Supporting information for:

Synthesis and characterization of cationic selenium-nitrogen heterocycles from *tert*-butyl-DAB (DAB = 1,4-di-*tert*-butyl-1,3-diazabutadiene) and SeX_4 *via* the reductive elimination of X_2 (X = Cl, Br): A distinct contrast with tellurium.

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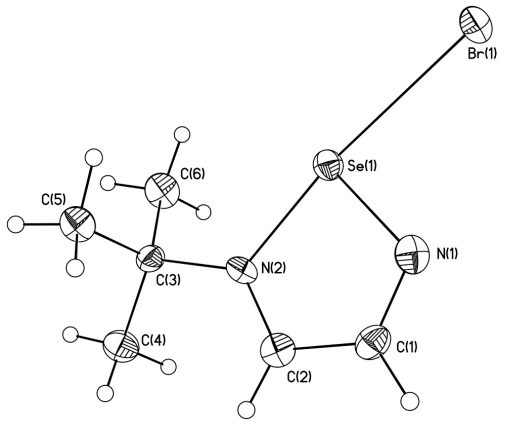

Figure S-1. Solid state structure of **5Br**. Ellipsoids are drawn to 50% probability, and the full labeling scheme is included.

Table S-1. Crystal data and structure refinement for 5Br.

Identification code	5Br
Empirical formula	$C_6 H_{11}BrN_2Se$
Formula weight	270.04
Temperature	150(2) K
Wavelength	.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 9.7366(19) Å alpha = 90 deg. b = 9.3214(19) Å beta = 104.47(3) deg. c = 10.070(2) Å gamma = 90 deg.
Volume	885.0(3) $Å^3$
Z, Calculated density	4, 2.027 Mg/m^3
Absorption coefficient	8.689 mm^{-1}
F(000)	520
Crystal size	0.20 x 0.18 x 0.15 mm
Theta range for data collection	2.16 to 27.52 deg.
Limiting indices	-12<=h<=12, -11<=k<=12, -13<=l<=13
Reflections collected / unique	3767 / 2022 [R(int) = 0.0634]
Completeness to theta = 27.52	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3556 and 0.2754
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2022 / 0 / 94
Goodness-of-fit on F^2	1.074
Final R indices [I>2sigma(I)]	R1 = 0.0487, wR2 = 0.1254
R indices (all data)	R1 = 0.0652, wR2 = 0.1323

Largest diff. peak and hole 1.146 and -1.235 e. $Å^{-3}$

Table S-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5Br. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	-2113(1)	-83(1)	3677(1)	24(1)
Se(1)	267(1)	369(1)	2673(1)	19(1)
N(1)	-881(5)	1346(5)	1284(5)	23(1)
C(1)	-199(6)	1841(6)	434(6)	23(1)
C(2)	1267(6)	1531(6)	674(5)	21(1)
N(2)	1767(5)	783(5)	1765(4)	18(1)
C(3)	3283(6)	367(6)	2319(5)	20(1)
C(6)	3329(6)	-1135(7)	2925(6)	28(1)
C(5)	3927(6)	1446(6)	3436(6)	24(1)
C(4)	4068(6)	387(8)	1181(6)	31(2)

Table S-3. Bond lengths [Å] and angles [deg] for 5br.

Br(1)-Se(1)	2.7820(10)
Se(1)-N(1)	1.804(5)
Se(1)-N(2)	1.945(4)
N(1)-C(1)	1.293(7)
C(1)-C(2)	1.417(7)
C(1)-H(1A)	.9500
C(2)-N(2)	1.289(7)
C(2)-H(2A)	.9500
N(2)-C(3)	1.493(7)
C(3)-C(5)	1.522(8)
C(3)-C(6)	1.523(8)
C(3)-C(4)	1.528(7)
C(6)-H(6A)	.9800
C(6)-H(6B)	.9800
C(6)-H(6C)	.9800
C(5)-H(5A)	.9800
C(5)-H(5B)	.9800
C(5)-H(5C)	.9800
C(4)-H(4A)	.9800

C(4)-H(4B)	.9800
C(4)-H(4C)	.9800

N(1)-Se(1)-N(2)	85.9(2)
N(1)-Se(1)-Br(1)	86.97(15)
N(2)-Se(1)-Br(1)	172.76(13)
C(1)-N(1)-Se(1)	111.8(4)
N(1)-C(1)-C(2)	118.5(5)
N(1)-C(1)-H(1A)	120.8
C(2)-C(1)-H(1A)	120.8
N(2)-C(2)-C(1)	113.9(5)
N(2)-C(2)-H(2A)	123.0
C(1)-C(2)-H(2A)	123.0
C(2)-N(2)-C(3)	125.9(4)
C(2)-N(2)-Se(1)	109.9(4)
C(3)-N(2)-Se(1)	124.1(3)
N(2)-C(3)-C(5)	106.9(4)
N(2)-C(3)-C(6)	108.4(4)
C(5)-C(3)-C(6)	110.2(4)
N(2)-C(3)-C(4)	110.5(4)
C(5)-C(3)-C(4)	110.8(5)
C(6)-C(3)-C(4)	109.9(5)
C(3)-C(6)-H(6A)	109.5

C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S-4. Anisotropic displacement parameters ($Å^2$ x 10^3) for 5br.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Br(1)	19(1)	24(1)	30(1)	1(1)	9(1)	-1(1)
Se(1)	18(1)	21(1)	20(1)	1(1)	6(1)	2(1)
N(1)	22(2)	21(3)	27(3)	-4(2)	7(2)	2(2)
C(1)	25(3)	19(3)	22(3)	3(2)	2(2)	3(2)
C(2)	25(3)	15(3)	23(3)	-2(2)	6(2)	1(2)
N(2)	19(2)	17(2)	20(2)	1(2)	10(2)	0(2)
C(3)	16(3)	29(3)	16(3)	3(2)	4(2)	3(2)
C(6)	28(3)	21(3)	35(3)	3(3)	9(3)	4(3)
C(5)	25(3)	18(3)	28(3)	1(2)	8(2)	1(2)
C(4)	28(3)	43(4)	25(3)	0(3)	13(3)	0(3)

Table S-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5br.

	x	y	z	U(eq)
H(1A)	-669	2400	-334	27
H(2A)	1831	1846	85	25
H(6A)	2808	-1143	3641	42
H(6B)	4318	-1411	3322	42
H(6C)	2892	-1815	2201	42
H(5A)	3740	2421	3073	35
H(5B)	4953	1290	3741	35
H(5C)	3501	1320	4214	35
H(4A)	3552	-202	411	47
H(4B)	5026	0	1534	47
H(4C)	4129	1375	870	47

Table S-6. Torsion angles [deg] for 5br.

N(2)-Se(1)-N(1)-C(1)	-1.3(4)
Br(1)-Se(1)-N(1)-C(1)	179.8(4)
Se(1)-N(1)-C(1)-C(2)	1.7(7)
N(1)-C(1)-C(2)-N(2)	-1.0(8)
C(1)-C(2)-N(2)-C(3)	-176.3(5)
C(1)-C(2)-N(2)-Se(1)	-.1(6)
N(1)-Se(1)-N(2)-C(2)	.8(4)
Br(1)-Se(1)-N(2)-C(2)	9.7(14)
N(1)-Se(1)-N(2)-C(3)	177.0(4)
Br(1)-Se(1)-N(2)-C(3)	-174.1(9)
C(2)-N(2)-C(3)-C(5)	97.4(6)
Se(1)-N(2)-C(3)-C(5)	-78.3(5)
C(2)-N(2)-C(3)-C(6)	-143.8(5)
Se(1)-N(2)-C(3)-C(6)	40.6(6)
C(2)-N(2)-C(3)-C(4)	-23.3(8)
Se(1)-N(2)-C(3)-C(4)	161.1(4)

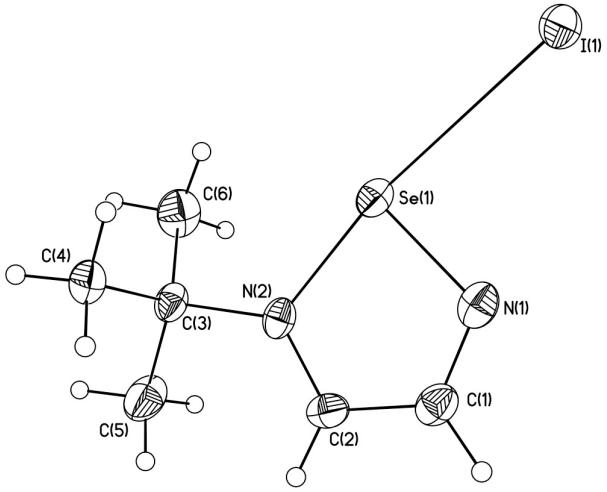

Figure S-2. Solid state structure of **5I**. Ellipsoids are drawn to 50% probability, and the full labeling scheme is included.

Table S-7. Crystal data and structure refinement for 5I.

Identification code	5I
Empirical formula	$C_6 H_{11} I N_2 Se$
Formula weight	317.03
Temperature	150(2) K
Wavelength	.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 10.251(2) Å alpha = 90 deg. b = 9.950(2) Å beta = 105.06(3) deg. c = 9.950(2) Å gamma = 90 deg.
Volume	948.0(3) $Å^3$
Z, Calculated density	4, 2.221 Mg/m^3
Absorption coefficient	7.154 mm^{-1}
F(000)	592
Crystal size	0.22 x 0.18 x 0.14 mm
Theta range for data collection	2.06 to 27.68 deg.
Limiting indices	-13<=h<=13, -11<=k<=12, -12<=l<=12
Reflections collected / unique	6589 / 2209 [R(int) = 0.0425]
Completeness to theta =	27.68 99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4341 and 0.3021
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2209 / 0 / 91

Goodness-of-fit on F^2	1.092
Final R indices [I>2sigma(I)]	R1 = 0.0398, wR2 = 0.1113
R indices (all data)	R1 = 0.0462, wR2 = 0.1160
Largest diff. peak and hole	1.187 and -1.646 e. $Å^{-3}$

Table S-8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5I. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
I(1)	2911(1)	4903(1)	3533(1)	27(1)
Se(1)	5405(1)	5420(1)	2604(1)	22(1)
N(2)	6857(4)	5772(4)	1700(4)	21(1)
N(1)	4324(4)	6374(4)	1165(4)	25(1)
C(2)	6384(5)	6489(5)	572(5)	24(1)
C(1)	4994(5)	6824(6)	307(5)	27(1)
C(3)	8299(5)	5308(6)	2279(5)	23(1)
C(4)	8948(5)	6331(6)	3431(5)	28(1)
C(5)	9009(6)	5334(8)	1096(6)	40(2)
C(6)	8283(6)	3853(6)	2843(6)	36(1)

Table S-9. Bond lengths [Å] and angles [deg] for 5I.

I(1)-Se(1)	2.9781(9)
Se(1)-N(1)	1.816(4)
Se(1)-N(2)	1.958(4)
N(2)-C(2)	1.299(6)
N(2)-C(3)	1.508(6)
N(1)-C(1)	1.301(6)
C(2)-C(1)	1.418(7)
C(2)-H(2A)	.9500
C(1)-H(1B)	.9500
C(3)-C(6)	1.511(8)
C(3)-C(4)	1.527(7)
C(3)-C(5)	1.537(7)
C(4)-H(4A)	.9800
C(4)-H(4B)	.9800
C(4)-H(4C)	.9800
C(5)-H(5A)	.9800
C(5)-H(5B)	.9800
C(5)-H(5C)	.9800
C(6)-H(6A)	.9800

C(6)-H(6B)	.9800
C(6)-H(6C)	.9800

N(1)-Se(1)-N(2)	86.07(18)
N(1)-Se(1)-I(1)	86.08(14)
N(2)-Se(1)-I(1)	171.06(11)
C(2)-N(2)-C(3)	126.6(4)
C(2)-N(2)-Se(1)	109.3(3)
C(3)-N(2)-Se(1)	124.0(3)
C(1)-N(1)-Se(1)	111.5(3)
N(2)-C(2)-C(1)	114.4(4)
N(2)-C(2)-H(2A)	122.8
C(1)-C(2)-H(2A)	122.8
N(1)-C(1)-C(2)	118.7(4)
N(1)-C(1)-H(1B)	120.7
C(2)-C(1)-H(1B)	120.7
N(2)-C(3)-C(6)	108.2(4)
N(2)-C(3)-C(4)	106.8(4)
C(6)-C(3)-C(4)	111.3(4)
N(2)-C(3)-C(5)	108.3(4)
C(6)-C(3)-C(5)	110.7(5)
C(4)-C(3)-C(5)	111.4(5)
C(3)-C(4)-H(4A)	109.5

C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5

Table S-10. Anisotropic displacement parameters ($Å^2$ x 10^3) for 5I.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
I(1)	26(1)	26(1)	30(1)	3(1)	8(1)	0(1)
Se(1)	22(1)	24(1)	18(1)	-1(1)	2(1)	4(1)
N(2)	20(2)	20(2)	21(2)	-4(2)	0(2)	1(2)
N(1)	27(2)	21(2)	25(2)	-3(2)	1(2)	1(2)
C(2)	30(3)	24(2)	20(2)	3(2)	6(2)	-1(2)
C(1)	30(3)	21(2)	25(2)	1(2)	1(2)	-1(2)
C(3)	19(2)	30(3)	18(2)	-3(2)	3(2)	4(2)
C(4)	24(2)	35(3)	25(2)	-1(2)	2(2)	-4(2)
C(5)	29(3)	69(4)	24(3)	3(3)	9(2)	12(3)
C(6)	34(3)	27(3)	45(3)	2(2)	7(2)	6(2)

Table S-11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5I.

	x	y	z	U(eq)
H(2A)	6925	6765	-26	29
H(1B)	4560	7365	-480	32
H(4A)	8480	6285	4173	43
H(4B)	8879	7275	3050	43
H(4C)	9902	6090	3811	43
H(5A)	8572	4667	375	60
H(5B)	9961	5083	1464	60
H(5C)	8945	6269	693	60
H(6A)	7870	3219	2080	54
H(6B)	7759	3842	3538	54
H(6C)	9211	3554	3278	54

Table S-12. Torsion angles [deg] for 5I.

