Ion Pairs of Weakly Coordinating Cations and Anions:

Synthesis and Application for Sulfide to Sulfoxide Oxidations

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Supporting Information

1. Spectroscopic data

1.1. IR spectroscopy

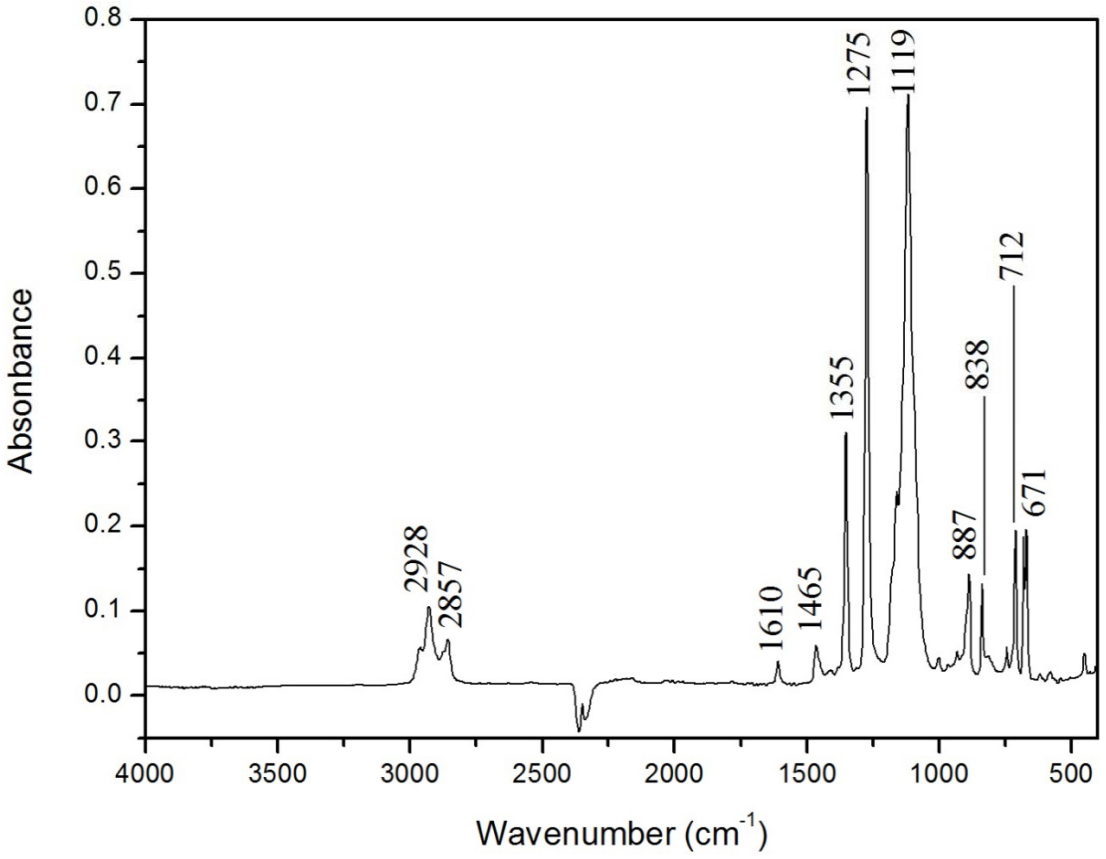

Figure S1. IR spectrum of neat $[P_{4,4,4,14}][B\{C_6H_3\text{-}3,5\text{-}(CF_3)_2\}_4]$ (**6b**).

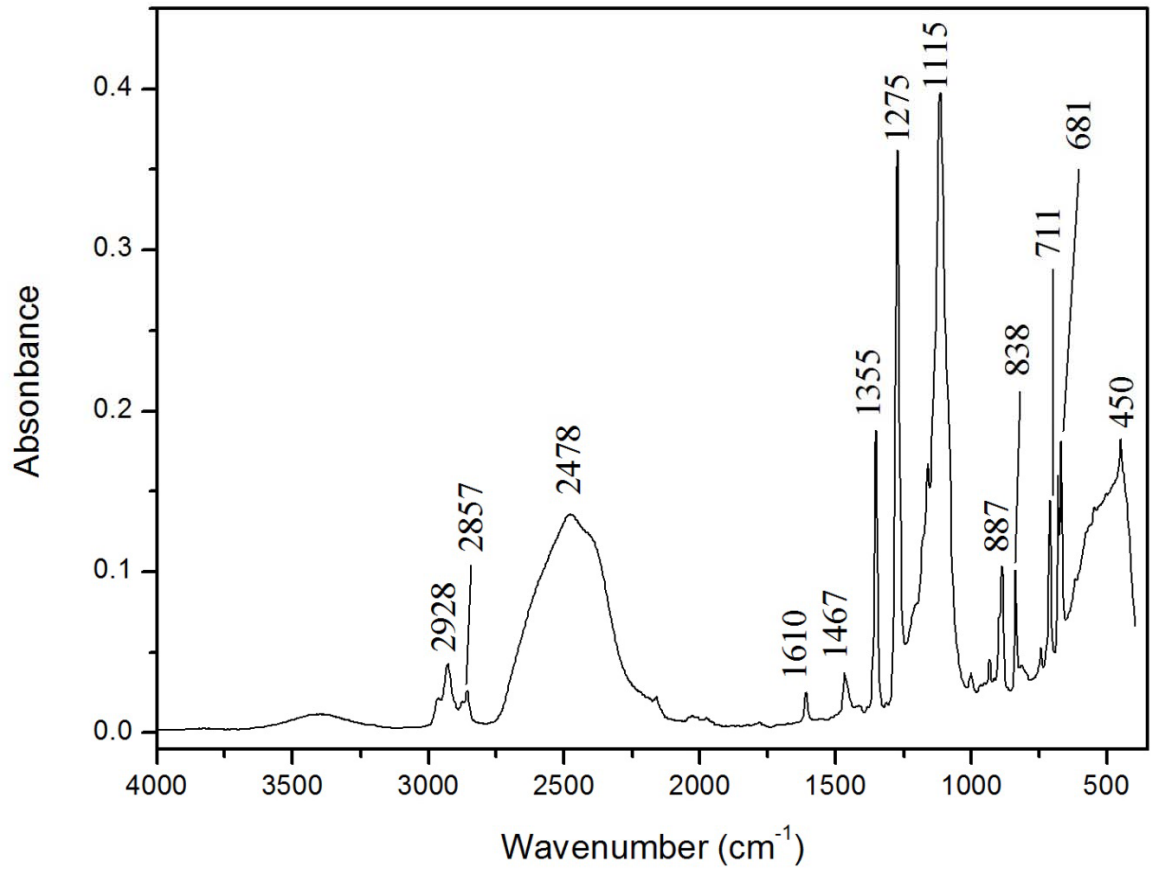

Figure S2. IR spectrum of a mixture of **6b** and D_2O.

