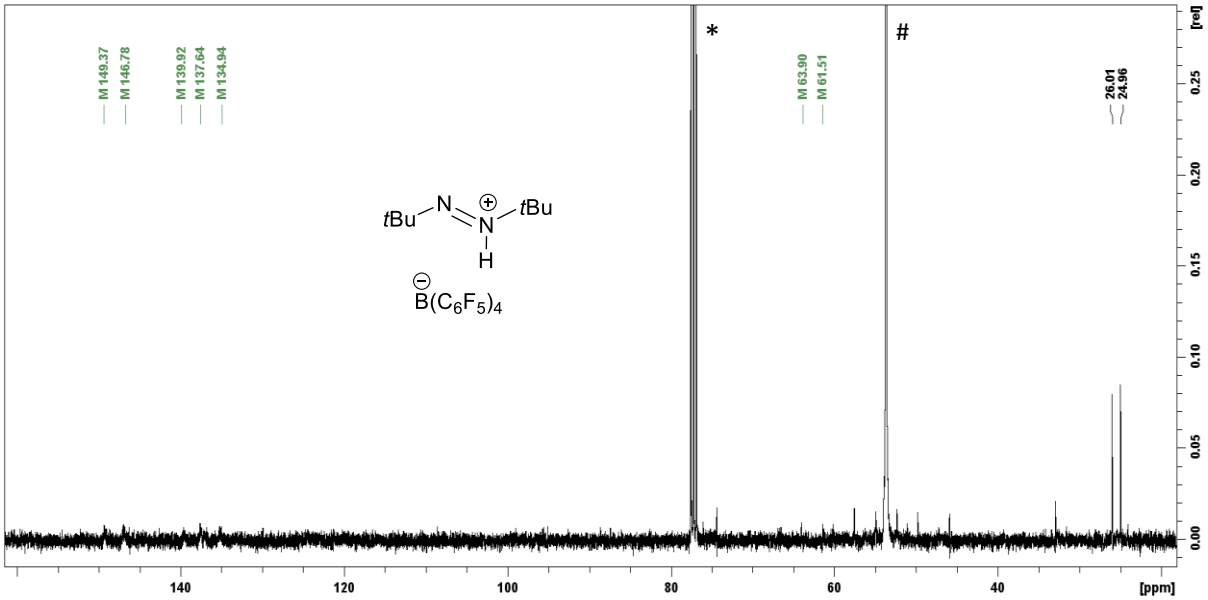


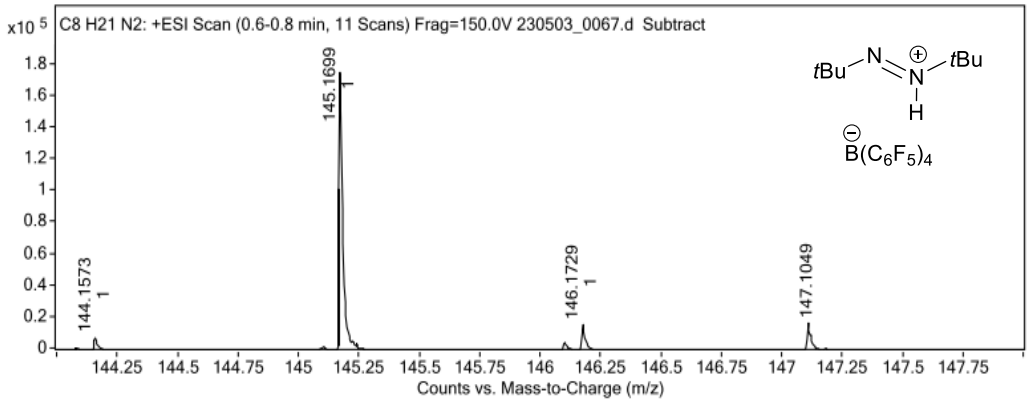
Figure S9. ^{13}C NMR (101 MHz) spectrum of the compound **3** in $CDCl_3/CH_2Cl_2$ (1:5) (*= $CDCl_3$, #= CH_2Cl_2).

Target Ion Species

Ion Species	*m/z*	*Ionic Formula*
M+	145.1699	C8 H21 N2

MFG Calculator Results

Target m/z	*Ionic Formula*	*Calc m/z*	*+/- (mDa)*	*+/- (ppm)*	*DBE*	*MFG Score*
145.1699	C8 H21 N2	145.1699	0.0	0.0	-0.5	87.93



Predicted Isotope Match Table

Isotope	*m/z*	*Calc m/z*	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	145.1699	145.1699	0.0	100.0	100.0	0.0
2	146.1729	146.1729	0.0	9.2	9.6	0.4

Figure S10. HRMS (ESI) spectrum of the compound **3**.