N(1)-Se(1)-N(2)-C(2)	.5(3)
I(1)-Se(1)-N(2)-C(2)	29.1(10)
N(1)-Se(1)-N(2)-C(3)	178.6(4)
I(1)-Se(1)-N(2)-C(3)	-152.7(6)
N(2)-Se(1)-N(1)-C(1)	-1.3(4)
I(1)-Se(1)-N(1)-C(1)	-177.0(3)
C(3)-N(2)-C(2)-C(1)	-177.7(4)
Se(1)-N(2)-C(2)-C(1)	.4(5)
Se(1)-N(1)-C(1)-C(2)	1.9(6)
N(2)-C(2)-C(1)-N(1)	-1.6(7)
C(2)-N(2)-C(3)-C(6)	-140.6(5)
Se(1)-N(2)-C(3)-C(6)	41.5(5)
C(2)-N(2)-C(3)-C(4)	99.5(5)
Se(1)-N(2)-C(3)-C(4)	-78.4(5)
C(2)-N(2)-C(3)-C(5)	-20.6(7)
Se(1)-N(2)-C(3)-C(5)	161.6(4)

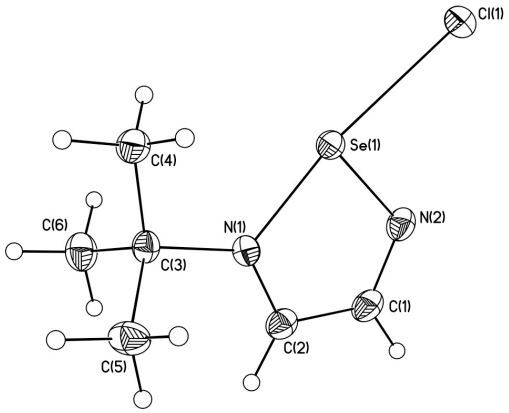

Figure S-3. Solid state structure of **5Cl**. Ellipsoids are drawn to 50% probability, and the full labeling scheme is included.

Table S-13. Crystal data and structure refinement for 5Cl.

Identification code	5Cl
Empirical formula	$C_6 H_{11}ClN_2Se$
Formula weight	225.58
Temperature	150(2) K
Wavelength	.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 8.2290(16) Å alpha = 90 deg. b = 10.646(2) Å beta = 108.74(3) deg. c = 10.347(2) Å gamma = 90 deg.
Volume	958.4(3) $Å^3$
Z, Calculated density	4, 1.745 Mg/m^3
Absorption coefficient	4.615 mm^{-1}
F(000)	448
Crystal size	0.10 x 0.05 x 0.05 mm
Theta range for data collection	2.61 to 27.65 deg.
Limiting indices	-10<=h<=10, -13<=k<=13, -13<=l<=13
Reflections collected / unique	7234 / 1999 [R(int) = 0.0686]
Completeness to theta =	27.65 99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8021 and 0.6554
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1999 / 0 / 91
Goodness-of-fit on F^2	1.105
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.0941
R indices (all data)	R1 = 0.0403, wR2 = 0.0966
Largest diff. peak and hole	1.118 and -1.353 e. $Å^{-3}$

Table S-14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5Cl. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Se(1)	2552(1)	4478(1)	8375(1)	18(1)
Cl(1)	2991(1)	2601(1)	10126(1)	24(1)
N(2)	659(3)	4827(2)	8813(2)	22(1)
N(1)	1977(3)	5927(2)	7203(2)	17(1)
C(4)	4641(4)	5638(2)	6668(3)	22(1)
C(3)	2954(3)	6351(2)	6276(2)	18(1)
C(2)	596(3)	6460(2)	7283(3)	21(1)
C(1)	-118(3)	5832(3)	8196(3)	24(1)
C(6)	1849(4)	6031(3)	4826(3)	26(1)
C(5)	3263(4)	7763(2)	6459(3)	26(1)

Table S-15. Bond lengths [Å] and angles [deg] for 5Cl.

Se(1)-N(2)	1.795(2)
Se(1)-N(1)	1.924(2)
Se(1)-Cl(1)	2.6432(8)
N(2)-C(1)	1.303(4)
N(1)-C(2)	1.297(3)
N(1)-C(3)	1.506(3)
C(4)-C(3)	1.519(4)
C(4)-H(4A)	.9800
C(4)-H(4B)	.9800
C(4)-H(4C)	.9800
C(3)-C(6)	1.522(4)
C(3)-C(5)	1.526(3)
C(2)-C(1)	1.428(4)
C(2)-H(2B)	.9500
C(1)-H(1A)	.9500
C(6)-H(6A)	.9800
C(6)-H(6B)	.9800
C(6)-H(6C)	.9800
C(5)-H(5A)	.9800

C(5)-H(5B)	.9800
C(5)-H(5C)	.9800

N(2)-Se(1)-N(1)	86.29(10)
N(2)-Se(1)-Cl(1)	85.53(8)
N(1)-Se(1)-Cl(1)	171.69(6)
C(1)-N(2)-Se(1)	112.06(18)
C(2)-N(1)-C(3)	124.6(2)
C(2)-N(1)-Se(1)	110.71(17)
C(3)-N(1)-Se(1)	124.66(16)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
N(1)-C(3)-C(4)	108.0(2)
N(1)-C(3)-C(6)	106.8(2)
C(4)-C(3)-C(6)	110.9(2)
N(1)-C(3)-C(5)	108.6(2)
C(4)-C(3)-C(5)	110.9(2)
C(6)-C(3)-C(5)	111.5(2)
N(1)-C(2)-C(1)	113.1(2)

N(1)-C(2)-H(2B)	123.4
C(1)-C(2)-H(2B)	123.4
N(2)-C(1)-C(2)	117.8(2)
N(2)-C(1)-H(1A)	121.1
C(2)-C(1)-H(1A)	121.1
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5

Table S-16. Anisotropic displacement parameters ($Å^2$ x 10^3) for 5Cl.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Se(1)	17(1)	19(1)	19(1)	1(1)	7(1)	1(1)
Cl(1)	26(1)	23(1)	22(1)	4(1)	7(1)	2(1)
N(2)	20(1)	28(1)	22(1)	-1(1)	10(1)	0(1)
N(1)	16(1)	18(1)	16(1)	1(1)	5(1)	-2(1)
C(4)	21(1)	22(1)	26(1)	2(1)	11(1)	1(1)
C(3)	18(1)	18(1)	17(1)	0(1)	8(1)	-2(1)
C(2)	19(1)	23(1)	20(1)	-3(1)	5(1)	2(1)
C(1)	20(1)	28(1)	25(1)	-3(1)	10(1)	2(1)
C(6)	26(1)	32(2)	19(1)	1(1)	6(1)	-2(1)
C(5)	26(1)	17(1)	35(2)	1(1)	11(1)	-2(1)

Table S-17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 5Cl.

	x	y	z	U(eq)
H(4A)	4411	4736	6543	33
H(4B)	5290	5807	7627	33
H(4C)	5311	5912	6089	33
H(2B)	108	7193	6785	25
H(1A)	-1127	6137	8348	28
H(6A)	1674	5120	4742	39
H(6B)	2426	6313	4183	39
H(6C)	736	6453	4618	39
H(5A)	3969	7938	7402	38
H(5B)	2160	8198	6258	38
H(5C)	3858	8058	5834	38

Table S-18. Torsion angles [deg] for 5Cl.

N(1)-Se(1)-N(2)-C(1)	-1.2(2)
Cl(1)-Se(1)-N(2)-C(1)	177.3(2)
N(2)-Se(1)-N(1)-C(2)	.89(18)
Cl(1)-Se(1)-N(1)-C(2)	-9.4(6)
N(2)-Se(1)-N(1)-C(3)	-176.7(2)
Cl(1)-Se(1)-N(1)-C(3)	173.0(3)
C(2)-N(1)-C(3)-C(4)	170.0(2)
Se(1)-N(1)-C(3)-C(4)	-12.7(3)
C(2)-N(1)-C(3)-C(6)	-70.6(3)
Se(1)-N(1)-C(3)-C(6)	106.6(2)
C(2)-N(1)-C(3)-C(5)	49.7(3)
Se(1)-N(1)-C(3)-C(5)	-133.08(19)
C(3)-N(1)-C(2)-C(1)	177.1(2)
Se(1)-N(1)-C(2)-C(1)	-.4(3)
Se(1)-N(2)-C(1)-C(2)	1.3(3)
N(1)-C(2)-C(1)-N(2)	-.6(4)

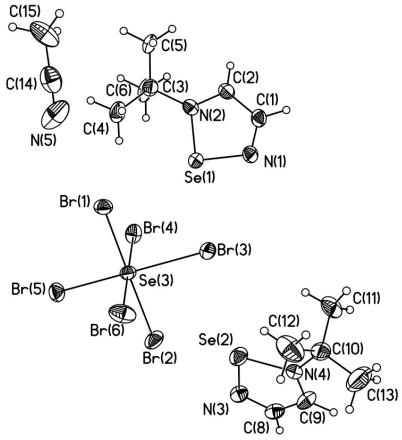

Figure S-4. Solid state structure of **$[5]_2[SeBr_6]$**. Ellipsoids are drawn to 50% probability, and the full labeling scheme is included.

Table S-19. Crystal data and structure refinement for $[5]_2[SeBr_6]$.

Identification code	$[5]_2[SeBr_6]$
Empirical formula	$C_{14}H_{25}Br_6N_5Se_3$
Formula weight	979.73
Temperature	150(2) K
Wavelength	.71073 Å
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 14.7569(8) Å alpha = 90 deg. b = 10.7682(5) Å beta = 93.392(3) deg. c = 17.0874(9) Å gamma = 90 deg.
Volume	2710.5(2) $Å^3$
Z, Calculated density	4, 2.401 Mg/m^3
Absorption coefficient	12.928 mm^{-1}
F(000)	1824
Crystal size	0.33 x 0.12 x 0.10 mm
Theta range for data collection	2.59 to 25.03 deg.
Limiting indices	-17<=h<=17, -12<=k<=12, -20<=l<=20
Reflections collected / unique	9149 / 4788 [R(int) = 0.0635]
Completeness to theta =	25.03 99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.3580 and 0.1020
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4788 / 164 / 253
Goodness-of-fit on F^2	1.036

Final R indices [I>2sigma(I)] R1 = 0.0860, wR2 = 0.2136
R indices (all data) R1 = 0.1202, wR2 = 0.2343
Largest diff. peak and hole 5.495 and -1.222 e. $Å^{-3}$

Table S-20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $[5]_2[SeBr_6]$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Se(1)	9088(1)	6335(1)	4796(1)	28(1)
N(1)	8841(8)	5006(11)	4195(7)	30(3)
C(1)	9384(10)	4955(14)	3633(8)	31(3)
C(2)	10026(10)	5926(14)	3551(8)	30(3)
N(2)	9995(8)	6740(10)	4129(6)	26(2)
C(3)	10563(11)	7912(14)	4214(8)	31(3)
C(6)	10215(12)	8824(14)	3609(10)	44(4)
C(5)	11542(11)	7575(14)	4133(11)	39(4)
C(4)	10454(13)	8378(16)	5034(9)	49(4)
Se(2)	5253(1)	5089(2)	6262(1)	38(1)
N(3)	4115(8)	5634(12)	6104(7)	32(3)
C(8)	3560(10)	4714(15)	5929(8)	32(3)
C(9)	3930(10)	3489(15)	5930(9)	35(3)
N(4)	4800(8)	3487(12)	6086(7)	32(3)
C(10)	5411(11)	2361(15)	6150(10)	37(3)

C(13)	4858(15)	1256(19)	6248(17)	80(7)
C(12)	6037(14)	2600(20)	6882(12)	64(6)
C(11)	5953(13)	2334(15)	5440(10)	45(4)
Se(3)	7546(1)	7764(1)	6618(1)	25(1)
Br(1)	9220(1)	7764(2)	6738(1)	31(1)
Br(2)	5740(1)	7746(2)	6478(1)	45(1)
Br(3)	7600(1)	5562(1)	5891(1)	36(1)
Br(4)	7577(1)	8888(1)	5247(1)	34(1)
Br(5)	7487(1)	9798(1)	7262(1)	35(1)
Br(6)	7526(1)	6690(2)	7918(1)	46(1)
N(5)	11520(13)	7998(19)	7067(11)	73(5)
C(14)	12111(15)	8226(17)	6726(10)	50(4)
C(15)	12904(15)	8512(19)	6311(10)	60(5)

Table S-21. Bond lengths [Å] and angles [deg] for $[5_2][SeBr_6]$.