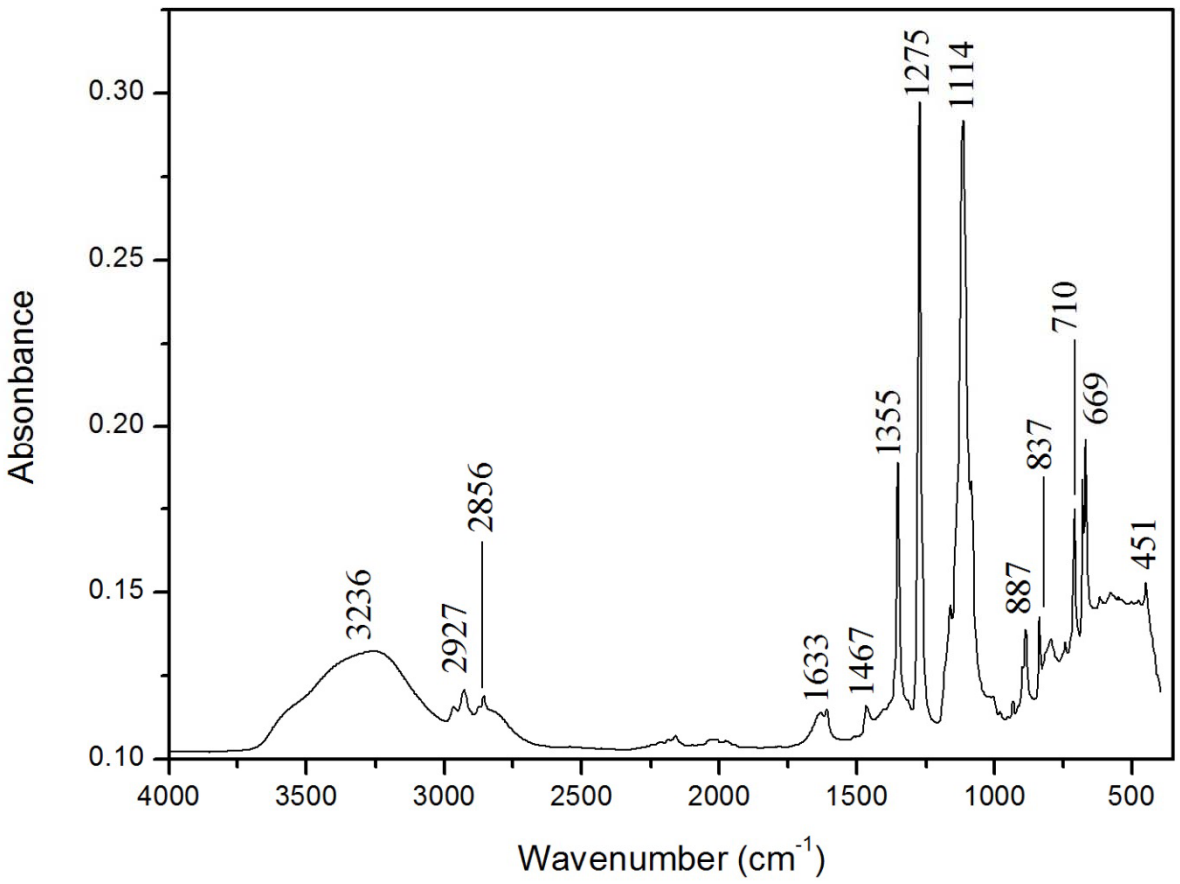

Figure S3. IR spectrum of a mixture of **6b** and H_2O_2.

1.2. NMR spectroscopy

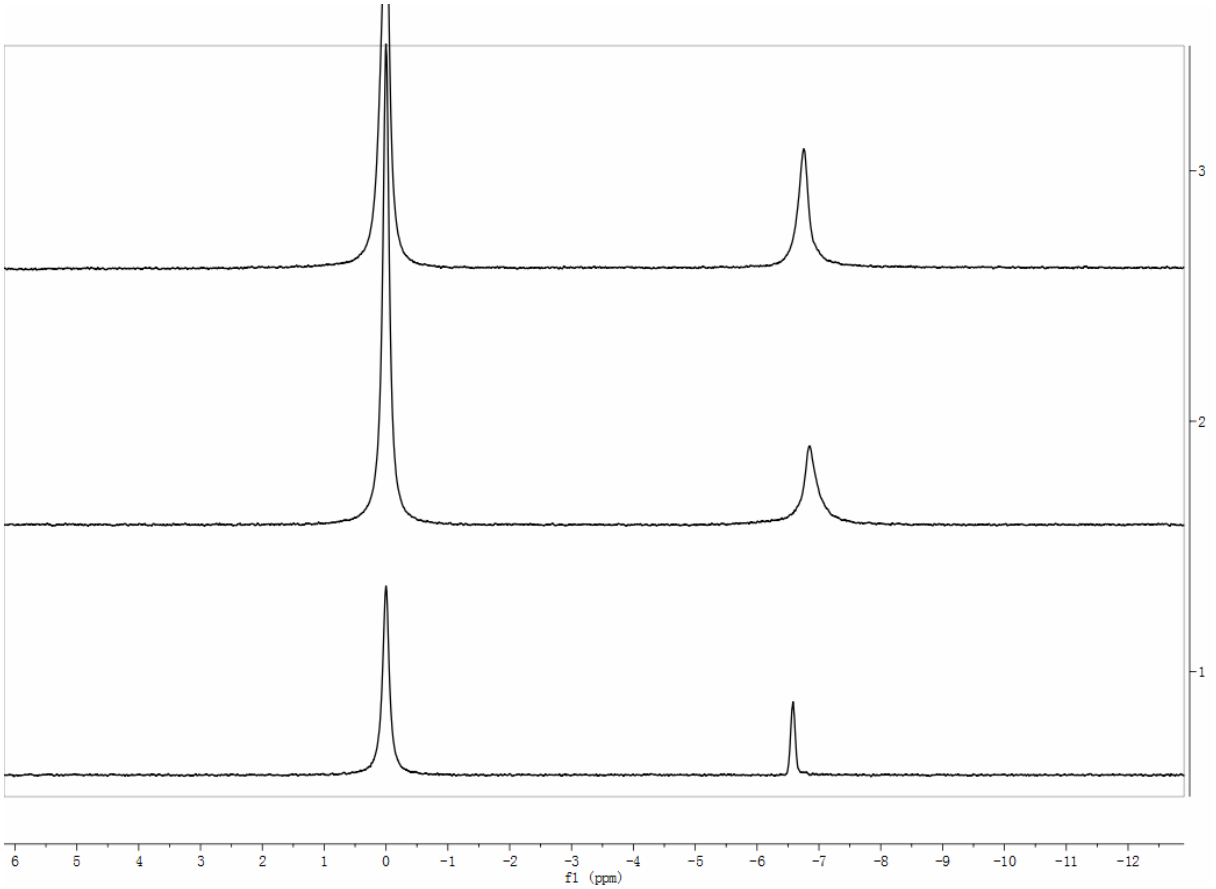

Figure S4. ^{11}B NMR spectra of neat **6b** (bottom), a mixture of **6b** and H_2O (middle) and a mixture of **6b** and aqueous H_2O_2 (top).