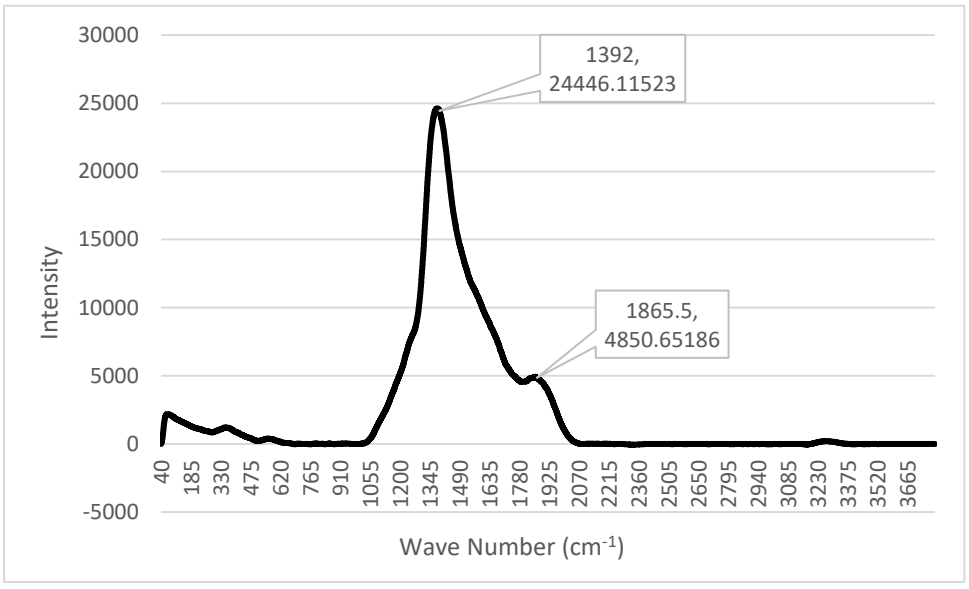


Figure S11. Raman Spectra (785 nm) of Compound **3**

Computational Details

The quantum chemical DFT calculations have been performed with the TURBOMOLE 7.4 suite of programs[1]4 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]5 The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO level of theory, which combines the TPSS meta-GGA density functional[3]6 with the BJ-damped DFT-D3 dispersion correction[4]7 and the def2-TZVP basis set,[5]8 using the Conductor-like Screening Model (COSMO) continuum solvation model[6]9 for CH_2Cl_2 solvent (dielectric constant $\varepsilon = 8.93$ and solvent radium $R_{solv} = 2.94$ Å). The density-fitting RI-J approach[5a, 7]8,10 is used to accelerate the geometry optimization and numerical harmonic frequency calculations[8]11 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]12 This choice of dispersion-corrected meta-GGA functional makes the efficient exploration of all potential reaction paths possible.

The final solvation free energies in CH_2Cl_2 solution are computed with the COSMO-RS solvation model[10]13 (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm program package[[11]14 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]6 and hybrid-meta-GGA PW6B95-D3[12]15 levels are performed using a larger def2-QZVP basis set.[5b, 13]8, 16 The final reaction Gibbs free energies (ΔG) are determined from the electronic single-point energies plus TPSS-D3 thermal corrections and COSMO-RS solvation free energies. In our discussion, higher-level PW6B95-D3 Gibbs free energies (in kcal/mol, at 298.15 K and 1 mol/L concentration) will be used in our discussion 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]17 which is the common standard in the field of DFT benchmarking.

Table S1. TPSS-D3/def2-TZVP + 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 CH_2Cl_2 solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP 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 energies (ΔG_T and ΔG_P) at the TPSS-D3 and PW6B95-D3 levels. (*t*Bu = CMe_3)

Reactions in CH_2Cl_2	ImF 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	Shift kcal /mol
Upon OEt_2 elimination, BF_3 may easily bind to an ester carbonyl oxygen														
$BF_3{\cdot}OEt_2$ + **R**	0	266.99	286.88	217.05	-32.81	-22.80	-1361.39237	-1362.77378	-1362.45819	0.00	0.00	*0.00*	0.00	
TSA	66i	265.47	286.77	227.55	-24.46	-17.17	-1361.38745	-1362.77009	-1362.43182	3.09	2.31	*16.55*	17.33	
A + OEt_2	0	265.96	286.16	216.89	-31.73	-21.41	-1361.38376	-1362.76475	-1362.44720	5.40	5.67	*6.90*	6.64	
..which induce *t*Bu^+ elimination from ester group, and then bind to the proximal nitrogen atom; proton transfer from *t*Bu^+ to N atom is kinietically less favorable														
A	0	181.79	197.10	151.04	-23.69	-17.01	-1127.56659	-1128.71189	-1128.49529	0.00	0.00	*0.00*	0.00	6.90
Ao$^-$ + *t*Bu^+	0	178.00	193.52	133.90	-120.71	-106.46	-1127.38258	-1128.52862	-1128.47887	115.47	115.01	*10.30*	10.76	17.20
TSB1	1208i	176.18	192.13	143.67	-31.56	-23.62	-1127.52662	-1128.66300	-1128.46868	25.08	30.68	*16.70*	11.10	23.60
B1 + $CH_2{=}CMe_2$	0	179.79	195.13	135.92	-36.34	-27.18	-1127.52257	-1128.66586	-1128.48656	27.62	28.89	*5.48*	4.21	12.38
TSB	65i	177.87	193.41	146.30	-37.93	-28.33	-1127.52150	-1128.66555	-1128.47454	28.29	29.08	*13.02*	12.23	19.92
B	0	182.10	197.25	151.86	-24.57	-18.17	-1127.57127	-1128.71324	-1128.49717	-2.94	-0.84	*-1.18*	-3.28	5.72
..followed by very fast CO_2 elimination and BF3 binding to the ester carbonyl oxygen														
TSC	189i	180.13	195.92	148.69	-17.55	-12.67	-1127.57199	-1128.71154	-1128.49176	-3.39	0.22	*2.21*	-1.40	9.11
Co + CO_2 + BF_3	0	179.43	194.94	126.04	-21.23	-12.21	-1127.57331	-1128.71748	-1128.52705	-4.22	-3.50	*-19.93*	-20.65	-13.03
C + CO_2	0	180.63	196.04	139.55	-24.33	-16.29	-1127.59062	-1128.73500	-1128.53254	-15.08	-14.50	*-23.38*	-23.96	-16.48
Further *t*Bu^+ elimination and binding to N-atom is kineitically even more facile, followed by easy CO2 elimination to produce **E** (*t*BuN)$_2$														
C	0	173.54	186.70	145.46	-21.16	-15.42	-938.88519	-939.84111	-939.63086	0.00	0.00	*0.00*	0.00	-16.48
Co$^-$ + *t*Bu^+	0	169.32	183.06	127.22	-123.64	-108.11	-938.69121	-939.64804	-939.61157	121.73	121.16	*12.11*	12.68	-4.37
TSD	89i	169.54	183.72	139.74	-33.55	-24.14	-938.84293	-939.79121	-939.60398	26.52	31.32	*16.87*	12.07	0.39
D	0	173.85	187.07	145.66	-25.38	-18.81	-938.89849	-939.85344	-939.64828	-8.35	-7.74	*-10.93*	-11.54	-27.41
TSE	133i	171.67	185.59	142.27	-13.02	-9.27	-938.90278	-939.85517	-939.64020	-11.04	-8.82	*-5.86*	-8.07	-22.34
E + CO_2 + BF_3	0	170.54	184.40	119.05	-15.13	-7.97	-938.90756	-939.86571	-939.67965	-14.03	-15.44	*-30.61*	-29.21	-47.09

Table S2. TPSS-D3/def2-TZVP + COSMO optimized Cartesian coordinates (in Å) in CH_2Cl_2 solution. Each structure is labeled by a specific name (See **Table S1**), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list).