Se(1)-N(1)	1.786(12)
Se(1)-N(2)	1.861(12)
N(1)-C(1)	1.288(19)
C(1)-C(2)	1.42(2)
C(1)-H(1B)	.9500
C(2)-N(2)	1.324(18)
C(2)-H(2A)	.9500
N(2)-C(3)	1.517(19)
C(3)-C(5)	1.50(2)
C(3)-C(6)	1.49(2)
C(3)-C(4)	1.51(2)
C(6)-H(6A)	.9800
C(6)-H(6B)	.9800
C(6)-H(6C)	.9800
C(5)-H(5A)	.9800
C(5)-H(5B)	.9800
C(5)-H(5C)	.9800
C(4)-H(4A)	.9800

C(4)-H(4B)	.9800
C(4)-H(4C)	.9800
Se(2)-N(3)	1.784(12)
Se(2)-N(4)	1.868(13)
N(3)-C(8)	1.308(19)
C(8)-C(9)	1.43(2)
C(8)-H(8A)	.9500
C(9)-N(4)	1.295(19)
C(9)-H(9A)	.9500
N(4)-C(10)	1.51(2)
C(10)-C(13)	1.46(2)
C(10)-C(11)	1.49(2)
C(10)-C(12)	1.53(2)
C(13)-H(13A)	.9800
C(13)-H(13B)	.9800
C(13)-H(13C)	.9800
C(12)-H(12A)	.9800
C(12)-H(12B)	.9800
C(12)-H(12C)	.9800
C(11)-H(11A)	.9800
C(11)-H(11B)	.9800
C(11)-H(11C)	.9800
Se(3)-Br(5)	2.454(2)

Se(3)-Br(1)	2.4660(19)
Se(3)-Br(6)	2.505(2)
Se(3)-Br(4)	2.639(2)
Se(3)-Br(2)	2.663(2)
Se(3)-Br(3)	2.681(2)
N(5)-C(14)	1.11(2)
C(14)-C(15)	1.44(3)
C(15)-H(15A)	.9800
C(15)-H(15B)	.9800
C(15)-H(15C)	.9800

N(1)-Se(1)-N(2)	88.0(5)
C(1)-N(1)-Se(1)	110.4(10)
N(1)-C(1)-C(2)	119.3(13)
N(1)-C(1)-H(1B)	120.4
C(2)-C(1)-H(1B)	120.4
N(2)-C(2)-C(1)	111.1(13)
N(2)-C(2)-H(2A)	124.4
C(1)-C(2)-H(2A)	124.4
C(2)-N(2)-C(3)	125.3(12)
C(2)-N(2)-Se(1)	111.1(10)
C(3)-N(2)-Se(1)	123.4(9)
C(5)-C(3)-C(6)	112.8(14)

C(5)-C(3)-C(4)	108.8(14)
C(6)-C(3)-C(4)	111.9(15)
C(5)-C(3)-N(2)	108.6(12)
C(6)-C(3)-N(2)	108.4(12)
C(4)-C(3)-N(2)	106.0(12)
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5

N(3)-Se(2)-N(4)	87.4(6)
C(8)-N(3)-Se(2)	110.9(11)
N(3)-C(8)-C(9)	117.7(13)
N(3)-C(8)-H(8A)	121.1
C(9)-C(8)-H(8A)	121.1
N(4)-C(9)-C(8)	112.1(14)
N(4)-C(9)-H(9A)	124.0
C(8)-C(9)-H(9A)	124.0
C(9)-N(4)-C(10)	126.5(13)
C(9)-N(4)-Se(2)	111.9(11)
C(10)-N(4)-Se(2)	121.6(10)
C(13)-C(10)-C(11)	114.1(17)
C(13)-C(10)-N(4)	109.1(14)
C(11)-C(10)-N(4)	107.6(13)
C(13)-C(10)-C(12)	111.1(18)
C(11)-C(10)-C(12)	109.9(15)
N(4)-C(10)-C(12)	104.5(13)
C(10)-C(13)-H(13A)	109.5
C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
Br(5)-Se(3)-Br(1)	91.42(7)
Br(5)-Se(3)-Br(6)	90.70(7)
Br(1)-Se(3)-Br(6)	89.49(7)
Br(5)-Se(3)-Br(4)	89.52(7)
Br(1)-Se(3)-Br(4)	90.23(7)
Br(6)-Se(3)-Br(4)	179.64(9)
Br(5)-Se(3)-Br(2)	89.14(7)
Br(1)-Se(3)-Br(2)	179.41(8)
Br(6)-Se(3)-Br(2)	90.66(7)
Br(4)-Se(3)-Br(2)	89.63(7)
Br(5)-Se(3)-Br(3)	178.98(8)

Br(1)-Se(3)-Br(3)	88.94(7)
Br(6)-Se(3)-Br(3)	90.25(7)
Br(4)-Se(3)-Br(3)	89.52(6)
Br(2)-Se(3)-Br(3)	90.49(7)
N(5)-C(14)-C(15)	178(2)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Table S-22. Anisotropic displacement parameters ($Å^2$ x 10^3) for $[5_2][SeBr_6]$.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Se(1)	28(1)	26(1)	30(1)	-3(1)	5(1)	-4(1)
N(1)	29(7)	22(6)	38(7)	-2(5)	1(5)	4(5)
C(1)	31(8)	33(7)	28(7)	-7(6)	-4(5)	-1(6)
C(2)	24(7)	37(7)	28(7)	-8(5)	-3(5)	5(6)
N(2)	32(6)	21(5)	25(6)	3(4)	5(5)	4(4)
C(3)	36(7)	33(7)	25(6)	-1(5)	6(6)	-9(5)
C(6)	57(10)	26(8)	48(8)	5(6)	-9(8)	-15(7)
C(5)	36(7)	27(8)	55(10)	-9(7)	5(7)	-14(6)
C(4)	66(12)	44(10)	40(7)	-9(6)	21(8)	-31(9)
Se(2)	24(1)	36(1)	54(1)	-3(1)	-1(1)	-2(1)
N(3)	26(6)	36(6)	32(7)	3(6)	-2(5)	0(5)

C(8) 21(6) 45(7) 29(7) 6(7) -2(6) -1(5)

C(9) 28(6) 32(6) 45(9) 12(7) 0(7) -6(5)

N(4) 28(6) 33(5) 37(7) -8(5) 11(5) -2(4)

C(10) 24(8) 37(6) 49(8) -1(7) 3(6) 4(5)

C(13) 55(13) 46(8) 140(20) 6(12) 27(12) -12(8)

C(12) 55(12) 82(15) 53(9) -13(10) -7(8) 25(9)

C(11) 55(11) 30(9) 51(8) 3(7) 11(7) 20(7)

Se(3) 21(1) 25(1) 29(1) 1(1) 4(1) 0(1)

Br(1) 22(1) 41(1) 30(1) -2(1) 3(1) 2(1)

Br(2) 21(1) 38(1) 75(1) -7(1) 3(1) -3(1)

Br(3) 36(1) 24(1) 50(1) -4(1) 14(1) -6(1)

Br(4) 43(1) 28(1) 31(1) 5(1) -2(1) -4(1)

Br(5) 36(1) 27(1) 41(1) -7(1) 2(1) 2(1)

Br(6) 52(1) 46(1) 41(1) 18(1) 20(1) 14(1)

N(5) 59(11) 88(13) 72(12) 12(11) -10(8) -32(11)

C(14) 74(13) 41(10) 36(10) 1(8) 3(8) 2(10)

C(15) 86(13) 59(12) 37(10) 7(9) 20(9) 30(11)

Table S-23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[5_2][SeBr_6]$.

	x	y	z	U(eq)
H(1B)	9356	4278	3276	37
H(2A)	10425	5982	3136	36
H(6A)	10575	9588	3655	66
H(6B)	9578	9014	3690	66
H(6C)	10263	8468	3085	66
H(5A)	11917	8325	4186	59
H(5B)	11611	7201	3617	59
H(5C)	11736	6980	4543	59
H(4A)	10809	9140	5121	74
H(4B)	10669	7745	5413	74
H(4C)	9812	8554	5103	74
H(8A)	2933	4856	5806	38
H(9A)	3580	2760	5829	42
H(13A)	4465	1122	5773	120

H(13B)	4483	1370	6697	120
H(13C)	5254	534	6339	120
H(12A)	6458	1905	6964	96
H(12B)	5671	2689	7339	96
H(12C)	6381	3368	6810	96
H(11A)	5549	2180	4975	67
H(11B)	6408	1671	5495	67
H(11C)	6259	3135	5385	67
H(15A)	12721	8751	5772	90
H(15B)	13298	7779	6306	90
H(15C)	13234	9199	6573	90

Table S-24. Torsion angles [deg] for $[5_2][SeBr_6]$.

N(2)-Se(1)-N(1)-C(1)	1.0(10)
Se(1)-N(1)-C(1)-C(2)	-2.9(17)
N(1)-C(1)-C(2)-N(2)	3.8(19)
C(1)-C(2)-N(2)-C(3)	-177.9(13)
C(1)-C(2)-N(2)-Se(1)	-2.6(14)
N(1)-Se(1)-N(2)-C(2)	1.0(10)
N(1)-Se(1)-N(2)-C(3)	176.4(11)
C(2)-N(2)-C(3)-C(5)	-50.7(18)
Se(1)-N(2)-C(3)-C(5)	134.4(11)
C(2)-N(2)-C(3)-C(6)	72.2(18)
Se(1)-N(2)-C(3)-C(6)	-102.6(13)
C(2)-N(2)-C(3)-C(4)	-167.5(14)
Se(1)-N(2)-C(3)-C(4)	17.7(17)
N(4)-Se(2)-N(3)-C(8)	-1.9(10)
Se(2)-N(3)-C(8)-C(9)	2.8(17)
N(3)-C(8)-C(9)-N(4)	-2(2)
C(8)-C(9)-N(4)-C(10)	178.8(13)
C(8)-C(9)-N(4)-Se(2)	.6(16)
N(3)-Se(2)-N(4)-C(9)	.7(11)

N(3)-Se(2)-N(4)-C(10)	-177.6(12)
C(9)-N(4)-C(10)-C(13)	-17(2)
Se(2)-N(4)-C(10)-C(13)	160.9(14)
C(9)-N(4)-C(10)-C(11)	107.2(18)
Se(2)-N(4)-C(10)-C(11)	-74.8(15)
C(9)-N(4)-C(10)-C(12)	-136.0(16)
Se(2)-N(4)-C(10)-C(12)	42.0(17)

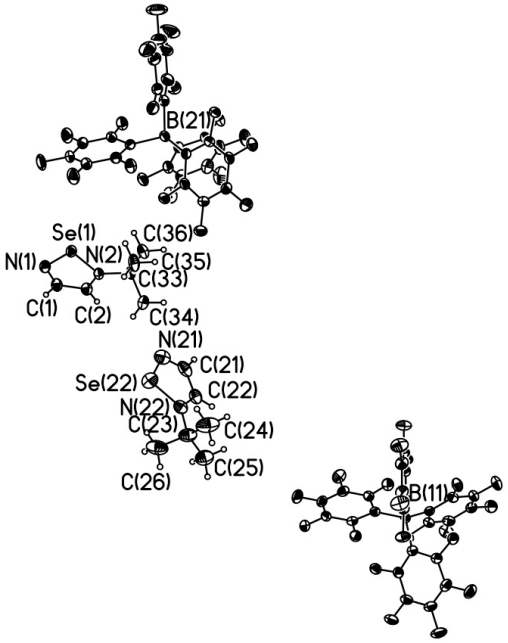

Figure S-5. Solid state structure of **[5][B(C_6F_5)$_4$]**. Ellipsoids are drawn to 50% probability, the full asymetric unit is shown, and the labeling scheme within the cationic rings is highlighted.

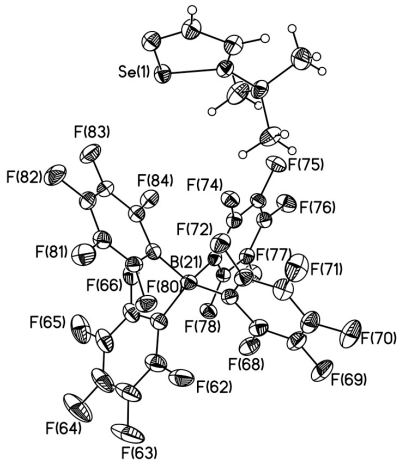

Figure S-6. Solid state structure of **[5][B(C_6F_5)$_4$]**. Ellipsoids are drawn to 50% probability, only one cation-anion unit is shown, and the labeling scheme highlights the anion. Carbons have the same number as the fluorine to which they are bound.