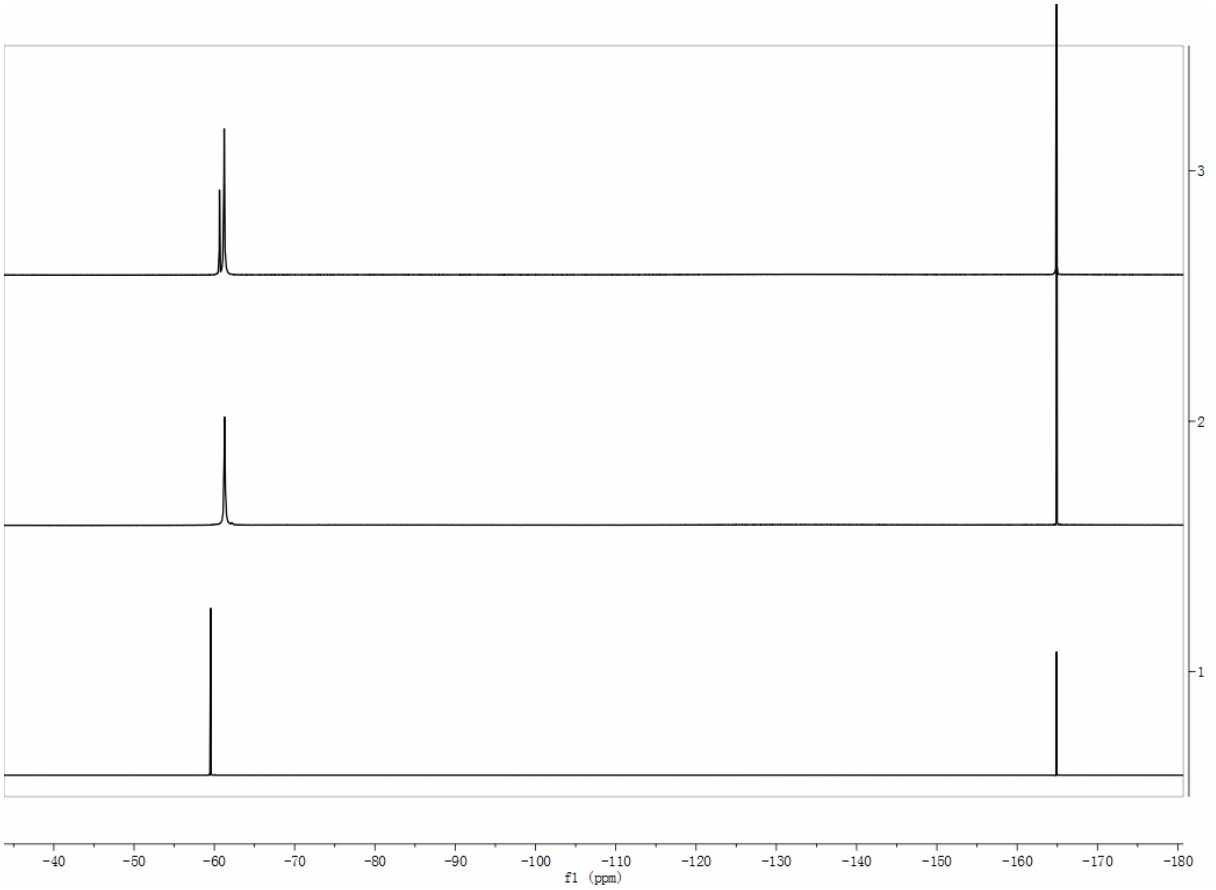

Figure S5. ^{19}F NMR spectra of neat **6b** (bottom), a mixture of **6b** and H_2O (middle) and a mixture of **6b** and aqueous H_2O_2 (top).

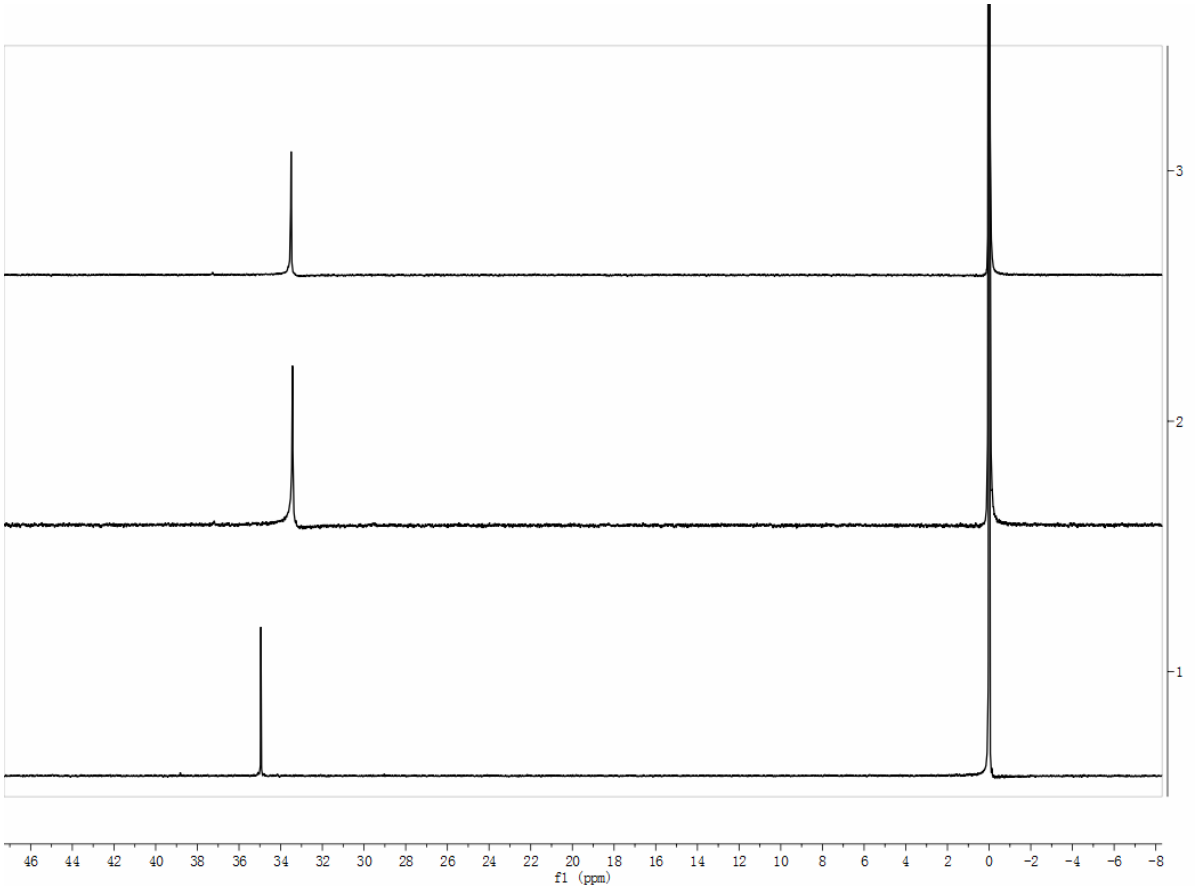

Figure S6. ^{31}P NMR spectra of neat **6b** (bottom), a mixture of **6b** and H_2O (middle) and a mixture of **6b** and aqueous H_2O_2 (top).