Ao⁻ : anion from tBu+ eliminationa of **A**
25
Energy = -969.7422769647

N	1.0702517	-1.4191399	-1.2172665
N	-0.0858994	-1.8014416	-1.4853341
C	2.0492581	-1.7495715	-2.2501557
O	2.5534360	-2.9310632	-2.0585284
O	2.3218877	-0.8842271	-3.0620495
C	-1.0624958	-1.4623778	-0.4679576
O	-1.5033609	-2.3314806	0.2564258
O	-1.4038914	-0.1899422	-0.5721010
C	-2.5221614	0.3864759	0.2683883
C	-2.1340372	0.2898090	1.7408291
C	-2.5601420	1.8342410	-0.2070921
C	-3.8189010	-0.3465714	-0.0614554
H	-2.8792824	0.8295046	2.3343306
H	-2.1029464	-0.7478837	2.0772048
H	-1.1580433	0.7551644	1.9089470
H	-1.6016811	2.3261833	-0.0182522
H	-2.7797187	1.8823647	-1.2775491
H	-3.3432071	2.3714972	0.3365667
H	-3.7867273	-1.3852589	0.2718849
H	-4.6446219	0.1595126	0.4492979
H	-4.0109463	-0.3163481	-1.1383524
B	3.7159533	-3.4788360	-2.8992353
F	3.3171558	-3.5795664	-4.2355485
F	4.8269584	-2.6415255	-2.7575771
F	3.9736210	-4.7446010	-2.3587966

A : BF_3 adduct of $(NCO_2tBu)_2$ at carbonyl
38
Energy = -1127.518402328

N	-1.7622407	-0.7621094	1.3612664
N	-2.5700520	-1.6877496	1.1641001
C	-0.5586288	-1.1443390	2.0295374
O	-0.2713542	-0.6529007	3.1442556
O	0.2067969	-1.8985736	1.3270598
C	-3.7290690	-1.2731629	0.3763417
O	-3.7539553	-1.5750709	-0.7968318
O	-4.6111712	-0.6976580	1.1532165
C	1.6567272	-2.2779898	1.7631347
C	2.4622620	-0.9927768	1.8704277
C	1.5628285	-3.0678302	3.0593033
C	2.0900561	-3.1395126	0.5884341
H	2.3936911	-0.4144809	0.9449176
H	2.1443174	-0.3787036	2.7142346
H	3.5102571	-1.2693708	2.0230308
H	0.8733433	-3.9094503	2.9499951
H	2.5580374	-3.4682374	3.2773671
H	1.2523358	-2.4429674	3.8977234
H	3.1126527	-3.4835921	0.7689175
H	1.4407338	-4.0130462	0.4870253
H	2.0735054	-2.5658644	-0.3419133
C	-5.9821205	-0.2848423	0.6251886
C	-5.7810939	0.7595473	-0.4665707
C	-6.7116770	-1.5334213	0.1449583
C	-6.6262241	0.3098848	1.8701279
H	-5.1722834	1.5894219	-0.0956571
H	-5.3083851	0.3284762	-1.3509797
H	-6.7614689	1.1541448	-0.7518389
H	-6.7524525	-2.2836421	0.9402552
H	-7.7374557	-1.2543720	-0.1162847
H	-6.2339252	-1.9632562	-0.7374264
H	-7.6328901	0.6571315	1.6192155
H	-6.7011163	-0.4402251	2.6622780
H	-6.0433509	1.1592420	2.2370029
B	-1.2274227	0.3224422	4.0445974
F	-2.4628887	-0.2859305	4.1020487
F	-0.5638098	0.3396704	5.2502161
F	-1.2302442	1.5373365	3.3968421

B1 : from tBu$^+$ proton transfer to **Ao⁻**
26
Energy = -970.1707547926

N	2.6258259	-0.5249726	-1.0165774
N	3.2878355	-0.1733123	-0.0482489
C	1.0803855	-0.7468699	-0.9907066
C	4.7738344	-0.2223998	-0.3967877
O	0.5756397	-0.0976560	-0.0326190
O	0.7175327	-1.4891488	-1.8661342
O	5.3963958	0.2000871	0.6575086
O	5.1336335	-0.6025681	-1.4852290
B	-0.9949019	-0.1533647	0.2749330
F	-1.2977830	-1.4721099	0.5679866
F	-1.1325584	0.6871835	1.3622967
F	-1.6427433	0.3139779	-0.8559998
H	3.1221599	-0.8175147	-1.8912705
C	6.9390211	0.2906800	0.6744587
C	7.3636072	1.2648924	-0.4156728
C	7.1947613	0.8343297	2.0710147
C	7.4866441	-1.1176296	0.4880279
H	7.1587193	0.8730803	-1.4136533
H	6.8646888	2.2296117	-0.2881614
H	8.4427430	1.4217674	-0.3227128

H	6.8109913	0.1489432	2.8313244
H	8.2742002	0.9422525	2.2109516
H	6.7266757	1.8140800	2.1982808
H	7.0770911	-1.7947976	1.2426996
H	7.2753621	-1.5067730	-0.5098479
H	8.5725006	-1.0752838	0.6176600