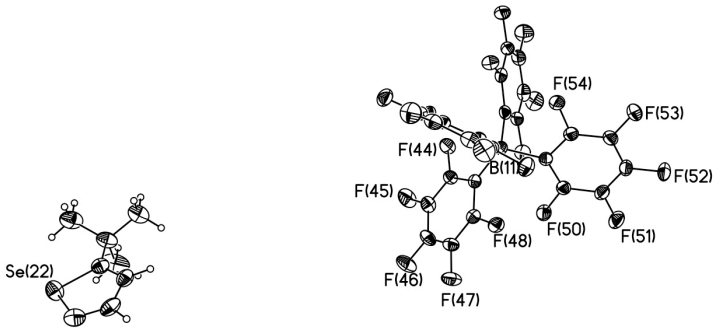

Figure S-7. Solid state structure of **[5][B(C_6F_5)$_4$]**. Ellipsoids are drawn to 50% probability, only one cation-anion unit is shown, and the labeling scheme highlights the anion. Carbons have the same number as the fluorine to which they are bound.

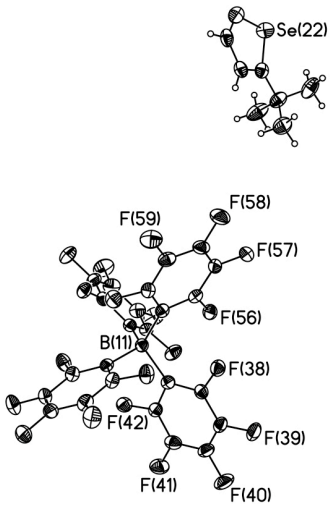

Figure S-8. Solid state structure of **[5][B(C_6F_5)$_4$]**. Ellipsoids are drawn to 50% probability, only one cation-anion unit is shown, and the labeling scheme highlights the anion. Carbons have the same number as the fluorine to which they are bound.

Table S-25. Crystal data and structure refinement for [5][B(C_6F_5)$_4$].

Identification code	[5][B(C_6F_5)$_4$]
Empirical formula	$C_{30}H_{11}BF_{20}N_2Se$
Formula weight	869.18
Temperature	150(2) K
Wavelength	.71073 Å
Crystal system, space group	Triclinic, *P*-1
Unit cell dimensions	
	a = 9.910(2) Å alpha = 68.87(3) deg.
	b = 17.185(3) Å beta = 78.32(3) deg.

c = 19.626(4) Å gamma = 81.81(3) deg.

Volume	3044.4(11) $Å^3$
Z, Calculated density	4, 1.896 Mg/m^3
Absorption coefficient	1.385 mm^{-1}
F(000)	1696
Crystal size	0.50 x 0.45 x 0.37 mm
Theta range for data collection	2.10 to 27.94 deg.
Limiting indices	-12<=h<=12, -22<=k<=22, -25<=l<=25
Reflections collected / unique	23198 / 14014 [R(int) = 0.0279]
Completeness to theta =	27.94 95.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6283 and 0.5444
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14014 / 0 / 979
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0400, wR2 = 0.0915
R indices (all data)	R1 = 0.0596, wR2 = 0.1012
Largest diff. peak and hole	.396 and -1.043 e. $Å^{-3}$

Table S-26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [5][$B(C_6F_5)_4$]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Se(1)	4292(1)	1017(1)	20(1)	27(1)
F(74)	1043(1)	3453(1)	-969(1)	29(1)
F(78)	-3074(2)	4473(1)	-1977(1)	30(1)
F(72)	2997(2)	3491(1)	-2316(1)	34(1)
F(80)	1809(2)	2894(1)	-3201(1)	36(1)
F(76)	-2568(2)	4871(1)	183(1)	39(1)
F(77)	-4055(2)	5062(1)	-887(1)	34(1)
F(66)	-2597(2)	2681(1)	-1635(1)	36(1)
F(68)	-929(2)	5293(1)	-3024(1)	37(1)
F(75)	6(2)	4040(1)	133(1)	36(1)
F(81)	3184(2)	1399(1)	-2895(1)	44(1)
F(84)	-551(2)	2160(1)	-738(1)	32(1)
F(70)	3444(2)	6302(1)	-3610(1)	54(1)
F(82)	2685(2)	266(1)	-1516(1)	47(1)
N(2)	5070(2)	1931(1)	31(1)	26(1)
F(83)	760(2)	670(1)	-473(1)	44(1)

F(69)	665(2)	6556(1)	-3638(1)	49(1)
F(62)	-148(2)	4290(1)	-3909(1)	49(1)
F(71)	4554(2)	4752(1)	-2948(1)	49(1)
N(1)	5994(2)	510(1)	-50(1)	29(1)
F(65)	-4400(2)	2406(1)	-2340(1)	62(1)
C(67)	933(3)	4305(2)	-2658(1)	26(1)
C(73)	-958(2)	3895(1)	-1526(1)	23(1)
C(2)	6407(3)	1788(2)	-12(1)	30(1)
C(80)	1543(3)	2371(2)	-2504(1)	27(1)
C(78)	-2248(3)	4327(1)	-1468(1)	24(1)
C(74)	-257(2)	3827(1)	-963(1)	25(1)
C(84)	385(3)	2025(2)	-1306(1)	26(1)
F(63)	-1991(3)	4035(2)	-4598(1)	79(1)
C(82)	2023(3)	1029(2)	-1671(2)	32(1)
B(21)	-178(3)	3585(2)	-2231(2)	25(1)
C(83)	1058(3)	1242(2)	-1144(1)	30(1)
C(77)	-2795(3)	4646(2)	-904(1)	26(1)
C(76)	-2048(3)	4551(2)	-360(1)	27(1)
C(1)	6912(3)	987(2)	-57(2)	30(1)
C(62)	-1195(3)	3822(2)	-3484(2)	40(1)
C(33)	4217(3)	2726(2)	71(2)	30(1)
C(72)	2342(3)	4228(2)	-2656(1)	29(1)
C(81)	2270(3)	1602(2)	-2363(1)	30(1)

C(79)	603(2)	2641(1)	-1988(1)	24(1)
C(75)	-763(3)	4130(2)	-385(1)	26(1)
C(68)	444(3)	5124(2)	-3004(1)	30(1)
C(66)	-2394(3)	3031(2)	-2380(2)	34(1)
C(70)	2630(3)	5663(2)	-3314(2)	38(1)
C(61)	-1280(3)	3509(2)	-2727(2)	31(1)
C(71)	3189(3)	4878(2)	-2977(2)	35(1)
C(69)	1242(3)	5784(2)	-3325(2)	36(1)
C(36)	2758(3)	2498(2)	436(2)	42(1)
F(64)	-4149(2)	3097(2)	-3837(2)	86(1)
C(35)	4245(3)	3302(2)	-725(2)	38(1)
C(65)	-3351(3)	2882(2)	-2732(2)	45(1)
C(34)	4866(4)	3093(2)	518(2)	48(1)
C(64)	-3226(4)	3219(2)	-3478(2)	57(1)
C(63)	-2145(4)	3692(2)	-3855(2)	55(1)
Se(22)	2628(1)	2112(1)	3683(1)	44(1)
N(22)	2946(2)	2958(2)	3989(1)	35(1)
C(22)	3293(3)	3605(2)	3408(2)	38(1)
N(21)	2978(3)	2762(2)	2762(1)	43(1)
C(23)	2701(3)	2904(2)	4791(2)	44(1)
C(21)	3293(3)	3475(2)	2737(2)	42(1)
C(26)	3109(4)	2002(2)	5223(2)	59(1)
C(25)	3575(4)	3507(2)	4891(2)	55(1)

C(24)	1161(4)	3132(3)	4992(2)	66(1)
F(56)	8715(2)	9517(1)	3627(1)	31(1)
F(48)	6780(2)	11398(1)	1633(1)	30(1)
F(42)	6163(2)	12007(1)	3811(1)	32(1)
F(50)	5808(2)	12594(1)	2310(1)	34(1)
F(54)	10612(2)	12092(1)	2376(1)	34(1)
F(60)	9784(2)	11588(1)	1309(1)	34(1)
F(38)	10637(2)	10598(1)	3650(1)	32(1)
F(44)	6166(2)	10243(1)	4234(1)	35(1)
F(57)	10431(2)	8412(1)	3125(1)	40(1)
F(39)	10908(2)	10770(1)	4893(1)	38(1)
F(51)	6103(2)	14202(1)	1721(1)	41(1)
F(52)	8625(2)	14797(1)	1412(1)	41(1)
F(59)	11486(2)	10486(1)	838(1)	42(1)
F(53)	10887(2)	13723(1)	1719(1)	44(1)
F(41)	6509(2)	12206(1)	5049(1)	45(1)
F(45)	3913(2)	9611(1)	4225(1)	48(1)
F(47)	4491(2)	10751(1)	1645(1)	42(1)
F(40)	8851(2)	11573(1)	5622(1)	50(1)
F(58)	11887(2)	8900(1)	1728(1)	45(1)
F(46)	3036(2)	9830(1)	2935(1)	49(1)
C(49)	8198(3)	12244(1)	2371(1)	23(1)
C(55)	9203(2)	10624(2)	2518(1)	24(1)

C(56)	9413(3)	9791(2)	2934(1)	26(1)
C(43)	6596(2)	10887(1)	2930(1)	23(1)
C(42)	7366(3)	11684(2)	4059(1)	26(1)
C(60)	9925(3)	10817(2)	1804(1)	26(1)
C(38)	9547(3)	10987(1)	3974(1)	26(1)
C(37)	8359(3)	11271(1)	3663(1)	24(1)
C(48)	6083(2)	10968(2)	2300(1)	24(1)
C(44)	5803(3)	10409(2)	3570(1)	26(1)
B(11)	8086(3)	11248(2)	2868(2)	23(1)
C(58)	11013(3)	9448(2)	1986(2)	32(1)
C(53)	9630(3)	13429(2)	1877(1)	31(1)
C(59)	10813(3)	10253(2)	1544(1)	30(1)
C(39)	9722(3)	11080(2)	4622(1)	30(1)
C(50)	7106(3)	12825(2)	2178(1)	26(1)
C(46)	4167(3)	10172(2)	2939(2)	33(1)
C(51)	7229(3)	13673(2)	1862(1)	30(1)
C(47)	4912(3)	10636(2)	2289(1)	29(1)
C(54)	9460(3)	12593(2)	2204(1)	27(1)
C(57)	10289(3)	9209(2)	2689(2)	30(1)
C(41)	7518(3)	11799(2)	4698(1)	33(1)
C(52)	8496(3)	13977(2)	1708(1)	31(1)
C(45)	4615(3)	10063(2)	3582(1)	31(1)
C(40)	8700(3)	11483(2)	4994(1)	33(1)

Table S-27. Bond lengths [Å] and angles [deg] for [5][$B(C_6F_5)_4$].

Se(1)-N(1)	1.787(2)
Se(1)-N(2)	1.854(2)
F(74)-C(74)	1.355(3)
F(78)-C(78)	1.349(3)
F(72)-C(72)	1.342(3)
F(80)-C(80)	1.337(3)
F(76)-C(76)	1.350(3)
F(77)-C(77)	1.348(3)
F(66)-C(66)	1.349(3)
F(68)-C(68)	1.356(3)
F(75)-C(75)	1.344(3)
F(81)-C(81)	1.349(3)
F(84)-C(84)	1.364(3)
F(70)-C(70)	1.341(3)
F(82)-C(82)	1.338(3)
N(2)-C(2)	1.304(3)
N(2)-C(33)	1.520(3)
F(83)-C(83)	1.333(3)
F(69)-C(69)	1.343(3)
F(62)-C(62)	1.350(4)

F(71)-C(71)	1.349(3)
N(1)-C(1)	1.304(3)
F(65)-C(65)	1.344(4)
C(67)-C(72)	1.384(4)
C(67)-C(68)	1.388(3)
C(67)-B(21)	1.647(4)
C(73)-C(74)	1.383(3)
C(73)-C(78)	1.389(3)
C(73)-B(21)	1.667(4)
C(2)-C(1)	1.423(4)
C(2)-H(32A)	.9500
C(80)-C(81)	1.375(3)
C(80)-C(79)	1.393(3)
C(78)-C(77)	1.390(3)
C(74)-C(75)	1.389(3)
C(84)-C(83)	1.371(3)
C(84)-C(79)	1.373(3)
F(63)-C(63)	1.346(4)
C(82)-C(81)	1.357(4)
C(82)-C(83)	1.376(4)
B(21)-C(79)	1.641(3)
B(21)-C(61)	1.648(4)
C(77)-C(76)	1.369(4)

C(76)-C(75)	1.373(4)
C(1)-H(31B)	.9500
C(62)-C(61)	1.375(4)
C(62)-C(63)	1.387(5)
C(33)-C(35)	1.515(4)
C(33)-C(36)	1.515(4)
C(33)-C(34)	1.525(4)
C(72)-C(71)	1.376(4)
C(68)-C(69)	1.360(4)
C(66)-C(65)	1.380(4)
C(66)-C(61)	1.381(4)
C(70)-C(71)	1.363(4)
C(70)-C(69)	1.365(4)
C(36)-H(36A)	.9800
C(36)-H(36B)	.9800
C(36)-H(36C)	.9800
F(64)-C(64)	1.340(4)
C(35)-H(35A)	.9800
C(35)-H(35B)	.9800
C(35)-H(35C)	.9800
C(65)-C(64)	1.354(5)
C(34)-H(34A)	.9800
C(34)-H(34B)	.9800