2. Characterization data of sulfoxides

Methyl phenyl sulfoxide: pale yellow oil. IR (cm^{-1}): 1032. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ = 2.60 (s, 3H), 7.39-7.40 (d, 3H), 7.53-7.55 (t, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ = 43.75, 123.29, 129.17, 130.81, 145.62.

Dimethyl sulfoxide: colorless liquid. IR (cm^{-1}): 1015. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ = 2.47 (s, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ = 41.30.

Dibutyl sulfoxide: white solid. M.p.: 30-32 ^{o}C. IR (cm^{-1}): 1023. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ = 0.98-1.01 (t, 6H), 1.48-1.52 (m, 4H), 1.83-1.87 (m, 4H), 2.94-2.99 (m, 4H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ = 13.53, 21.78, 23.95, 52.50.

Ethyl phenyl sulfoxide: yellow oil. IR (cm^{-1}): 1018. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ = 1.03-1.07 (t, 3H), 2.58-2.67 (m, 1H), 2.73-2.82 (m, 1H), 7.33 -7.40 (m, 3H), 7.47-7.49 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ = 6.06, 50.49, 124.38, 129.33, 131.08, 143.78.

Phenyl isopropyl sulfoxide: yellow oil. IR (cm^{-1}): 1020. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ = 1.04-1.06 (d, 3H), 1.14-1.15 (d, 3H), 2.73 - 2.77 (m, 3H), 7.41-7.44 (m, 3H), 7.50-7.52 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ = 13.82, 15.84, 54.45, 124.91, 128.83, 130.93, 141.68.

Phenyl allyl sulfoxide: yellow oil. IR (cm^{-1}): 1037. ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K, ppm): δ = 3.39-3.52 (m, 2H), 5.08-5.13 (d, 1H), 5.22-5.25 (d, 1H), 5.51-5.59 (m, 1H), 7.41 - 7.45 (m, 3H), 7.51-7.53 (m, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz, 298 K, ppm): δ = 59.76, 122.85, 123.27, 124.19, 128.01, 130.06, 141.85.

2-(Phenylsulfinyl)ethanol: pale yellow oil. IR (cm^{-1}): 3343, 1018. ^{1}H NMR ([D_6]DMSO, 400 MHz, 298 K, ppm): δ = 2.83-2.98 (m, 1H), 2.99-3.04 (m, 1H), 3.64-3.70 (m, 1H), 3.80-3.88 (m, 1H), 5.08 - 5.12 (t, 1H), 7.50-7.58 (m, 3H), 7.588-7.67 (m, 2H). ^{13}C NMR ([D_6]DMSO, 100 MHz, 298 K, ppm): δ = 54.32, 59.92, 123.78, 129.20, 130.65, 144.

3. X-Ray single crystal structure analyses

4a: Twin refinement (twin operation: inversion).

7a: Hydrogen atoms could be located in the difference Fourier maps and were allowed to refine freely.

2b: Four CF_3-Groups are disordered over two positions.

The butyl-Group of the cation is disordered over two positions.

Diffractometer: Kappa APEX II (BRUKER AXS); sealed tube

5b: Three CF_3 groups are disordered over two positions.

3.1. X-ray data of compound 2b

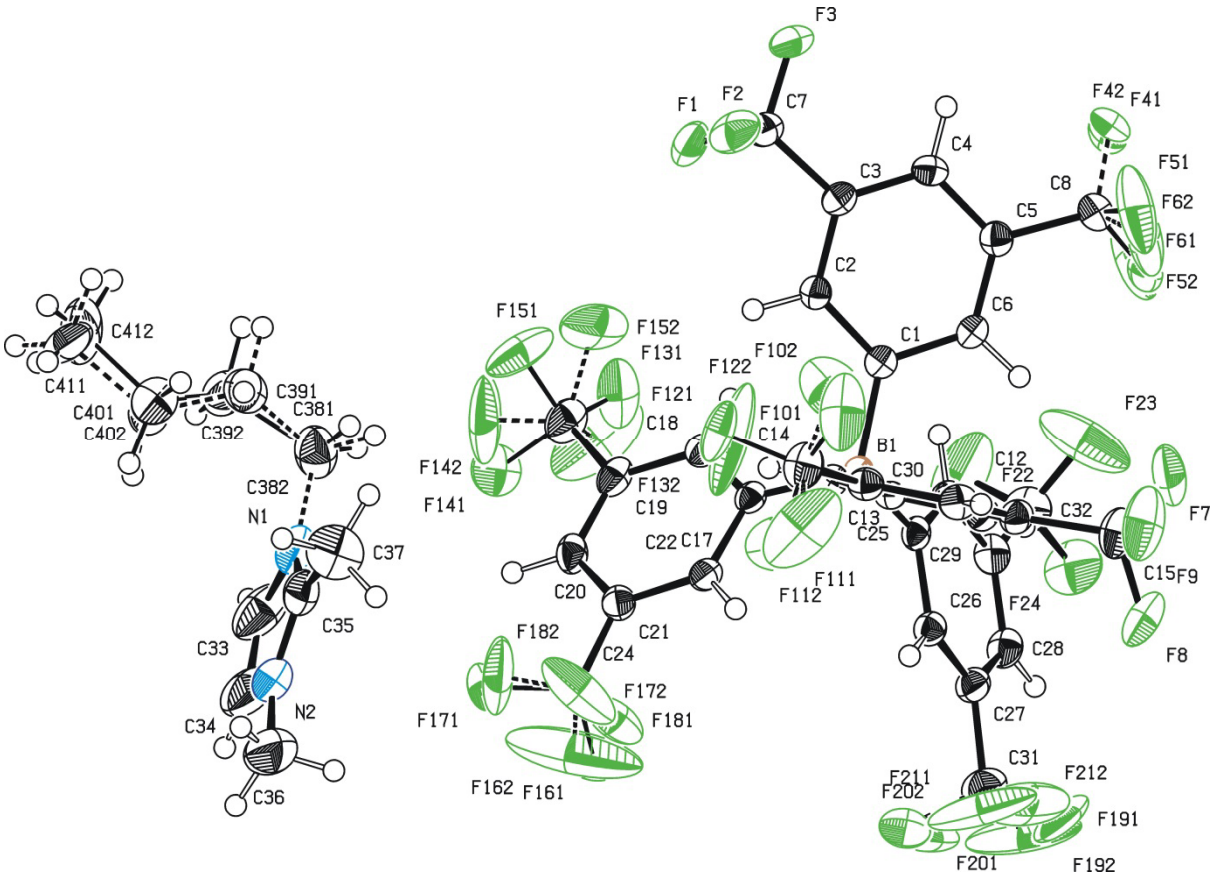

Figure S7. ORTEP drawing of compound **2b** with 50 % ellipsoids.