$BF_3{\cdot}OEt_2$: adduct of BF_3 and OEt_2
19
Energy = -558.5640588309

B	0.9862194	-0.1981947	-0.0522432
F	1.2508381	-1.5169312	-0.3798362
F	1.2569916	0.0730371	1.2808994
F	1.5612025	0.7139927	-0.9163165
H	0.0232444	2.4488931	0.8358518
C	-1.0257301	2.2584128	0.5989474
C	-1.1589243	1.2983518	-0.5651059
H	-1.4964241	3.2048791	0.3120493
H	-1.5331445	1.8863845	1.4937267
O	-0.5843698	-0.0385611	-0.2703006
H	-2.1988846	1.1031358	-0.8315346
H	-0.6171268	1.6345465	-1.4473523
C	-1.4657465	-0.9370767	0.5176067
C	-2.3786808	-1.7062869	-0.4116025
H	-2.0079364	-0.3093464	1.2275270
H	-0.7854319	-1.5895136	1.0633463
H	-3.0104690	-2.3682561	0.1899925
H	-3.0332623	-1.0385279	-0.9795771
H	-1.7960269	-2.3151746	-1.1076096

BF_3 : Lewis acid
4
Energy = -324.7315643384

B	0.0518657	-1.1606050	0.1432304
F	-1.2165303	-1.3129052	-0.2037342
F	0.3626461	-0.8254685	1.3856124
F	1.0095756	-1.3436112	-0.7521525

B : *t*Bu^+ binding to N-atom of **Ao**$^-$
38
Energy = -1127.526494709

N	0.7175931	-0.7583195	-0.4089081
N	-0.3079690	-1.2192150	0.0956357
C	2.0042102	-1.5795115	-0.0142889
O	2.4505387	-1.3358519	1.1451233
O	2.3724059	-2.3331415	-0.8792092
C	-1.6577900	-0.8271973	-0.2977673
O	-2.1294412	-1.3164692	-1.3002090
O	-2.1721035	-0.1172591	0.6667797
C	0.8917502	0.3565540	-1.4645955
C	-0.1481634	1.4528601	-1.2330138
C	2.3118192	0.9070402	-1.3003806
C	0.7181373	-0.3266196	-2.8355345
H	-1.1504145	1.1527967	-1.5433564
H	-0.1551814	1.7819582	-0.1920016
H	0.1396713	2.2989833	-1.8624701
H	3.0695295	0.1352216	-1.4589449
H	2.4525525	1.6684358	-2.0716485
H	2.4492693	1.3693237	-0.3217158
H	0.8436887	0.4508076	-3.5950334
H	1.4753864	-1.0975203	-2.9868816
H	-0.2769371	-0.7640103	-2.9349300
C	-3.6700581	0.2322413	0.6893150
C	-3.9853071	1.0820903	-0.5341157
C	-4.4545984	-1.0711542	0.7456838
C	-3.7753967	1.0256348	1.9827540
H	-3.3500852	1.9719497	-0.5630311
H	-3.8692080	0.5147711	-1.4597540
H	-5.0263524	1.4118507	-0.4607129
H	-4.1212914	-1.6849689	1.5872103
H	-5.5107662	-0.8264207	0.8967889
H	-4.3610498	-1.6394230	-0.1816293
H	-4.8142389	1.3396854	2.1199166
H	-3.4785195	0.4127737	2.8379258
H	-3.1430743	1.9168081	1.9430086
B	1.8722171	-0.4203100	2.3076255
F	0.8877002	-1.1565411	2.9383216
F	2.9718743	-0.1827417	3.1065688
F	1.3703109	0.7480282	1.7344000

CO_2 : carbon dioxide
3
Energy = -188.6982055112

C	-0.0001041	-0.0000121	-0.0000002
O	1.1684675	0.0000478	0.0000226
O	-1.1687003	-0.0000818	-0.0000157

Co$^-$: anion of **C** after *t*Bu_3^+ elimination
22
Energy = -781.0616083724

N	-0.1073264	1.2414980	-2.3382956
N	-1.3373895	1.2660635	-2.1894607
C	-2.1439335	0.4120818	-1.3300826
O	-2.1994835	0.9027380	-0.1156931
O	-2.7912083	-0.4926450	-1.8319343
C	0.8243031	0.3240238	-1.5713701
C	0.2555246	-1.0248697	-1.1155726
C	1.9923519	0.0988268	-2.5424769
C	1.2866177	1.1696979	-0.3695467
H	-0.4709070	-0.9346182	-0.3057728
H	-0.2017639	-1.5646520	-1.9493494
H	1.0892499	-1.6264527	-0.7369363

H	2.3852952	1.0569121	-2.8954728
H	2.7939542	-0.4495515	-2.0373851
H	1.6664598	-0.4849751	-3.4101142
H	2.0948723	0.6423746	0.1482402
H	1.6628698	2.1420562	-0.7030264
H	0.4591921	1.3274071	0.3275362
B	-3.0965710	0.3158434	0.9675207
F	-2.8587591	1.1111896	2.0989366
F	-4.4402113	0.4011572	0.5817675
F	-2.7235226	-1.0133791	1.2156834

C : BF_3 adduct at ester carbonyl

35

Energy = -938.8460855039

N	0.4716635	0.4080790	-2.3233382
N	-0.5681699	-0.2002774	-2.5676846
C	-1.5986845	-0.7218557	-1.7710923
O	-1.7355444	-1.9680707	-1.6017368
O	-2.5362494	0.1380489	-1.5170230
C	0.9481107	0.7387795	-0.9401244
C	0.1314939	0.1753923	0.2192143
C	2.3931969	0.2055839	-0.9173900
C	0.9519113	2.2811115	-0.9311666
H	-0.8606880	0.6275563	0.2867032
H	0.0471604	-0.9136901	0.1667649
H	0.6605287	0.4132566	1.1469480
H	2.9555757	0.5855508	-1.7742630
H	2.8765410	0.5458295	0.0033057
H	2.4004101	-0.8869669	-0.9399052
H	1.4200599	2.6204490	-0.0023094
H	1.5215942	2.6719501	-1.7781512
H	-0.0687386	2.6728211	-0.9751318
C	-3.9675137	-0.2729879	-1.0931954
C	-4.5638106	-1.1393524	-2.1930187
C	-3.8895731	-0.9588886	0.2635274
C	-4.6413462	1.0884908	-1.0085061
H	-4.4844620	-0.6401908	-3.1629101
H	-4.0898164	-2.1203093	-2.2442798
H	-5.6258447	-1.2816585	-1.9688396
H	-3.3649480	-0.3280036	0.9867636
H	-4.9124102	-1.1090116	0.6234167
H	-3.3990591	-1.9309856	0.2008920
H	-5.6825195	0.9464593	-0.7046364
H	-4.1453461	1.7213895	-0.2674925
H	-4.6254997	1.5902861	-1.9796402
B	-0.6765363	-3.0908229	-2.0024070
F	-1.1806727	-4.2250540	-1.3991728
F	-0.6798607	-3.1608041	-3.3836325
F	0.5548132	-2.7076304	-1.4869733