C(34)-H(34C)	.9800
C(64)-C(63)	1.360(6)
Se(22)-N(21)	1.743(3)
Se(22)-N(22)	1.847(2)
N(22)-C(22)	1.300(4)
N(22)-C(23)	1.514(4)
C(22)-C(21)	1.413(4)
C(22)-H(22A)	.9500
N(21)-C(21)	1.289(4)
C(23)-C(26)	1.516(5)
C(23)-C(25)	1.527(5)
C(23)-C(24)	1.528(5)
C(21)-H(21A)	.9500
C(26)-H(26A)	.9800
C(26)-H(26B)	.9800
C(26)-H(26C)	.9800
C(25)-H(25A)	.9800
C(25)-H(25B)	.9800
C(25)-H(25C)	.9800
C(24)-H(24A)	.9800
C(24)-H(24B)	.9800
C(24)-H(24C)	.9800
F(56)-C(56)	1.341(3)

F(48)-C(48)	1.350(3)
F(42)-C(42)	1.349(3)
F(50)-C(50)	1.347(3)
F(54)-C(54)	1.351(3)
F(60)-C(60)	1.340(3)
F(38)-C(38)	1.356(3)
F(44)-C(44)	1.342(3)
F(57)-C(57)	1.332(3)
F(39)-C(39)	1.349(3)
F(51)-C(51)	1.344(3)
F(52)-C(52)	1.330(3)
F(59)-C(59)	1.351(3)
F(53)-C(53)	1.346(3)
F(41)-C(41)	1.352(3)
F(45)-C(45)	1.330(3)
F(47)-C(47)	1.349(3)
F(40)-C(40)	1.336(3)
F(58)-C(58)	1.351(3)
F(46)-C(46)	1.341(3)
C(49)-C(50)	1.377(3)
C(49)-C(54)	1.393(3)
C(49)-B(11)	1.643(3)
C(55)-C(56)	1.379(3)

C(55)-C(60)	1.382(3)
C(55)-B(11)	1.653(4)
C(56)-C(57)	1.384(4)
C(43)-C(44)	1.382(3)
C(43)-C(48)	1.384(3)
C(43)-B(11)	1.647(4)
C(42)-C(41)	1.378(4)
C(42)-C(37)	1.401(3)
C(60)-C(59)	1.381(4)
C(38)-C(37)	1.382(4)
C(38)-C(39)	1.384(4)
C(37)-B(11)	1.651(4)
C(48)-C(47)	1.372(4)
C(44)-C(45)	1.385(4)
C(58)-C(59)	1.354(4)
C(58)-C(57)	1.365(4)
C(53)-C(54)	1.365(4)
C(53)-C(52)	1.372(4)
C(39)-C(40)	1.380(4)
C(50)-C(51)	1.376(3)
C(46)-C(45)	1.364(4)
C(46)-C(47)	1.364(4)
C(51)-C(52)	1.363(4)

C(41)-C(40)	1.368(4)

N(1)-Se(1)-N(2)	88.03(10)
C(2)-N(2)-C(33)	126.8(2)
C(2)-N(2)-Se(1)	110.51(17)
C(33)-N(2)-Se(1)	122.70(16)
C(1)-N(1)-Se(1)	111.20(17)
C(72)-C(67)-C(68)	112.5(2)
C(72)-C(67)-B(21)	127.9(2)
C(68)-C(67)-B(21)	119.2(2)
C(74)-C(73)-C(78)	112.5(2)
C(74)-C(73)-B(21)	120.5(2)
C(78)-C(73)-B(21)	126.5(2)
N(2)-C(2)-C(1)	113.8(2)
N(2)-C(2)-H(32A)	123.1
C(1)-C(2)-H(32A)	123.1
F(80)-C(80)-C(81)	115.0(2)
F(80)-C(80)-C(79)	119.1(2)
C(81)-C(80)-C(79)	125.9(2)
F(78)-C(78)-C(73)	121.2(2)
F(78)-C(78)-C(77)	114.6(2)
C(73)-C(78)-C(77)	124.3(2)
F(74)-C(74)-C(73)	118.8(2)

F(74)-C(74)-C(75)	115.8(2)
C(73)-C(74)-C(75)	125.3(2)
F(84)-C(84)-C(83)	115.3(2)
F(84)-C(84)-C(79)	121.1(2)
C(83)-C(84)-C(79)	123.6(2)
F(82)-C(82)-C(81)	120.2(2)
F(82)-C(82)-C(83)	121.1(2)
C(81)-C(82)-C(83)	118.8(2)
C(79)-B(21)-C(67)	111.6(2)
C(79)-B(21)-C(61)	102.22(19)
C(67)-B(21)-C(61)	116.0(2)
C(79)-B(21)-C(73)	114.6(2)
C(67)-B(21)-C(73)	100.65(19)
C(61)-B(21)-C(73)	112.3(2)
F(83)-C(83)-C(84)	120.1(2)
F(83)-C(83)-C(82)	119.1(2)
C(84)-C(83)-C(82)	120.8(2)
F(77)-C(77)-C(76)	119.0(2)
F(77)-C(77)-C(78)	120.8(2)
C(76)-C(77)-C(78)	120.2(2)
F(76)-C(76)-C(77)	120.3(2)
F(76)-C(76)-C(75)	121.3(2)
C(77)-C(76)-C(75)	118.4(2)

N(1)-C(1)-C(2)	116.5(2)
N(1)-C(1)-H(31B)	121.8
C(2)-C(1)-H(31B)	121.8
F(62)-C(62)-C(61)	120.1(3)
F(62)-C(62)-C(63)	116.2(3)
C(61)-C(62)-C(63)	123.6(3)
C(35)-C(33)-C(36)	110.8(2)
C(35)-C(33)-N(2)	105.6(2)
C(36)-C(33)-N(2)	107.8(2)
C(35)-C(33)-C(34)	112.3(2)
C(36)-C(33)-C(34)	111.3(3)
N(2)-C(33)-C(34)	108.8(2)
F(72)-C(72)-C(71)	114.0(2)
F(72)-C(72)-C(67)	121.4(2)
C(71)-C(72)-C(67)	124.6(2)
F(81)-C(81)-C(82)	119.8(2)
F(81)-C(81)-C(80)	121.9(2)
C(82)-C(81)-C(80)	118.3(2)
C(84)-C(79)-C(80)	112.5(2)
C(84)-C(79)-B(21)	126.7(2)
C(80)-C(79)-B(21)	120.7(2)
F(75)-C(75)-C(76)	119.8(2)
F(75)-C(75)-C(74)	120.9(2)

C(76)-C(75)-C(74)	119.3(2)
F(68)-C(68)-C(69)	116.5(2)
F(68)-C(68)-C(67)	118.7(2)
C(69)-C(68)-C(67)	124.8(3)
F(66)-C(66)-C(65)	115.9(3)
F(66)-C(66)-C(61)	118.7(2)
C(65)-C(66)-C(61)	125.4(3)
F(70)-C(70)-C(71)	119.5(3)
F(70)-C(70)-C(69)	121.5(3)
C(71)-C(70)-C(69)	119.0(3)
C(62)-C(61)-C(66)	112.5(3)
C(62)-C(61)-B(21)	127.8(3)
C(66)-C(61)-B(21)	119.5(2)
F(71)-C(71)-C(70)	119.6(2)
F(71)-C(71)-C(72)	121.1(2)
C(70)-C(71)-C(72)	119.3(3)
F(69)-C(69)-C(68)	120.2(3)
F(69)-C(69)-C(70)	120.0(3)
C(68)-C(69)-C(70)	119.8(2)
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5

H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
F(65)-C(65)-C(64)	120.0(3)
F(65)-C(65)-C(66)	120.6(3)
C(64)-C(65)-C(66)	119.5(3)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
F(64)-C(64)-C(65)	121.0(4)
F(64)-C(64)-C(63)	120.8(4)
C(65)-C(64)-C(63)	118.2(3)
F(63)-C(63)-C(64)	119.6(3)
F(63)-C(63)-C(62)	119.5(4)
C(64)-C(63)-C(62)	120.8(3)

N(21)-Se(22)-N(22)	90.17(12)
C(22)-N(22)-C(23)	127.2(3)
C(22)-N(22)-Se(22)	108.8(2)
C(23)-N(22)-Se(22)	123.77(19)
N(22)-C(22)-C(21)	112.9(3)
N(22)-C(22)-H(22A)	123.5
C(21)-C(22)-H(22A)	123.5
C(21)-N(21)-Se(22)	109.2(2)
N(22)-C(23)-C(26)	105.4(3)
N(22)-C(23)-C(25)	110.3(3)
C(26)-C(23)-C(25)	111.5(3)
N(22)-C(23)-C(24)	106.8(3)
C(26)-C(23)-C(24)	111.8(3)
C(25)-C(23)-C(24)	110.9(3)
N(21)-C(21)-C(22)	118.9(3)
N(21)-C(21)-H(21A)	120.5
C(22)-C(21)-H(21A)	120.5
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5

C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(50)-C(49)-C(54)	113.6(2)
C(50)-C(49)-B(11)	126.0(2)
C(54)-C(49)-B(11)	119.7(2)
C(56)-C(55)-C(60)	112.4(2)
C(56)-C(55)-B(11)	120.0(2)
C(60)-C(55)-B(11)	127.4(2)
F(56)-C(56)-C(55)	118.0(2)
F(56)-C(56)-C(57)	117.1(2)
C(55)-C(56)-C(57)	124.9(2)
C(44)-C(43)-C(48)	112.3(2)
C(44)-C(43)-B(11)	126.5(2)

C(48)-C(43)-B(11)	120.8(2)
F(42)-C(42)-C(41)	115.5(2)
F(42)-C(42)-C(37)	119.5(2)
C(41)-C(42)-C(37)	124.9(2)
F(60)-C(60)-C(59)	115.3(2)
F(60)-C(60)-C(55)	120.6(2)
C(59)-C(60)-C(55)	124.2(2)
F(38)-C(38)-C(37)	121.2(2)
F(38)-C(38)-C(39)	115.4(2)
C(37)-C(38)-C(39)	123.4(2)
C(38)-C(37)-C(42)	113.1(2)
C(38)-C(37)-B(11)	127.2(2)
C(42)-C(37)-B(11)	119.5(2)
F(48)-C(48)-C(47)	115.7(2)
F(48)-C(48)-C(43)	118.7(2)
C(47)-C(48)-C(43)	125.5(2)
F(44)-C(44)-C(43)	120.6(2)
F(44)-C(44)-C(45)	115.4(2)
C(43)-C(44)-C(45)	124.0(2)
C(49)-B(11)-C(43)	114.6(2)
C(49)-B(11)-C(37)	99.08(18)
C(43)-B(11)-C(37)	113.22(19)
C(49)-B(11)-C(55)	113.19(19)

C(43)-B(11)-C(55)	102.44(19)
C(37)-B(11)-C(55)	114.9(2)
F(58)-C(58)-C(59)	120.4(2)
F(58)-C(58)-C(57)	121.6(2)
C(59)-C(58)-C(57)	118.0(2)
F(53)-C(53)-C(54)	121.2(2)
F(53)-C(53)-C(52)	119.7(2)
C(54)-C(53)-C(52)	119.2(2)
F(59)-C(59)-C(58)	118.3(2)
F(59)-C(59)-C(60)	120.9(2)
C(58)-C(59)-C(60)	120.8(2)
F(39)-C(39)-C(40)	119.6(2)
F(39)-C(39)-C(38)	119.5(2)
C(40)-C(39)-C(38)	121.0(2)
F(50)-C(50)-C(51)	114.8(2)
F(50)-C(50)-C(49)	121.3(2)
C(51)-C(50)-C(49)	123.8(2)
F(46)-C(46)-C(45)	121.6(2)
F(46)-C(46)-C(47)	120.2(3)
C(45)-C(46)-C(47)	118.2(2)
F(51)-C(51)-C(52)	120.0(2)
F(51)-C(51)-C(50)	120.2(2)
C(52)-C(51)-C(50)	119.8(2)

F(47)-C(47)-C(46)	119.3(2)
F(47)-C(47)-C(48)	121.2(2)
C(46)-C(47)-C(48)	119.5(2)
F(54)-C(54)-C(53)	116.1(2)
F(54)-C(54)-C(49)	119.6(2)
C(53)-C(54)-C(49)	124.3(2)
F(57)-C(57)-C(58)	119.0(2)
F(57)-C(57)-C(56)	121.2(2)
C(58)-C(57)-C(56)	119.8(2)
F(41)-C(41)-C(40)	119.1(2)
F(41)-C(41)-C(42)	121.4(3)
C(40)-C(41)-C(42)	119.5(2)
F(52)-C(52)-C(51)	120.3(2)
F(52)-C(52)-C(53)	120.4(2)
C(51)-C(52)-C(53)	119.3(2)
F(45)-C(45)-C(46)	119.6(2)
F(45)-C(45)-C(44)	119.9(2)
C(46)-C(45)-C(44)	120.5(2)
F(40)-C(40)-C(41)	120.3(3)
F(40)-C(40)-C(39)	121.6(3)
C(41)-C(40)-C(39)	118.1(2)

Table S-28. Anisotropic displacement parameters ($Å^2$ x 10^3) for [5][$B(C_6F_5)_4$].