Operator:	*** Herdtweck ***		
Molecular Formula:	$C_{41}\ H_{29}\ B\ F_{24}\ N_2$ $[(C_{32}\ H_{12}\ B\ F_{24})^-]$, $[(C_9\ H_{17}\ N_2)^+]$		
Crystal Color / Shape	Colorless block		
Crystal Size	Approximate size of crystal fragment used for data collection: $0.38 \times 0.51 \times 0.51$ mm		
Molecular Weight:	1016.47 a.m.u.		
F_{000}:	2040		
Systematic Absences:	h0l: l≠2n; 0k0: k≠2n		
Space Group:	Monoclinic	*P* $2_1/c$	(I.T.-No.: 14)

Cell Constants:	Least-squares refinement of 9688 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 1.82° < θ < 25.50°; Mo(K_α); λ = 71.073 pm
	a = 2013.91(5) pm
	b = 1393.55(3) pm β = 111.2143(9)°
	c = 1625.59(4) pm
	V = 4253.03(18)· 10^6 pm^3; Z = 4; D_{calc} = 1.587 g cm^{-3}; Mos. = 0.67
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); sealed tube; graphite monochromator; 50 kV; 30 mA; λ = 71.073 pm; Mo(K_α)
Temperature:	(-150±1) °C; (123±1) K
Measurement Range:	1.82° < θ < 25.50°; h: -24/24, k: -16/16, l: -19/19
Measurement Time:	2 × 10 s per film
Measurement Mode:	measured: 9 runs; 4878 films / scaled: 9 runs; 4878 films
	φ- and ω-movement; Increment: Δφ/Δω = 0.50°; dx = 45.0 mm
LP - Correction:	Yes [2]
Intensity Correction	No/Yes; during scaling [2]
Absorption Correction:	Multi-scan; during scaling; μ = 0.167 mm^{-1} [2]
	Correction Factors: T_{min} = 0.6736 T_{max} = 0.7452
Reflection Data:	137576 reflections were integrated and scaled
	4050 reflections systematic absent and rejected
	2 obvious wrong intensity and rejected
	133524 reflections to be merged
	7872 independent reflections
	0.019 R_{int}: (basis F_o^2)
	7872 independent reflections (all) were used in refinements
	6806 independent reflections with $I_o > 2\sigma(I_o)$
	99.4 % completeness of the data set
	785 parameter full-matrix refinement
	10.0 reflections per parameter
Solution:	Direct Methods [3, 6]; Difference Fourier syntheses
Refinement Parameters:	In the asymmetric unit:
	68+18 Non-hydrogen atoms with anisotropic displacement parameters
Hydrogen Atoms:	In the difference map(s) calculated from the model containing all non-hydrogen atoms, not all of the hydrogen positions could be determined from the highest peaks. For this reason, the hydrogen atoms were placed in calculated positions (d_{C-H} = 95, 98, 99 pm). Isotropic displacement parameters were calculated from the parent carbon atom (U_H = 1.2/1.5 U_C). The hydrogen atoms were included in the structure factor calculations but not refined.
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4, 5, 6]
Extinction Correction:	no
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$
	with a: 0.0401; b: 3.0998; P: [Maximum(0 or F_o^2)+2*F_c^2]/3
Shift/Err:	Less than 0.001 in the last cycle of refinement:
Residual Electron Density:	+0.47 e_0^-/Å^3; -0.43 e_0^-/Å^3
R_1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$
[$F_o > 4\sigma(F_o)$; N=6806]:	= 0.0396
[all reflctns; N=7872]:	= 0.0472
w_{R2}:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$
[$F_o > 4\sigma(F_o)$; N=6806]:	= 0.0937
[all reflections; N=7872]:	= 0.1006
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$ = 1.020
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$