D : tBu$^+$ binding to N-atom of **Co**$^-$

35

Energy = -938.8654489841

N	-0.0395057	1.2092725	-2.3357160
N	-1.2688888	1.2643661	-2.2584165
C	-2.2071173	0.3988101	-1.3435608
O	-2.1373740	0.8896299	-0.1670228
O	-2.8280021	-0.4836311	-1.8735179
C	0.8196576	0.2918973	-1.5435681
C	0.2173559	-1.0473668	-1.1021559
C	2.0225543	0.0488503	-2.4741674
C	1.2543939	1.1566750	-0.3346597
H	-0.5010409	-0.9574085	-0.2867564
H	-0.2430595	-1.5717268	-1.9437975
H	1.0439752	-1.6629047	-0.7359954
H	2.4469793	0.9980444	-2.8102340
H	2.7847017	-0.5107219	-1.9253228
H	1.7225372	-0.5367682	-3.3483525
H	2.0184794	0.5962488	0.2114029
H	1.6839955	2.1052171	-0.6672471
H	0.4069894	1.3507956	0.3264349
C	-2.0066812	2.2709379	-3.1593151
C	-2.5273540	1.4658674	-4.3627369
C	-3.1587520	2.8651785	-2.3409997
C	-1.0175339	3.3462030	-3.5981416
H	-1.6961888	1.0012988	-4.9006546
H	-3.2365766	0.6960437	-4.0545450
H	-3.0332800	2.1646613	-5.0349452
H	-2.7899879	3.3940399	-1.4586847
H	-3.6835909	3.5778556	-2.9821184
H	-3.8807537	2.1041953	-2.0313640
H	-1.5731345	4.0807906	-4.1873847
H	-0.5754196	3.8515995	-2.7348339
H	-0.2178928	2.9327208	-4.2147049
B	-2.9929200	0.3058397	1.0343517
F	-2.6187015	1.0951635	2.1082639
F	-4.3306497	0.4520418	0.7012559
F	-2.6192734	-1.0223131	1.1948916

E : (tBuN)$_2$

28

Energy = -425.4282620030

N	-0.0347817	1.2555754	-0.8097017
N	-0.8926959	0.5147979	-0.3115124
C	-0.2346175	2.7154632	-0.5334734
C	-1.4658541	3.0282515	0.3153280
C	1.0554251	3.1641268	0.1717020
C	-0.3348825	3.3697572	-1.9208001
H	-2.3795497	2.6820626	-0.1767766
H	-1.4042810	2.5379956	1.2914090
H	-1.5348242	4.1107646	0.4673501
H	1.9317160	2.8921776	-0.4249317

H	1.0456480	4.2503183	0.3094736
H	1.1413333	2.6889512	1.1548045
H	-0.3671342	4.4592395	-1.8168275
H	0.5301664	3.0993564	-2.5342418
H	-1.2441730	3.0417343	-2.4358716
C	-0.6928364	-0.9451013	-0.5876632
C	-1.9829332	-1.3938963	-1.2926481
C	0.5383269	-1.2579096	-1.4365599
C	-0.5923653	-1.5992496	0.7997214
H	-2.8591685	-1.1213901	-0.6961897
H	-2.0686864	-0.9192629	-2.2760257
H	-1.9734232	-2.4801744	-1.4297690
H	1.4521340	-0.9119395	-0.9445098
H	0.6070927	-2.3404011	-1.5888293
H	0.4767821	-0.7674362	-2.4125296
H	-0.5595984	-2.6887206	0.6958030
H	0.3167792	-1.2708160	1.3147931
H	-1.4575540	-1.3292202	1.4131259

N(*t*Bu)N(*t*Bu)H$^+$: **3**$^+$
29
Energy = -425.8604747670

N	-0.1227665	1.2882667	-0.7450294
N	-0.9216853	0.4616023	-0.2960660
C	-0.2342031	2.7690487	-0.5258448
C	-1.4644086	3.0672780	0.3175694
C	1.0763197	3.1692258	0.1729646
C	-0.3196492	3.3764392	-1.9364242
H	-2.3779594	2.7322752	-0.1802862
H	-1.3998416	2.5880382	1.2977994
H	-1.5192401	4.1493018	0.4594148
H	1.9489516	2.8836611	-0.4227385
H	1.0817337	4.2561058	0.2858175
H	1.1464997	2.7104889	1.1628045
H	-0.3233373	4.4645877	-1.8368794
H	0.5440980	3.0923247	-2.5455445
H	-1.2379635	3.0642140	-2.4408384
C	-0.6854541	-0.9656601	-0.5926880
C	-1.9835846	-1.4151764	-1.3000634
C	0.5521296	-1.2398827	-1.4408235
C	-0.5878194	-1.6211567	0.8031968
H	-2.8580212	-1.1806798	-0.6891021
H	-2.0817847	-0.9314397	-2.2757276
H	-1.9280863	-2.4974055	-1.4450667
H	1.4749076	-0.9186489	-0.9422161
H	0.6316637	-2.3173554	-1.5991627
H	0.4869818	-0.7726742	-2.4311499
H	-0.5301819	-2.7036535	0.6611855
H	0.3099758	-1.2843767	1.3287157
H	-1.4693413	-1.3855874	1.4033969
H	0.6888072	0.9786064	-1.3136454