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Se(1)	24(1)	26(1)	32(1)	-13(1)	-3(1)	0(1)
F(74)	22(1)	34(1)	33(1)	-15(1)	-9(1)	6(1)
F(78)	27(1)	33(1)	32(1)	-15(1)	-12(1)	7(1)
F(72)	28(1)	29(1)	43(1)	-9(1)	-10(1)	5(1)
F(80)	47(1)	32(1)	23(1)	-8(1)	-4(1)	7(1)
F(76)	40(1)	48(1)	35(1)	-27(1)	-6(1)	10(1)
F(77)	26(1)	36(1)	42(1)	-21(1)	-8(1)	11(1)
F(66)	31(1)	34(1)	49(1)	-20(1)	-7(1)	-2(1)
F(68)	34(1)	30(1)	40(1)	-6(1)	-8(1)	10(1)
F(75)	35(1)	47(1)	32(1)	-20(1)	-14(1)	7(1)
F(81)	53(1)	42(1)	36(1)	-21(1)	-4(1)	18(1)
F(84)	32(1)	29(1)	30(1)	-8(1)	2(1)	1(1)
F(70)	57(1)	35(1)	59(1)	-7(1)	9(1)	-17(1)

F(82)	62(1)	29(1)	45(1)	-13(1)	-15(1)	21(1)
N(2)	27(1)	21(1)	27(1)	-8(1)	-4(1)	1(1)
F(83)	60(1)	27(1)	34(1)	-1(1)	-6(1)	2(1)
F(69)	61(1)	24(1)	48(1)	-1(1)	-7(1)	4(1)
F(62)	61(1)	54(1)	29(1)	-14(1)	-13(1)	8(1)
F(71)	30(1)	45(1)	67(1)	-16(1)	0(1)	-6(1)
N(1)	28(1)	27(1)	29(1)	-11(1)	-1(1)	1(1)
F(65)	33(1)	72(1)	105(2)	-56(1)	-21(1)	0(1)
C(67)	29(1)	25(1)	22(1)	-10(1)	-4(1)	3(1)
C(73)	24(1)	19(1)	25(1)	-8(1)	-4(1)	-1(1)
C(2)	26(1)	28(1)	33(1)	-10(1)	-2(1)	-2(1)
C(80)	31(1)	26(1)	25(1)	-9(1)	-9(1)	3(1)
C(78)	25(1)	23(1)	26(1)	-8(1)	-8(1)	-1(1)
C(74)	20(1)	23(1)	30(1)	-10(1)	-5(1)	3(1)
C(84)	25(1)	28(1)	27(1)	-11(1)	-4(1)	-1(1)
F(63)	88(2)	115(2)	47(1)	-39(1)	-40(1)	24(1)
C(82)	36(2)	24(1)	38(2)	-14(1)	-15(1)	10(1)
B(21)	24(1)	25(1)	25(1)	-9(1)	-6(1)	4(1)
C(83)	38(2)	23(1)	28(1)	-5(1)	-10(1)	0(1)
C(77)	22(1)	23(1)	32(1)	-10(1)	-5(1)	4(1)
C(76)	29(1)	28(1)	25(1)	-13(1)	-2(1)	1(1)
C(1)	25(1)	28(1)	35(1)	-10(1)	-2(1)	-1(1)
C(62)	43(2)	47(2)	37(2)	-21(1)	-16(1)	13(1)

C(33)	30(1)	21(1)	36(1)	-10(1)	-7(1)	5(1)
C(72)	31(1)	26(1)	27(1)	-8(1)	-4(1)	4(1)
C(81)	32(1)	32(1)	29(1)	-17(1)	-7(1)	7(1)
C(79)	22(1)	25(1)	27(1)	-12(1)	-6(1)	1(1)
C(75)	27(1)	29(1)	26(1)	-11(1)	-9(1)	-1(1)
C(68)	28(1)	29(1)	29(1)	-9(1)	-4(1)	5(1)
C(66)	29(1)	36(1)	47(2)	-26(1)	-15(1)	10(1)
C(70)	42(2)	31(1)	36(2)	-9(1)	5(1)	-9(1)
C(61)	32(1)	30(1)	34(1)	-18(1)	-12(1)	10(1)
C(71)	29(1)	37(2)	38(2)	-14(1)	1(1)	-3(1)
C(69)	46(2)	24(1)	31(1)	-6(1)	-2(1)	2(1)
C(36)	36(2)	32(1)	48(2)	-13(1)	5(1)	10(1)
F(64)	65(2)	131(2)	106(2)	-80(2)	-54(1)	19(1)
C(35)	38(2)	29(1)	39(2)	-4(1)	-7(1)	4(1)
C(65)	32(2)	51(2)	71(2)	-42(2)	-20(2)	11(1)
C(34)	60(2)	36(2)	59(2)	-28(2)	-23(2)	13(1)
C(64)	44(2)	78(2)	78(3)	-56(2)	-38(2)	23(2)
C(63)	61(2)	73(2)	46(2)	-36(2)	-32(2)	25(2)
Se(22)	46(1)	45(1)	40(1)	-14(1)	3(1)	-16(1)
N(22)	26(1)	41(1)	36(1)	-11(1)	-4(1)	-1(1)
C(22)	31(2)	36(2)	43(2)	-10(1)	-5(1)	4(1)
N(21)	28(1)	58(2)	38(1)	-16(1)	-1(1)	-1(1)
C(23)	37(2)	65(2)	33(2)	-18(1)	-2(1)	-12(2)

C(21)	32(2)	44(2)	36(2)	-4(1)	-2(1)	9(1)
C(26)	65(2)	70(2)	34(2)	4(2)	-13(2)	-29(2)
C(25)	50(2)	66(2)	54(2)	-24(2)	-10(2)	-12(2)
C(24)	38(2)	125(4)	48(2)	-48(2)	3(2)	-9(2)
F(56)	40(1)	27(1)	22(1)	-4(1)	-4(1)	-2(1)
F(48)	34(1)	34(1)	20(1)	-6(1)	-4(1)	-5(1)
F(42)	29(1)	36(1)	34(1)	-16(1)	-4(1)	2(1)
F(50)	23(1)	29(1)	45(1)	-8(1)	-5(1)	0(1)
F(54)	24(1)	33(1)	40(1)	-4(1)	-9(1)	-5(1)
F(60)	38(1)	32(1)	24(1)	-4(1)	3(1)	-4(1)
F(38)	28(1)	35(1)	32(1)	-11(1)	-8(1)	1(1)
F(44)	42(1)	41(1)	20(1)	-6(1)	-2(1)	-17(1)
F(57)	58(1)	26(1)	40(1)	-14(1)	-21(1)	8(1)
F(39)	45(1)	37(1)	32(1)	-3(1)	-20(1)	-7(1)
F(51)	37(1)	28(1)	52(1)	-6(1)	-12(1)	6(1)
F(52)	56(1)	23(1)	40(1)	-2(1)	-14(1)	-11(1)
F(59)	38(1)	54(1)	33(1)	-21(1)	13(1)	-8(1)
F(53)	38(1)	38(1)	50(1)	0(1)	-13(1)	-18(1)
F(41)	53(1)	48(1)	37(1)	-26(1)	0(1)	2(1)
F(45)	46(1)	60(1)	34(1)	-10(1)	8(1)	-31(1)
F(47)	40(1)	57(1)	35(1)	-16(1)	-16(1)	-7(1)
F(40)	71(1)	57(1)	28(1)	-19(1)	-15(1)	-10(1)
F(58)	41(1)	48(1)	53(1)	-33(1)	-5(1)	10(1)

F(46)	33(1)	67(1)	54(1)	-25(1)	-5(1)	-21(1)
C(49)	27(1)	24(1)	19(1)	-8(1)	-4(1)	-2(1)
C(55)	20(1)	28(1)	24(1)	-9(1)	-4(1)	-2(1)
C(56)	28(1)	30(1)	21(1)	-9(1)	-5(1)	-4(1)
C(43)	23(1)	22(1)	23(1)	-8(1)	-3(1)	-1(1)
C(42)	28(1)	25(1)	25(1)	-6(1)	-5(1)	-5(1)
C(60)	23(1)	27(1)	26(1)	-7(1)	-4(1)	-3(1)
C(38)	30(1)	21(1)	26(1)	-4(1)	-5(1)	-4(1)
C(37)	26(1)	22(1)	22(1)	-5(1)	-2(1)	-8(1)
C(48)	22(1)	25(1)	24(1)	-8(1)	-2(1)	1(1)
C(44)	27(1)	29(1)	22(1)	-10(1)	-3(1)	-4(1)
B(11)	24(1)	23(1)	21(1)	-7(1)	-3(1)	-2(1)
C(58)	25(1)	38(1)	41(2)	-25(1)	-8(1)	4(1)
C(53)	30(1)	33(1)	28(1)	-6(1)	-6(1)	-11(1)
C(59)	25(1)	41(2)	28(1)	-18(1)	0(1)	-4(1)
C(39)	36(2)	27(1)	26(1)	-2(1)	-12(1)	-8(1)
C(50)	24(1)	28(1)	26(1)	-7(1)	-4(1)	-4(1)
C(46)	22(1)	40(1)	42(2)	-19(1)	-2(1)	-10(1)
C(51)	32(1)	26(1)	31(1)	-7(1)	-9(1)	3(1)
C(47)	29(1)	36(1)	28(1)	-16(1)	-9(1)	0(1)
C(54)	27(1)	28(1)	26(1)	-6(1)	-7(1)	-3(1)
C(57)	34(1)	25(1)	34(1)	-11(1)	-15(1)	2(1)
C(41)	42(2)	28(1)	28(1)	-12(1)	2(1)	-7(1)

C(52)	43(2)	23(1)	27(1)	-5(1)	-9(1)	-7(1)
C(45)	32(1)	34(1)	26(1)	-10(1)	3(1)	-10(1)
C(40)	48(2)	32(1)	23(1)	-9(1)	-8(1)	-11(1)

Table S-29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [5][$B(C_6F_5)_4$].

	x	y	z	U(eq)
H(32A)	6990	2182	-13	36
H(31B)	7868	809	-90	36
H(36A)	2773	2091	936	63
H(36B)	2374	2254	143	63
H(36C)	2183	3002	466	63
H(35A)	3699	3828	-736	57
H(35B)	3854	3033	-996	57
H(35C)	5202	3419	-958	57
H(34A)	4306	3596	562	72
H(34B)	5803	3240	267	72
H(34C)	4907	2679	1013	72
H(22A)	3523	4112	3432	46
H(21A)	3522	3906	2275	50
H(26A)	2517	1634	5156	89

H(26B)	2999	1929	5750	89
H(26C)	4076	1862	5042	89
H(25A)	3464	3433	5418	82
H(25B)	3272	4084	4614	82
H(25C)	4549	3390	4705	82
H(24A)	620	2762	4893	100
H(24B)	932	3714	4695	100
H(24C)	944	3067	5519	100

Table S-30. Torsion angles [deg] for [5][$B(C_6F_5)_4$].

N(1)-Se(1)-N(2)-C(2)	-.21(18)
N(1)-Se(1)-N(2)-C(33)	178.81(19)
N(2)-Se(1)-N(1)-C(1)	.22(19)
C(33)-N(2)-C(2)-C(1)	-178.8(2)
Se(1)-N(2)-C(2)-C(1)	.1(3)
C(74)-C(73)-C(78)-F(78)	178.5(2)
B(21)-C(73)-C(78)-F(78)	6.4(4)
C(74)-C(73)-C(78)-C(77)	-1.0(3)
B(21)-C(73)-C(78)-C(77)	-173.1(2)
C(78)-C(73)-C(74)-F(74)	-177.0(2)
B(21)-C(73)-C(74)-F(74)	-4.4(3)
C(78)-C(73)-C(74)-C(75)	1.5(3)
B(21)-C(73)-C(74)-C(75)	174.1(2)
C(72)-C(67)-B(21)-C(79)	-17.9(3)
C(68)-C(67)-B(21)-C(79)	170.0(2)
C(72)-C(67)-B(21)-C(61)	-134.4(3)
C(68)-C(67)-B(21)-C(61)	53.4(3)
C(72)-C(67)-B(21)-C(73)	104.1(3)

C(68)-C(67)-B(21)-C(73)	-68.0(3)
C(74)-C(73)-B(21)-C(79)	50.3(3)
C(78)-C(73)-B(21)-C(79)	-138.2(2)
C(74)-C(73)-B(21)-C(67)	-69.7(3)
C(78)-C(73)-B(21)-C(67)	101.9(3)
C(74)-C(73)-B(21)-C(61)	166.3(2)
C(78)-C(73)-B(21)-C(61)	-22.1(3)
F(84)-C(84)-C(83)-F(83)	1.2(4)
C(79)-C(84)-C(83)-F(83)	-178.1(2)
F(84)-C(84)-C(83)-C(82)	179.8(2)
C(79)-C(84)-C(83)-C(82)	.5(4)
F(82)-C(82)-C(83)-F(83)	-1.5(4)
C(81)-C(82)-C(83)-F(83)	176.8(2)
F(82)-C(82)-C(83)-C(84)	180.0(2)
C(81)-C(82)-C(83)-C(84)	-1.8(4)
F(78)-C(78)-C(77)-F(77)	.2(3)
C(73)-C(78)-C(77)-F(77)	179.8(2)
F(78)-C(78)-C(77)-C(76)	-179.0(2)
C(73)-C(78)-C(77)-C(76)	.6(4)
F(77)-C(77)-C(76)-F(76)	-.2(4)
C(78)-C(77)-C(76)-F(76)	179.0(2)
F(77)-C(77)-C(76)-C(75)	-179.7(2)
C(78)-C(77)-C(76)-C(75)	-.5(4)