3.2. X-ray data of compound 5a

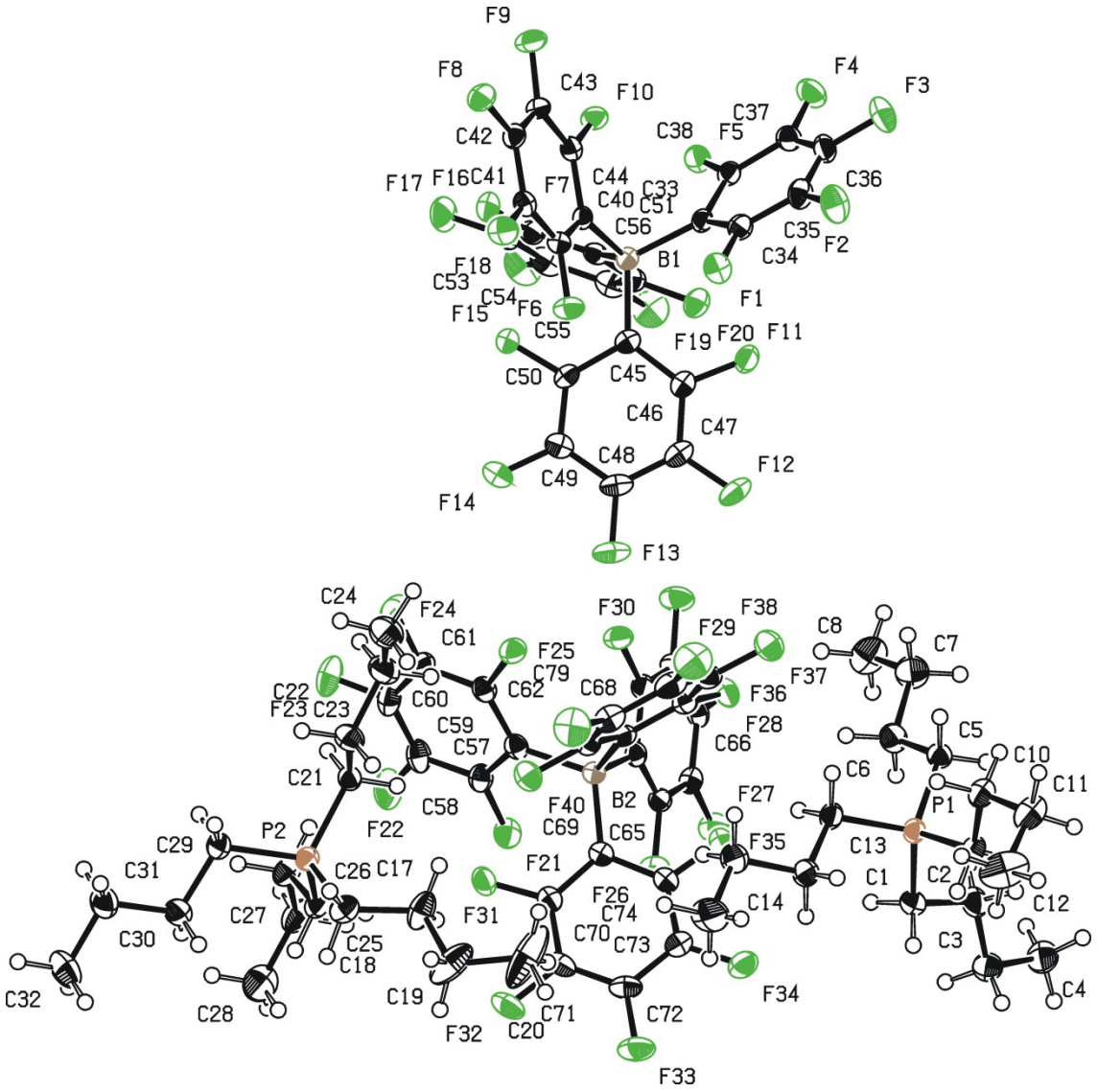

Figure S8. ORTEP drawing of compound **5a** with 50 % ellipsoids.

Operator:	*** Herdtweck ***
Molecular Formula:	C_{40} H_{36} B F_{20} P $[(C_{16}$ H_{36} $P)^{+}]$, $[(C_{24}$ B $F_{20})^{-}]$
Crystal Color / Shape	Colorless fragment
Crystal Size	*Approximate size of crystal fragment used for data collection:* 0.48 × 0.56 × 0.61 mm
Molecular Weight:	938.47 a.m.u.
F_{000}:	3808
Systematic Absences:	0kl: l≠2n; h0l: h≠2n; 00l: l≠2n
Space Group:	Orthorhombic *P ca*2_1 (I.T.-No.: 29)
Cell Constants:	Least-squares refinement of 9712 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 0.91° < θ < 25.40°; Mo(K_α); λ = 71.073 pm *a* = 1895.91(7) pm *b* = 2229.87(8) pm *c* = 1924.49(7) pm *V* = 8136.0(5)· 10^6 pm^3; *Z* = 8; D_{calc} = 1.532 g cm^{-3}; Mos. = 0.67
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); rotating anode; graphite monochromator; 50 kV; 40 mA; λ = 71.073 pm; Mo(K_α)
Temperature:	(-150±1) °C; (123±1) K

Measurement Range:	$0.91° < \theta < 25.40°$; h: -22/22, k: -26/26, l: -23/23	
Measurement Time:	2×5 s per film	
Measurement Mode:	measured: 10 runs; 4833 films / scaled: 10 runs; 4833 films φ- and ω-movement; Increment: $\Delta\varphi/\Delta\omega = 0.50°$; dx = 50.0 mm	
LP - Correction:	Yes [2]	
Intensity Correction	No/Yes; during scaling [2]	
Absorption Correction:	Multi-scan; during scaling; $\mu = 0.190$ mm^{-1} [2]	
	Correction Factors: T_{min} = 0.6499	T_{max} = 0.7452
Reflection Data:	239019	reflections were integrated and scaled
	7959	reflections systematic absent and rejected
	231060	reflections to be merged
	14933	independent reflections
	0.036	R_{int}: (basis F_o^2)
	14933	independent reflections (all) were used in refinements
	14524	independent reflections with $I_o > 2\sigma(I_o)$
	99.6 %	completeness of the data set
	1126	parameter full-matrix refinement
	13.3	reflections per parameter
Solution:	Direct Methods [3]; Difference Fourier syntheses	
Refinement Parameters:	In the asymmetric unit:	
	124	Non-hydrogen atoms with anisotropic displacement parameters
Hydrogen Atoms:	In the difference map(s) calculated from the model containing all non-hydrogen atoms, not all of the hydrogen positions could be determined from the highest peaks. For this reason, the hydrogen atoms were placed in calculated positions (d_{C-H} = 98, 99 pm). Isotropic displacement parameters were calculated from the parent carbon atom (U_H = 1.2/1.5 U_C). The hydrogen atoms were included in the structure factor calculations but not refined.	
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4]	
Extinction Correction:	no	
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$	
	with a: 0.0402; b: 1.9728; P: [Maximum(0 or F_o^2)+2*F_c^2]/3	
Shift/Err:	Less than 0.001 in the last cycle of refinement:	
Residual Electron Density:	+0.27 e_0^-/Å^3; -0.22 e_0^-/Å^3	
R_1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$	
[$F_o > 4\sigma(F_o)$; N=14524]:		= 0.0245
[all reflections; N=14933]:		= 0.0257
w_{R2}:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	
[$F_o > 4\sigma(F_o)$; N=14524]:		= 0.0667
[all reflections; N=14933]:		= 0.0682
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$	= 1.046
Flack's Parameter :	x = 0.45(5)	
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$ Twin refinement (twin operation: inversion) The correct enantiomere could **not** be proved by Flack's Parameter.	