OEt_2 : diethyl ether
15
Energy = -233.8037752212

H	-2.4467365	-0.3555488	-0.5659141
C	-2.4633475	0.7390841	-0.5540457
C	-1.2728798	1.2836815	0.2144867
H	-3.3952576	1.0667615	-0.0812608
H	-2.4531516	1.1002579	-1.5875264
O	-0.0726166	0.8374932	-0.4300978
H	-1.2883007	2.3852387	0.2358201
H	-1.2813501	0.9282402	1.2574202
C	1.1032019	1.3117814	0.2389663
C	2.3217406	0.7977478	-0.5062441
H	1.0994661	0.9548940	1.2814346
H	1.0912990	2.4133416	0.2619370
H	3.2357547	1.1460970	-0.0137261
H	2.3313732	-0.2969428	-0.5209652
H	2.3240526	1.1614549	-1.5388831

R : $(NCO_2tBu)_2$
34
Energy = -802.7697973713

N	0.3310352	0.4344214	-0.3256830
N	-0.3265410	-0.4085224	0.3140287
C	1.6700884	-0.0176803	-0.6724519
O	1.8962365	-0.3795488	-1.8078168
O	2.4773603	0.1462330	0.3550730
C	-1.6653874	0.0428329	0.6617120
O	-1.8874864	0.4205901	1.7927115
O	-2.4772212	-0.1413402	-0.3587495
C	3.9708781	-0.0998030	0.2246493
C	4.1953550	-1.5692630	-0.1160945
C	4.5373799	0.8558766	-0.8198499
C	4.4670414	0.2364629	1.6253966
H	3.6954505	-2.2117812	0.6149918
H	3.8313233	-1.8070900	-1.1171276
H	5.2698820	-1.7748488	-0.0760715
H	4.2777533	1.8898463	-0.5734419
H	5.6284299	0.7658164	-0.8160203
H	4.1724076	0.6180723	-1.8205657
H	5.5510499	0.0932193	1.6656585
H	4.2417405	1.2772017	1.8749696
H	3.9995636	-0.4174803	2.3670525
C	-3.9717747	0.0959946	-0.2233396
C	-4.5251774	-0.8472625	0.8393297
C	-4.2049502	1.5689392	0.0957485
C	-4.4736253	-0.2658741	-1.6156495
H	-4.2585538	-1.8829595	0.6080929
H	-4.1569567	-0.5905752	1.8341653
H	-5.6169254	-0.7659920	0.8397781

H	-3.7147310	2.2035688	-0.6486655
H	-5.2812330	1.7659379	0.0598277
H	-3.8360847	1.8251053	1.0904724
H	-5.5588022	-0.1306065	-1.6518257
H	-4.0149430	0.3793897	-2.3702814
H	-4.2425819	-1.3088803	-1.8500241

*t*Bu$^+$: CMe_3^+
13
Energy = -157.7248403638

C	0.0023381	-0.0018618	-0.0120737
C	-1.3663517	-0.5074637	-0.0095209
C	1.1347795	-0.9215899	0.0131734
C	0.2403235	1.4355835	0.0008905
H	-2.0825030	0.2117402	-0.4144218
H	-1.4652566	-1.5036809	-0.4420275
H	-1.6114913	-0.5966528	1.0693285
H	2.0517929	-0.4726308	-0.3761946
H	1.3181662	-1.0823236	1.0959554
H	0.9152287	-1.8977862	-0.4206893
H	1.2085439	1.7119229	0.4233649
H	0.2908813	1.6849940	-1.0807460
H	-0.5939127	2.0106301	0.4079341

TSA : OEt_2-elimination and BF_3 binding
53
Energy = -1361.317742090

N	0.4253995	0.4472248	-1.7744667
N	-0.2682239	-0.5393969	-2.0829422
C	1.8088237	0.1231764	-1.4834697
O	2.1763413	0.0010518	-0.3284939
O	2.5131605	0.1190468	-2.5900590
C	-1.6502782	-0.1979349	-2.3930183
O	-1.9897925	-0.1198221	-3.5546440
O	-2.3519661	-0.1222516	-1.2828239
C	4.0305999	-0.0291092	-2.5547684
C	4.6159816	1.1449415	-1.7785468
C	4.3728485	-1.3863640	-1.9504758
C	4.3828067	0.0372960	-4.0349908
H	4.2756620	2.0939323	-2.2035345
H	4.3462440	1.1008862	-0.7219928
H	5.7067551	1.1033324	-1.8615540
H	3.8405832	-2.1845312	-2.4764540
H	5.4479483	-1.5556670	-2.0685173
H	4.1276986	-1.4244749	-0.8878006
H	5.4679593	-0.0453941	-4.1473371
H	3.9106367	-0.7837903	-4.5817780
H	4.0575773	0.9879910	-4.4668062
C	-3.8577388	0.0778422	-1.3226255
C	-4.1532286	1.4226915	-1.9780155
C	-4.4912243	-1.1026568	-2.0504296
C	-4.2136426	0.0835128	0.1585954
H	-3.5995491	2.2218788	-1.4760471
H	-3.8971710	1.4150206	-3.0388421
H	-5.2232576	1.6308390	-1.8771631
H	-4.1912347	-2.0457147	-1.5836866
H	-5.5796358	-1.0128861	-1.9742121
H	-4.2168435	-1.1162058	-3.1066617
H	-5.2922731	0.2307171	0.2670993
H	-3.9415256	-0.8681569	0.6231968
H	-3.6947946	0.8950577	0.6760573
B	0.8644306	-0.1484046	1.6370272
F	0.2887215	-1.2774724	1.2234667
F	1.9821717	-0.2016241	2.3610118
F	0.2747336	1.0263323	1.4120457
O	-0.6226492	-0.3072058	3.8151367
C	-0.3200683	0.7322812	4.7676469
C	0.9252141	0.3441855	5.5436422
H	-1.1689998	0.8605981	5.4516179
H	-0.1756016	1.6783106	4.2248298
H	1.1813708	1.1404508	6.2509615
H	0.7545795	-0.5791294	6.1064165
H	1.7731005	0.1928355	4.8704222
C	-1.9739187	-0.2204933	3.3173030
C	-2.9928704	-0.8090266	4.2868292
H	-1.9729838	-0.7832558	2.3812292
H	-2.2078940	0.8281004	3.0842873
H	-3.9948849	-0.7555457	3.8453924
H	-2.7605105	-1.8585282	4.4930261
H	-3.0163504	-0.2628639	5.2352417