Se(1)-N(1)-C(1)-C(2)	-.2(3)
N(2)-C(2)-C(1)-N(1)	.0(4)
C(2)-N(2)-C(33)-C(35)	85.6(3)
Se(1)-N(2)-C(33)-C(35)	-93.3(2)
C(2)-N(2)-C(33)-C(36)	-155.9(3)
Se(1)-N(2)-C(33)-C(36)	25.2(3)
C(2)-N(2)-C(33)-C(34)	-35.1(4)
Se(1)-N(2)-C(33)-C(34)	146.0(2)
C(68)-C(67)-C(72)-F(72)	176.8(2)
B(21)-C(67)-C(72)-F(72)	4.3(4)
C(68)-C(67)-C(72)-C(71)	-1.9(4)
B(21)-C(67)-C(72)-C(71)	-174.5(3)
F(82)-C(82)-C(81)-F(81)	.1(4)
C(83)-C(82)-C(81)-F(81)	-178.1(2)
F(82)-C(82)-C(81)-C(80)	178.4(2)
C(83)-C(82)-C(81)-C(80)	.1(4)
F(80)-C(80)-C(81)-F(81)	.2(4)
C(79)-C(80)-C(81)-F(81)	-178.7(2)
F(80)-C(80)-C(81)-C(82)	-178.1(2)
C(79)-C(80)-C(81)-C(82)	3.1(4)
F(84)-C(84)-C(79)-C(80)	-176.9(2)
C(83)-C(84)-C(79)-C(80)	2.3(4)
F(84)-C(84)-C(79)-B(21)	-.5(4)

C(83)-C(84)-C(79)-B(21)	178.7(2)
F(80)-C(80)-C(79)-C(84)	177.0(2)
C(81)-C(80)-C(79)-C(84)	-4.2(4)
F(80)-C(80)-C(79)-B(21)	.4(4)
C(81)-C(80)-C(79)-B(21)	179.2(2)
C(67)-B(21)-C(79)-C(84)	131.8(3)
C(61)-B(21)-C(79)-C(84)	-103.6(3)
C(73)-B(21)-C(79)-C(84)	18.2(4)
C(67)-B(21)-C(79)-C(80)	-52.1(3)
C(61)-B(21)-C(79)-C(80)	72.5(3)
C(73)-B(21)-C(79)-C(80)	-165.7(2)
F(76)-C(76)-C(75)-F(75)	-.8(4)
C(77)-C(76)-C(75)-F(75)	178.7(2)
F(76)-C(76)-C(75)-C(74)	-178.6(2)
C(77)-C(76)-C(75)-C(74)	.9(4)
F(74)-C(74)-C(75)-F(75)	-.7(3)
C(73)-C(74)-C(75)-F(75)	-179.3(2)
F(74)-C(74)-C(75)-C(76)	177.0(2)
C(73)-C(74)-C(75)-C(76)	-1.5(4)
C(72)-C(67)-C(68)-F(68)	-177.9(2)
B(21)-C(67)-C(68)-F(68)	-4.6(3)
C(72)-C(67)-C(68)-C(69)	1.5(4)
B(21)-C(67)-C(68)-C(69)	174.8(2)

F(62)-C(62)-C(61)-C(66)	-178.6(2)
C(63)-C(62)-C(61)-C(66)	1.7(4)
F(62)-C(62)-C(61)-B(21)	-3.6(4)
C(63)-C(62)-C(61)-B(21)	176.8(3)
F(66)-C(66)-C(61)-C(62)	179.7(2)
C(65)-C(66)-C(61)-C(62)	-1.1(4)
F(66)-C(66)-C(61)-B(21)	4.2(3)
C(65)-C(66)-C(61)-B(21)	-176.6(2)
C(79)-B(21)-C(61)-C(62)	-105.0(3)
C(67)-B(21)-C(61)-C(62)	16.7(4)
C(73)-B(21)-C(61)-C(62)	131.7(3)
C(79)-B(21)-C(61)-C(66)	69.8(3)
C(67)-B(21)-C(61)-C(66)	-168.5(2)
C(73)-B(21)-C(61)-C(66)	-53.5(3)
F(70)-C(70)-C(71)-F(71)	-.2(4)
C(69)-C(70)-C(71)-F(71)	-178.6(3)
F(70)-C(70)-C(71)-C(72)	178.1(3)
C(69)-C(70)-C(71)-C(72)	-.2(4)
F(72)-C(72)-C(71)-F(71)	.9(4)
C(67)-C(72)-C(71)-F(71)	179.7(2)
F(72)-C(72)-C(71)-C(70)	-177.4(2)
C(67)-C(72)-C(71)-C(70)	1.4(4)
F(68)-C(68)-C(69)-F(69)	.2(4)

C(67)-C(68)-C(69)-F(69)	-179.2(2)
F(68)-C(68)-C(69)-C(70)	178.8(2)
C(67)-C(68)-C(69)-C(70)	-.6(4)
F(70)-C(70)-C(69)-F(69)	.1(4)
C(71)-C(70)-C(69)-F(69)	178.5(3)
F(70)-C(70)-C(69)-C(68)	-178.5(3)
C(71)-C(70)-C(69)-C(68)	-.1(4)
F(66)-C(66)-C(65)-F(65)	-.8(4)
C(61)-C(66)-C(65)-F(65)	-180.0(2)
F(66)-C(66)-C(65)-C(64)	179.3(3)
C(61)-C(66)-C(65)-C(64)	.1(4)
F(65)-C(65)-C(64)-F(64)	1.1(5)
C(66)-C(65)-C(64)-F(64)	-179.0(3)
F(65)-C(65)-C(64)-C(63)	-179.5(3)
C(66)-C(65)-C(64)-C(63)	.5(5)
F(64)-C(64)-C(63)-F(63)	-.7(5)
C(65)-C(64)-C(63)-F(63)	179.9(3)
F(64)-C(64)-C(63)-C(62)	179.6(3)
C(65)-C(64)-C(63)-C(62)	.1(5)
F(62)-C(62)-C(63)-F(63)	-.7(4)
C(61)-C(62)-C(63)-F(63)	178.9(3)
F(62)-C(62)-C(63)-C(64)	179.0(3)
C(61)-C(62)-C(63)-C(64)	-1.4(5)

N(21)-Se(22)-N(22)-C(22)	-1.3(2)
N(21)-Se(22)-N(22)-C(23)	173.7(2)
C(23)-N(22)-C(22)-C(21)	-173.5(3)
Se(22)-N(22)-C(22)-C(21)	1.2(3)
N(22)-Se(22)-N(21)-C(21)	.9(2)
C(22)-N(22)-C(23)-C(26)	-149.5(3)
Se(22)-N(22)-C(23)-C(26)	36.5(3)
C(22)-N(22)-C(23)-C(25)	-29.0(4)
Se(22)-N(22)-C(23)-C(25)	157.0(2)
C(22)-N(22)-C(23)-C(24)	91.5(4)
Se(22)-N(22)-C(23)-C(24)	-82.5(3)
Se(22)-N(21)-C(21)-C(22)	-.5(3)
N(22)-C(22)-C(21)-N(21)	-.6(4)
C(60)-C(55)-C(56)-F(56)	-176.8(2)
B(11)-C(55)-C(56)-F(56)	-1.7(3)
C(60)-C(55)-C(56)-C(57)	2.8(4)
B(11)-C(55)-C(56)-C(57)	178.0(2)
C(56)-C(55)-C(60)-F(60)	176.3(2)
B(11)-C(55)-C(60)-F(60)	1.6(4)
C(56)-C(55)-C(60)-C(59)	-3.1(4)
B(11)-C(55)-C(60)-C(59)	-177.9(2)
F(38)-C(38)-C(37)-C(42)	-177.7(2)
C(39)-C(38)-C(37)-C(42)	1.8(3)

F(38)-C(38)-C(37)-B(11)	-3.8(4)
C(39)-C(38)-C(37)-B(11)	175.7(2)
F(42)-C(42)-C(37)-C(38)	178.8(2)
C(41)-C(42)-C(37)-C(38)	-.6(3)
F(42)-C(42)-C(37)-B(11)	4.4(3)
C(41)-C(42)-C(37)-B(11)	-175.0(2)
C(44)-C(43)-C(48)-F(48)	-178.0(2)
B(11)-C(43)-C(48)-F(48)	-4.4(3)
C(44)-C(43)-C(48)-C(47)	1.2(4)
B(11)-C(43)-C(48)-C(47)	174.8(2)
C(48)-C(43)-C(44)-F(44)	178.1(2)
B(11)-C(43)-C(44)-F(44)	4.9(4)
C(48)-C(43)-C(44)-C(45)	-1.2(4)
B(11)-C(43)-C(44)-C(45)	-174.3(2)
C(50)-C(49)-B(11)-C(43)	17.9(3)
C(54)-C(49)-B(11)-C(43)	-172.2(2)
C(50)-C(49)-B(11)-C(37)	-102.9(3)
C(54)-C(49)-B(11)-C(37)	67.0(3)
C(50)-C(49)-B(11)-C(55)	134.8(2)
C(54)-C(49)-B(11)-C(55)	-55.2(3)
C(44)-C(43)-B(11)-C(49)	-132.2(2)
C(48)-C(43)-B(11)-C(49)	55.2(3)
C(44)-C(43)-B(11)-C(37)	-19.5(3)

C(48)-C(43)-B(11)-C(37)	167.9(2)
C(44)-C(43)-B(11)-C(55)	104.9(3)
C(48)-C(43)-B(11)-C(55)	-67.8(3)
C(38)-C(37)-B(11)-C(49)	-105.5(3)
C(42)-C(37)-B(11)-C(49)	68.1(3)
C(38)-C(37)-B(11)-C(43)	132.7(2)
C(42)-C(37)-B(11)-C(43)	-53.7(3)
C(38)-C(37)-B(11)-C(55)	15.5(3)
C(42)-C(37)-B(11)-C(55)	-171.0(2)
C(56)-C(55)-B(11)-C(49)	168.3(2)
C(60)-C(55)-B(11)-C(49)	-17.4(4)
C(56)-C(55)-B(11)-C(43)	-67.8(3)
C(60)-C(55)-B(11)-C(43)	106.5(3)
C(56)-C(55)-B(11)-C(37)	55.4(3)
C(60)-C(55)-B(11)-C(37)	-130.2(3)
F(58)-C(58)-C(59)-F(59)	1.3(4)
C(57)-C(58)-C(59)-F(59)	-177.6(2)
F(58)-C(58)-C(59)-C(60)	-179.8(2)
C(57)-C(58)-C(59)-C(60)	1.3(4)
F(60)-C(60)-C(59)-F(59)	.6(4)
C(55)-C(60)-C(59)-F(59)	-179.9(2)
F(60)-C(60)-C(59)-C(58)	-178.3(2)
C(55)-C(60)-C(59)-C(58)	1.2(4)

F(38)-C(38)-C(39)-F(39)	-1.7(3)
C(37)-C(38)-C(39)-F(39)	178.8(2)
F(38)-C(38)-C(39)-C(40)	178.4(2)
C(37)-C(38)-C(39)-C(40)	-1.1(4)
C(54)-C(49)-C(50)-F(50)	-179.0(2)
B(11)-C(49)-C(50)-F(50)	-8.6(4)
C(54)-C(49)-C(50)-C(51)	-1.1(4)
B(11)-C(49)-C(50)-C(51)	169.3(2)
F(50)-C(50)-C(51)-F(51)	1.1(4)
C(49)-C(50)-C(51)-F(51)	-177.0(2)
F(50)-C(50)-C(51)-C(52)	179.6(2)
C(49)-C(50)-C(51)-C(52)	1.6(4)
F(46)-C(46)-C(47)-F(47)	.5(4)
C(45)-C(46)-C(47)-F(47)	179.8(2)
F(46)-C(46)-C(47)-C(48)	-178.6(2)
C(45)-C(46)-C(47)-C(48)	.7(4)
F(48)-C(48)-C(47)-F(47)	-.9(3)
C(43)-C(48)-C(47)-F(47)	179.9(2)
F(48)-C(48)-C(47)-C(46)	178.2(2)
C(43)-C(48)-C(47)-C(46)	-1.1(4)
F(53)-C(53)-C(54)-F(54)	1.9(4)
C(52)-C(53)-C(54)-F(54)	-178.0(2)
F(53)-C(53)-C(54)-C(49)	-178.7(2)