3.3. X-ray data of compound 6b

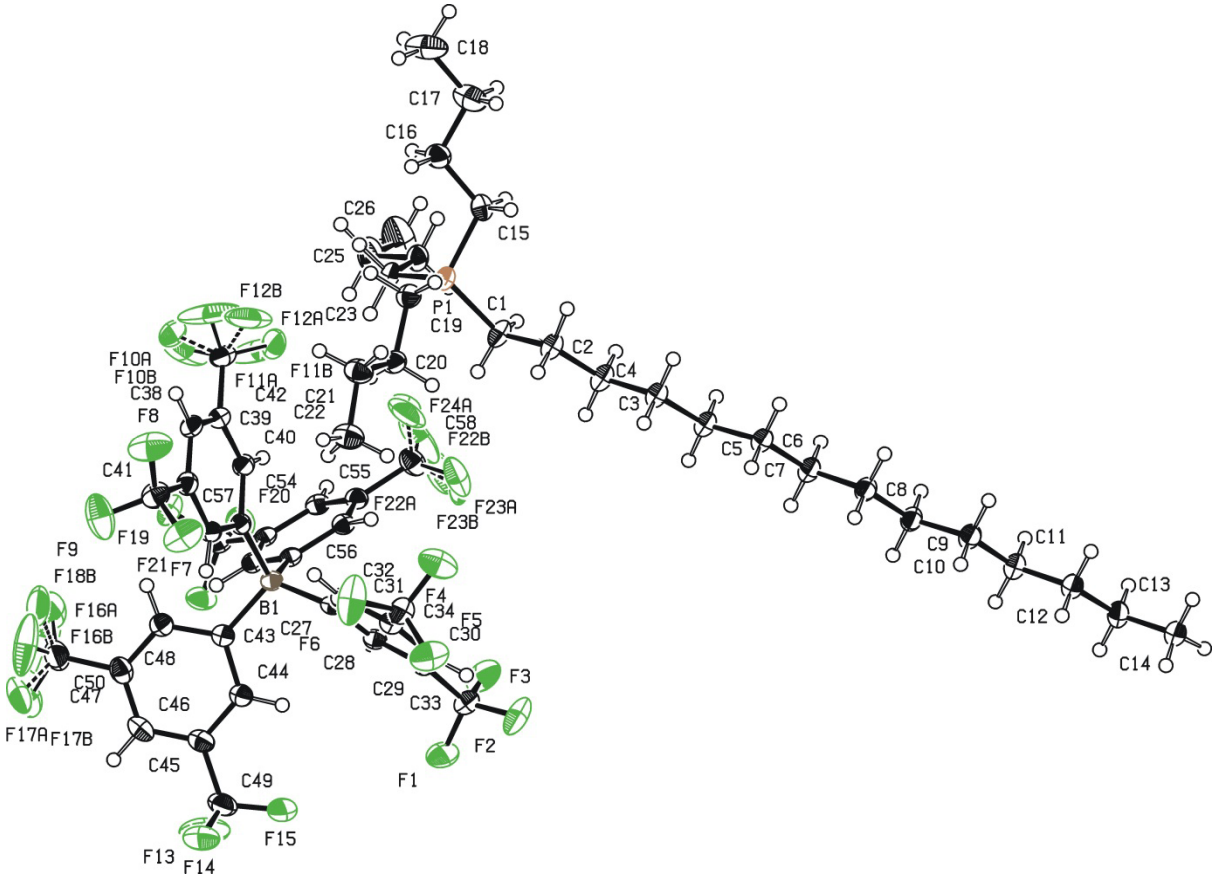

Figure S9. ORTEP drawing of compound **6b** with 50 % ellipsoids.

Operator:	*** Herdtweck ***
Molecular Formula:	$C_{58}\ H_{68}\ B\ F_{24}\ P$ $[(C_{32}\ H_{12}\ B\ F_{24})^-]$, $[(C_{26}\ H_{56}\ P)^+]$
Crystal Color / Shape	Colorless fragment
Crystal Size	Approximate size of crystal fragment used for data collection: 0.56 × 0.59 × 0.59 mm
Molecular Weight:	1262.90 a.m.u.
F_{000}:	1304
Systematic Absences:	none
Space Group:	Triclinic $P\bar{1}$ (I.T.-No.: 2)
ell Constants:	Least-squares refinement of 9093 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 1.19° < θ < 25.43°; Mo(K_α); λ = 71.073 pm *a* = 1297.32(4) pm α = 105.4144(14)° *b* = 1404.01(4) pm β = 97.8526(13)° *c* = 1803.89(5) pm γ = 97.5892(13)° *V* = 3088.64(16)· 10^6 pm^3; *Z* = 2; D_{calc} = 1.358 g cm^{-3}; Mos. = 0.67
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); rotating anode; graphite monochromator; 50 kV; 40 mA; λ = 71.073 pm; Mo(K_α)
Temperature:	(-150±1) °C; (123±1) K
Measurement Range:	1.19° < θ < 25.43°; h: -15/15, k: -16/16, l: -21/21
Measurement Time:	2 × 5 s per film
Measurement Mode:	measured: 9 runs; 5070 films / scaled: 9 runs; 5070 films φ- and ω-movement; Increment: Δφ/Δω = 0.50°; dx = 45.0 mm
LP - Correction:	Yes [2]
Intensity Correction	No/Yes; during scaling [2]
Absorption Correction:	Multi-scan; during scaling; μ = 0.153 mm^{-1} [2] Correction Factors: T_{min} = 0.6784 T_{max} = 0.7452
Reflection Data:	95414 reflections were integrated and scaled 95414 reflections to be merged 11372 independent reflections 0.030 R_{int}: (basis F_o^2) 11372 independent reflections (all) were used in refinements

	10444	independent reflections with $I_o > 2\sigma(I_o)$
	99.6 %	completeness of the data set
	845	parameter full-matrix refinement
	13.5	reflections per parameter
Solution:	Direct Methods [3]; Difference Fourier syntheses	
Refinement Parameters:	In the asymmetric unit:	
	93	Non-hydrogen atoms with anisotropic displacement parameters
Hydrogen Atoms:	In the difference map(s) calculated from the model containing all non-hydrogen atoms, not all of the hydrogen positions could be determined from the highest peaks. For this reason, the hydrogen atoms were placed in calculated positions (d_{C-H} = 95, 98, 99 pm). Isotropic displacement parameters were calculated from the parent carbon atom (U_H = 1.2/1.5 U_C). The hydrogen atoms were included in the structure factor calculations but not refined.	
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4]	
Extinction Correction:	no	
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$	
	with a: 0.0394; b: 1.6926; P: [Maximum(0 or F_o^2)+2$*F_c^2$]/3	
Shift/Err:	Less than 0.001 in the last cycle of refinement:	
Residual Electron Density:	+0.53 $e_0^-/Å^3$; -0.50 $e_0^-/Å^3$	
R_1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$	
[$F_o > 4\sigma(F_o)$; N=10444]:		= 0.0363
[all reflections; N=11372]:		= 0.0399
w_{R2}:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	
[$F_o > 4\sigma(F_o)$; N=10444]:		= 0.0889
[all reflections; N=11372]:		= 0.0929
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$	= 1.015
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$	