TSB1 : proton transfer from *t*Bu$^+$
38
Energy = -1127.488453881

N	0.1313495	-0.3695283	-0.2356700
N	0.9082813	-0.3425718	0.7185038
C	-1.2937085	-0.7490082	0.0266764
C	2.3195495	-0.0588742	0.2907898
O	-1.9867487	0.3062480	0.2363712
O	-1.5467667	-1.9250888	-0.0989437
O	2.9787193	0.1573217	1.4014886
O	2.6716198	-0.0637700	-0.8649805
B	-3.5634165	0.2898192	0.2643102
F	-3.9779854	-0.5805988	1.2597959
F	-3.9009486	1.6067728	0.5345443
F	-3.9815418	-0.1101933	-1.0041153
H	0.3539205	-0.1506295	-1.5870179
C	0.5005367	0.0493223	-2.9604309
C	-0.8328854	0.1215458	-3.3043390
H	1.0535593	-0.8646276	-3.1714905
H	1.0851139	0.9666063	-2.9138010
C	-1.5726517	1.4152393	-3.2739006

C	-1.6140772	-1.1015576	-3.6474219
H	-0.9408261	2.2492602	-2.9637562
H	-1.9661293	1.6201646	-4.2788372
H	-2.4458579	1.3378652	-2.6153438
H	-1.0328334	-2.0159154	-3.5160931
H	-2.5359870	-1.1508477	-3.0575069
H	-1.9236094	-1.0287709	-4.6995371
C	4.4647484	0.4997991	1.3687129
C	4.6468387	1.7952672	0.5859193
C	4.7739070	0.6805916	2.8486679
C	5.2161177	-0.6830585	0.7683149
H	4.4079282	1.6649683	-0.4711007
H	4.0246222	2.5899403	1.0078437
H	5.6948063	2.0995936	0.6687881
H	4.5717480	-0.2410944	3.4012548
H	5.8326019	0.9313586	2.9616762
H	4.1752186	1.4915883	3.2725771
H	4.9936395	-1.6002282	1.3212551
H	4.9709178	-0.8228527	-0.2860513
H	6.2889894	-0.4830688	0.8510030

TSB : *t*Bu$^+$ binding to N-atom

38

Energy = -1127.492548743

N	0.6125279	-0.5971661	-0.2226633
N	-0.3420809	-1.1839074	0.3183466
C	1.9192451	-1.1412270	0.1291514
O	2.6181525	-0.4663721	0.9856199
O	2.2977933	-2.1122746	-0.5057938
C	-1.6382186	-0.7036410	-0.1701551
O	-1.8930147	-0.5393972	-1.3484866
O	-2.4222012	-0.5879466	0.8807210
C	1.3441760	1.0498763	-2.7099364
C	0.7758067	2.3500479	-2.3424186
C	2.7327154	0.7531602	-2.3677852
C	0.5282618	0.1045163	-3.4557820
H	-0.2859271	2.4387332	-2.5706987
H	0.9952449	2.5717655	-1.2917319
H	1.3335789	3.1119545	-2.9140116
H	2.9432998	-0.3175370	-2.3346417
H	3.3032374	1.1475602	-3.2335756
H	3.0777333	1.2910856	-1.4831467
H	-0.0001623	0.6030451	-4.2787249
H	1.0442174	-0.8008218	-3.7685036
H	-0.2748714	-0.1261525	-2.7260599
C	-3.8441345	-0.0820099	0.7445937
C	-3.8152255	1.3172562	0.1372290
C	-4.6425878	-1.0827988	-0.0848055
C	-4.3076491	-0.0548186	2.1958836
H	-3.1557693	1.9712262	0.7158672
H	-3.4867566	1.2961328	-0.9035027
H	-4.8273253	1.7320126	0.1744981
H	-4.5856384	-2.0807419	0.3598192
H	-5.6910835	-0.7677625	-0.0895544
H	-4.2863024	-1.1225155	-1.1155914
H	-5.3428594	0.2967812	2.2350154
H	-4.2608047	-1.0558883	2.6335938
H	-3.6848017	0.6225229	2.7869643
B	2.2154389	0.8505499	1.6763808
F	1.0112452	0.6883306	2.3573394
F	3.2679522	1.1253858	2.5439395
F	2.1051068	1.8482436	0.6894154

TSC : CO_2 elimination

38

Energy = -1127.518024342

N	1.1014565	-0.2999356	-0.6965462
N	0.1357250	-0.8496884	-0.1752093
C	2.8627126	-0.8381936	0.1828938
O	2.8896915	-0.2324634	1.2284806
O	3.3585872	-1.6063967	-0.5652727
C	-1.2388411	-0.8085984	-0.6564085
O	-1.5948502	-1.5674654	-1.5349140
O	-1.9339661	-0.0319998	0.1456002
C	1.1023753	0.5911010	-1.9253017
C	-0.1488639	1.4695464	-2.0222361
C	2.3608554	1.4598190	-1.8113916
C	1.2193243	-0.3745697	-3.1229921
H	-1.0373814	0.9047040	-2.3105454
H	-0.3348156	1.9993670	-1.0848955
H	0.0290953	2.2100785	-2.8072987
H	3.2641639	0.8448341	-1.7658073
H	2.4296468	2.0904643	-2.7016754
H	2.3170752	2.1045411	-0.9305622
H	1.3106648	0.2272746	-4.0323321
H	2.1074122	-1.0045405	-3.0296960
H	0.3327289	-1.0078552	-3.1998951
C	-3.4544984	0.0030316	0.0898626
C	-3.8882304	0.5119834	-1.2801024
C	-3.9824583	-1.3902354	0.4114323
C	-3.7805344	1.0012718	1.1930672
H	-3.4411545	1.4885578	-1.4877774
H	-3.6188024	-0.1897999	-2.0716605
H	-4.9764505	0.6299064	-1.2761358
H	-3.5837580	-1.7391956	1.3685170
H	-5.0728415	-1.3360380	0.4927320
H	-3.7280598	-2.1066825	-0.3716997
H	-4.8663166	1.1169632	1.2611998
H	-3.4041305	0.6470601	2.1566764
H	-3.3375374	1.9768329	0.9737698
B	1.7909534	0.8993918	2.2778702
F	0.9493631	-0.0065910	2.8112740

F 2.7683275 1.3816798 3.0728809
F 1.2867386 1.7443935 1.3504818

TSD1 : proton transfer from *t*Bu+
35
Energy = -938.8190472929
N -1.3810224 -0.8641281 -0.4473507
N -0.5810303 -0.7201225 0.4724765
C -0.7410206 -0.0790393 1.7996111
O -0.1254301 1.0499535 1.9555141
O -1.2749826 -0.7441815 2.6675877
C -2.7522786 -0.2602089 -0.5057692
C -3.1187399 0.7834692 0.5492957
C -2.8012355 0.3555133 -1.9167917
C -3.6798332 -1.4898768 -0.4281583
H -3.2209889 0.3523726 1.5469458
H -2.3943892 1.6013716 0.5705414
H -4.0887252 1.2071057 0.2706720
H -2.5087624 -0.3824764 -2.6683955
H -3.8238741 0.6863916 -2.1211314
H -2.1310535 1.2169703 -1.9810075
H -4.7076467 -1.1585488 -0.6046782
H -3.4111054 -2.2285467 -1.1882068
H -3.6237330 -1.9542351 0.5606067
C 2.6592377 -1.6200363 -0.5462145
C 2.7620471 -0.9308718 -1.8553587
C 3.7605456 -1.4299813 0.4269723
C 1.5225123 -2.3720637 -0.2183884
H 1.9336221 -1.1713331 -2.5228316
H 2.7990409 0.1527122 -1.6844615
H 3.7137697 -1.1975056 -2.3334007
H 4.0142940 -0.3689536 0.5201070
H 3.5329950 -1.8562474 1.4048715
H 4.6550542 -1.9282966 0.0235127
H 1.6003370 -3.0357547 0.6431016
H 0.7423890 -1.5000214 0.1737218
H 0.9338417 -2.7575687 -1.0535716
B 0.6943461 1.7846344 0.8806517
F 1.0911300 2.9721858 1.4820143
F 1.7992741 0.9822625 0.5534000
F -0.1004312 2.0165958 -0.2458652

TSD : *t*Bu+ binding to N-atom
35
Energy = -938.8178525862
N -1.0282900 -1.1110912 -0.2817978
N -0.1352732 -0.5801083 0.3593843
C -0.1389813 0.4093975 1.4292327
O 0.2843315 1.5954756 1.0990080
O -0.3132978 0.0078644 2.5690599
C -2.4993699 -0.7696361 -0.2088687
C -2.8822714 0.4053484 0.6879958
C -2.8799525 -0.4971232 -1.6738904
C -3.1416230 -2.0813377 0.2760150
H -2.7019724 0.1931879 1.7438034
H -2.3543586 1.3178840 0.3992718
H -3.9539793 0.5886177 0.5595011
H -2.5700479 -1.3294385 -2.3122567
H -3.9666364 -0.3860707 -1.7417855
H -2.4061374 0.4217532 -2.0279481
H -4.2301485 -1.9705869 0.2503295
H -2.8569411 -2.9147609 -0.3723601
H -2.8376641 -2.3065604 1.3028310
C 2.3359339 -2.1544191 -0.2845730
C 2.0359990 -1.9430556 -1.7049958
C 3.3212451 -1.3210217 0.4093692
C 1.7337028 -3.3143911 0.3928493
H 0.9461201 -1.9866251 -1.8545184
H 2.4515690 -1.0195081 -2.1034857
H 2.4261378 -2.8072991 -2.2689069
H 3.3699754 -0.3086749 0.0046259
H 3.1999184 -1.3320240 1.4938526
H 4.3023292 -1.7895601 0.1922782
H 2.3368678 -4.1965034 0.1116405
H 1.7564582 -3.2292505 1.4796393
H 0.7221395 -3.5093110 0.0219541
B 0.5948583 2.0972777 -0.3155713
F 0.9560411 3.4325540 -0.1459047
F 1.6527792 1.3537022 -0.8582691
F -0.5492174 1.9777563 -1.1162565

TSE : CO_2 elimination
35
Energy = -938.8540123044
N 0.5190778 0.3205959 -2.0403799
N -0.4431579 -0.0657243 -1.3780191
C -0.5983085 -0.7991079 0.6531851
O -0.2848817 0.2141925 1.2274346
O -0.9588172 -1.9158371 0.5767496
C 1.9138050 0.0211789 -1.5908642
C 2.0696249 -1.1984430 -0.6778933
C 2.6737909 -0.2079279 -2.9087816
C 2.4059534 1.3135871 -0.9131600
H 1.7774900 -0.9986081 0.3544972
H 1.4972884 -2.0501630 -1.0576485
H 3.1265433 -1.4808370 -0.6579533
H 2.5321765 0.6409365 -3.5833306
H 3.7412208 -0.3235557 -2.6985387
H 2.3176183 -1.1151060 -3.4080623
H 3.4750547 1.2179768 -0.7003623
H 2.2565463 2.1745858 -1.5714798
H 1.8716196 1.4852109 0.0250415

C	-1.8008021	0.2466594	-1.9705524
C	-2.3707361	-1.1151675	-2.4080084
C	-2.6570127	0.8565468	-0.8523599
C	-1.6990848	1.2023908	-3.1584736
H	-1.7535664	-1.5513427	-3.1994960
H	-2.4171160	-1.8133377	-1.5689557
H	-3.3829677	-0.9658446	-2.7959453
H	-2.1986697	1.7670201	-0.4559488
H	-3.6385045	1.1105859	-1.2628224
H	-2.8163140	0.1511721	-0.0308679
H	-2.7085633	1.3935045	-3.5351687
H	-1.2482297	2.1533428	-2.8597176
H	-1.0954131	0.7749686	-3.9621910
B	0.4295078	0.2376450	3.0480089
F	1.1935384	1.3343891	2.9081172
F	-0.7227402	0.3518277	3.7321935
F	1.0488301	-0.9604875	3.0581162

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