3.4. X-ray data of compound 7a

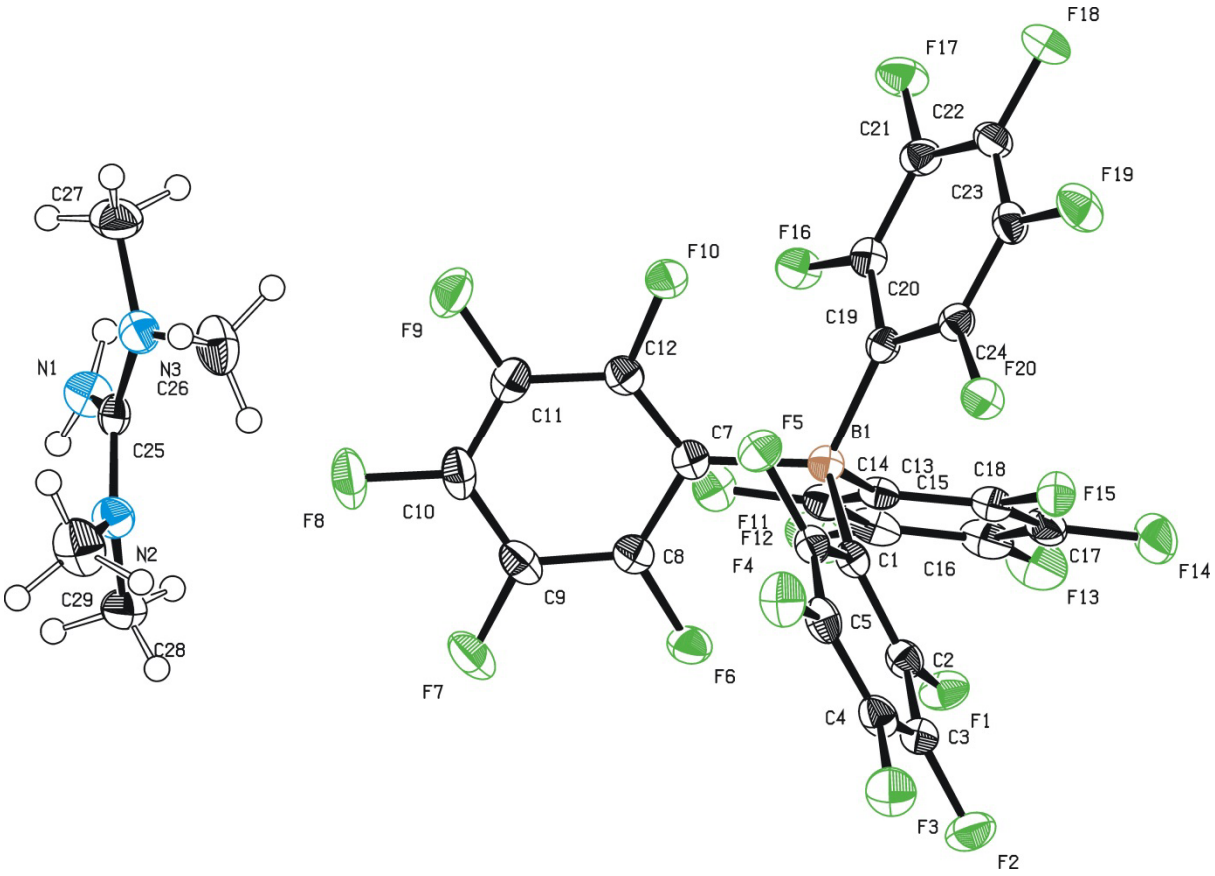

Figure S10. ORTEP drawing of compound **7a** with 50 % ellipsoids.

Operator:	*** Herdtweck ***
Molecular Formula:	$C_{29}\ H_{14}\ B\ F_{20}\ N_3$ $[(C_{24}\ B\ F_{20})^-]$, $[(C_5\ H_{14}\ N_3)^+]$
Crystal Color / Shape	Colorless fragment
Crystal Size	Approximate size of crystal fragment used for data collection: 0.10 × 0.25 × 0.36 mm
Molecular Weight:	795.24 a.m.u.
F_{000}:	788
Systematic Absences:	none
Space Group:	Triclinic $P\bar{1}$ (I.T.-No.: 2)
Cell Constants:	Least-squares refinement of 9961 reflections with the programs "APEX suite" and "SAINT" [1,2]; theta range 1.41° < θ < 25.43°; Mo(K_α); λ = 71.073 pm *a* = 815.71(2) pm α = 89.4091(12)° *b* = 1271.09(4) pm β = 83.9006(12)° *c* = 1455.97(4) pm γ = 81.7908(12)° *V* = 1485.66(7)· 10^6 pm^3; *Z* = 2; D_{calc} = 1.778 g cm^{-3}; Mos. = 0.72
Diffractometer:	Kappa APEX II (Area Diffraction System; BRUKER AXS); rotating anode; graphite monochromator; 50 kV; 40 mA; λ = 71.073 pm; Mo(K_α)
Temperature:	(-150±1) °C; (123±1) K
Measurement Range:	1.41° < θ < 25.43°; h: -9/9, k: -15/15, l: -17/17
Measurement Time:	2 × 5 s per film
Measurement Mode:	measured: 7 runs; 3291 films / scaled: 7 runs; 3291 films φ- and ω-movement; Increment: Δφ/Δω = 0.50°; dx = 35.0 mm
LP - Correction:	Yes [2]
Intensity Correction	No/Yes; during scaling [2]
Absorption Correction:	Multi-scan; during scaling; μ = 0.194 mm^{-1} [2]

	Correction Factors:	T_{min} = 0.6491 T_{max} = 0.7452
Reflection Data:	51233	reflections were integrated and scaled
	51233	reflections to be merged
	5423	independent reflections
	0.039	R_{int}: (basis F_o^2)
	5423	independent reflections (all) were used in refinements
	5014	independent reflections with $I_o > 2\sigma(I_o)$
	98.9 %	completeness of the data set
	534	parameter full-matrix refinement
	10.2	reflections per parameter
Solution:	Direct Methods [3]; Difference Fourier syntheses	
Refinement Parameters:	In the asymmetric unit:	
	53	Non-hydrogen atoms with anisotropic displacement parameters
	14	Hydrogen atoms with isotropic displacement parameters
Hydrogen Atoms:	All hydrogen atom positions were found in the difference map calculated from the model containing all non-hydrogen atoms. The hydrogen positions were refined with individual isotropic displacement parameters.	
Atomic Form Factors:	For neutral atoms and anomalous dispersion [4]	
Extinction Correction:	no	
Weighting Scheme:	$w^{-1} = \sigma^2(F_o^2)+(a*P)^2+b*P$	
	with a: 0.0426; b: 0.6762; P: [Maximum(0 or F_o^2)+2$*F_c^2$]/3	
Shift/Err:	Less than 0.001 in the last cycle of refinement:	
Residual Electron Density:	+0.29 $e_0^-/Å^3$; -0.19 $e_0^-/Å^3$	
R_1:	$\Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma\|F_o\|$	
[$F_o > 4\sigma(F_o)$; N=5014]:		= 0.0296
[all reflections; N=5423]:		= 0.0322
w_{R2}:	$[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$	
[$F_o > 4\sigma(F_o)$; N=5014]:		= 0.0778
[all reflections; N=5423]:		= 0.0808
Goodness of fit:	$[\Sigma w(F_o^2-F_c^2)^2/(NO-NV)]^{1/2}$	= 1.031
Remarks:	Refinement expression $\Sigma w(F_o^2-F_c^2)^2$	

4. References

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