C(52)-C(53)-C(54)-C(49)	1.3(4)
C(50)-C(49)-C(54)-F(54)	179.0(2)
B(11)-C(49)-C(54)-F(54)	7.9(3)
C(50)-C(49)-C(54)-C(53)	-.4(4)
B(11)-C(49)-C(54)-C(53)	-171.5(2)
F(58)-C(58)-C(57)-F(57)	-1.4(4)
C(59)-C(58)-C(57)-F(57)	177.5(2)
F(58)-C(58)-C(57)-C(56)	179.5(2)
C(59)-C(58)-C(57)-C(56)	-1.6(4)
F(56)-C(56)-C(57)-F(57)	.0(4)
C(55)-C(56)-C(57)-F(57)	-179.7(2)
F(56)-C(56)-C(57)-C(58)	179.1(2)
C(55)-C(56)-C(57)-C(58)	-.6(4)
F(42)-C(42)-C(41)-F(41)	.5(3)
C(37)-C(42)-C(41)-F(41)	180.0(2)
F(42)-C(42)-C(41)-C(40)	179.3(2)
C(37)-C(42)-C(41)-C(40)	-1.3(4)
F(51)-C(51)-C(52)-F(52)	-.5(4)
C(50)-C(51)-C(52)-F(52)	-179.1(2)
F(51)-C(51)-C(52)-C(53)	178.0(2)
C(50)-C(51)-C(52)-C(53)	-.5(4)
F(53)-C(53)-C(52)-F(52)	-2.2(4)
C(54)-C(53)-C(52)-F(52)	177.7(2)

F(53)-C(53)-C(52)-C(51)	179.2(2)
C(54)-C(53)-C(52)-C(51)	-.9(4)
F(46)-C(46)-C(45)-F(45)	-.5(4)
C(47)-C(46)-C(45)-F(45)	-179.8(2)
F(46)-C(46)-C(45)-C(44)	178.7(2)
C(47)-C(46)-C(45)-C(44)	-.6(4)
F(44)-C(44)-C(45)-F(45)	.8(4)
C(43)-C(44)-C(45)-F(45)	-179.9(2)
F(44)-C(44)-C(45)-C(46)	-178.3(2)
C(43)-C(44)-C(45)-C(46)	.9(4)
F(41)-C(41)-C(40)-F(40)	.3(4)
C(42)-C(41)-C(40)-F(40)	-178.5(2)
F(41)-C(41)-C(40)-C(39)	-179.3(2)
C(42)-C(41)-C(40)-C(39)	2.0(4)
F(39)-C(39)-C(40)-F(40)	-.3(4)
C(38)-C(39)-C(40)-F(40)	179.6(2)
F(39)-C(39)-C(40)-C(41)	179.2(2)
C(38)-C(39)-C(40)-C(41)	-.9(4)

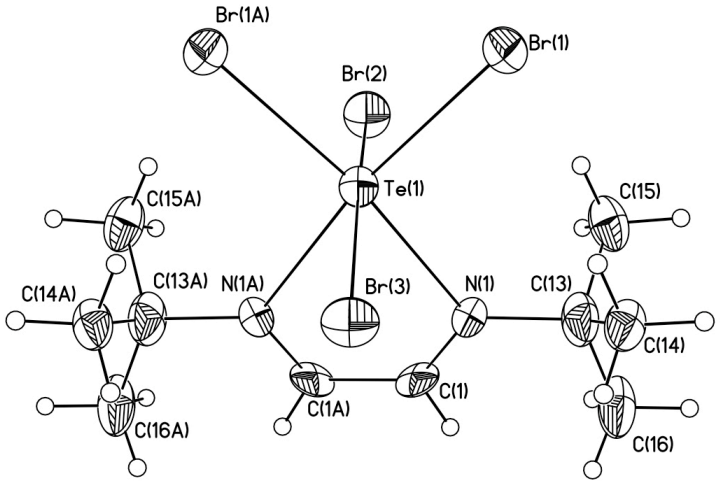

Figure S-9. Solid state structure of **6Br**. Ellipsoids are drawn to 50% probability, and the full labeling scheme is included.

Table S-31. Crystal data and structure refinement for 6Br.

Identification code	6Br
Empirical formula	$C_{10}H_{20}Br_4N_2Te$
Formula weight	615.52
Temperature	150(2) K
Wavelength	.71073 Å
Crystal system, space group	Orthorhombic, *Pnma*
Unit cell dimensions	a = 13.5284(10) Å alpha = 90 deg. b = 18.4929(12) Å beta = 90 deg. c = 6.9942(6)(2) Å gamma = 90 deg.
Volume	1749.8(2) $Å^3$
Z, Calculated density	4, 2.336 Mg/m^3
Absorption coefficient	10.819 mm^{-1}
F(000)	1144
Crystal size	0.15 x 0.13 x 0.08 mm
Theta range for data collection	3.01 to 24.99 deg.
Limiting indices	-15<=h<=16, -21<=k<=21, -8<=l<=8
Reflections collected / unique	8891 / 1576 [R(int) = 0.148]
Completeness to theta =	24.99 98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4975 and 0.2937
Refinement method	Full-matrix least-squares on F^2

Data / restraints / parameters	1576 / 0 / 85
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0703, wR2 = 0.1703
R indices (all data)	R1 = 0.1091, wR2 = 0.1919
Largest diff. peak and hole	1.879 and -1.606 e. $Å^{-3}$

Table S-32. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5I. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Te(1)	-74(1)	2500	393(2)	27(1)
Br(1)	-1042(1)	3493(1)	-1572(2)	37(1)
Br(2)	1493(2)	2500	-1903(3)	41(1)
Br(3)	-1310(2)	2500	3358(3)	37(1)
N(1)	974(7)	3271(5)	2434(15)	22(2)
C(1)	1552(9)	2890(7)	3468(17)	29(3)
C(13)	980(11)	4065(7)	2470(20)	42(4)
C(14)	-69(9)	4313(7)	2960(20)	37(4)
C(15)	1297(10)	4302(8)	450(20)	43(4)
C(16)	1703(11)	4363(8)	3950(20)	52(5)

Table S-33. Bond lengths [Å] and angles [deg] for 6Br.

Te(1)-N(1)	2.466(10)
Te(1)-N(1)#1	2.466(10)
Te(1)-Br(1)	2.6419(16)
Te(1)-Br(1)#1	2.6419(16)
Te(1)-Br(2)	2.659(2)
Te(1)-Br(3)	2.664(2)
N(1)-C(1)	1.279(15)
N(1)-C(13)	1.468(17)
C(1)-C(1)#1	1.44(3)
C(1)-H(1A)	.9500
C(13)-C(16)	1.529(19)
C(13)-C(14)	1.530(18)
C(13)-C(15)	1.54(2)
C(14)-H(14A)	.9800
C(14)-H(14B)	.9800
C(14)-H(14C)	.9800
C(15)-H(15A)	.9800
C(15)-H(15B)	.9800
C(15)-H(15C)	.9800

C(16)-H(16A)	.9800
C(16)-H(16B)	.9800
C(16)-H(16C)	.9800

N(1)-Te(1)-N(1)#1	70.7(5)
N(1)-Te(1)-Br(1)	100.6(2)
N(1)#1-Te(1)-Br(1)	171.2(2)
N(1)-Te(1)-Br(1)#1	171.2(2)
N(1)#1-Te(1)-Br(1)#1	100.6(2)
Br(1)-Te(1)-Br(1)#1	88.11(7)
N(1)-Te(1)-Br(2)	83.8(2)
N(1)#1-Te(1)-Br(2)	83.8(2)
Br(1)-Te(1)-Br(2)	94.66(6)
Br(1)#1-Te(1)-Br(2)	94.66(6)
N(1)-Te(1)-Br(3)	84.8(2)
N(1)#1-Te(1)-Br(3)	84.8(2)
Br(1)-Te(1)-Br(3)	95.37(6)
Br(1)#1-Te(1)-Br(3)	95.37(6)
Br(2)-Te(1)-Br(3)	166.02(8)
C(1)-N(1)-C(13)	122.6(11)
C(1)-N(1)-Te(1)	111.1(8)
C(13)-N(1)-Te(1)	126.2(8)
N(1)-C(1)-C(1)#1	123.5(7)

N(1)-C(1)-H(1A)	118.3
C(1)#1-C(1)-H(1A)	118.3
N(1)-C(13)-C(16)	112.0(11)
N(1)-C(13)-C(14)	107.3(11)
C(16)-C(13)-C(14)	109.5(13)
N(1)-C(13)-C(15)	105.8(12)
C(16)-C(13)-C(15)	109.9(12)
C(14)-C(13)-C(15)	112.2(13)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5

C(13)-C(16)-H(16C) 109.5

H(16A)-C(16)-H(16C) 109.5

H(16B)-C(16)-H(16C) 109.5

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z

Table S-34. Anisotropic displacement parameters (A^2 x 10^3) for 6Br.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Te(1)	25(1)	26(1)	29(1)	0	0(1)	0
Br(1)	41(1)	31(1)	38(1)	2(1)	-8(1)	4(1)
Br(2)	38(1)	45(1)	39(1)	0	10(1)	0
Br(3)	30(1)	49(1)	34(1)	0	4(1)	0
N(1)	14(6)	23(5)	30(6)	-5(5)	0(5)	0(4)
C(1)	26(8)	37(7)	26(7)	-7(6)	-9(6)	-14(6)

C(13)	46(10)	24(8)	58(10)	2(7)	-8(8)	-9(7)
C(14)	31(8)	30(7)	50(9)	-7(7)	-14(7)	8(6)
C(15)	36(9)	31(8)	62(10)	11(8)	0(8)	-4(6)
C(16)	45(10)	27(8)	84(12)	-4(9)	-25(10)	0(7)

Table S-35. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 6Br.

	x	y	z	U(eq)
H(1A)	2007	3133	4281	35
H(14A)	-536	4106	2035	55
H(14B)	-103	4842	2898	55
H(14C)	-240	4150	4248	55
H(15A)	1978	4145	218	64
H(15B)	1257	4830	357	64
H(15C)	857	4082	-495	64
H(16A)	1539	4168	5213	78
H(16B)	1656	4892	3981	78
H(16C)	2378	4221	3606	78

Table S-36. Torsion angles [deg] for 6Br.

N(1)#1-Te(1)-N(1)-C(1)	2.2(9)
Br(2)-Te(1)-N(1)-C(1)	-83.4(8)
Br(3)-Te(1)-N(1)-C(1)	88.5(8)
N(1)#1-Te(1)-N(1)-C(13)	-179.5(9)
Br(2)-Te(1)-N(1)-C(13)	95.0(10)
Br(3)-Te(1)-N(1)-C(13)	-93.2(10)
C(13)-N(1)-C(1)-C(1)#1	179.5(9)
Te(1)-N(1)-C(1)-C(1)#1	-2.2(9)
C(1)-N(1)-C(13)-C(16)	-3.4(19)
Te(1)-N(1)-C(13)-C(16)	178.4(9)
C(1)-N(1)-C(13)-C(14)	-123.7(13)
Te(1)-N(1)-C(13)-C(14)	58.2(14)
C(1)-N(1)-C(13)-C(15)	116.3(13)
Te(1)-N(1)-C(13)-C(15)	-61.9(13)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z

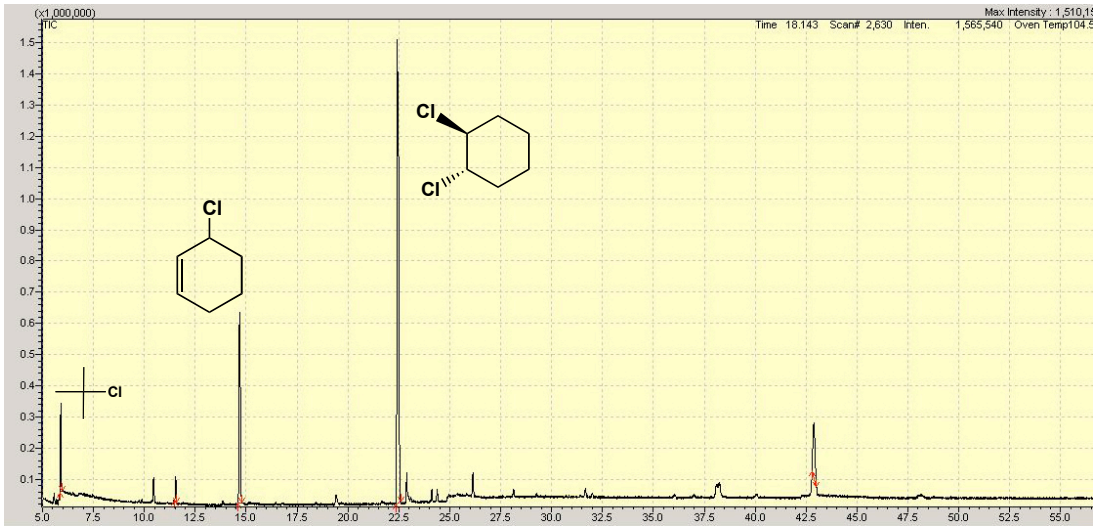

Figure S-10. Chromatogram from GC-MS study of the supernatant from the reaction of *tert*-butyl DAB with $SeCl_4$ in the presence of cyclohexene

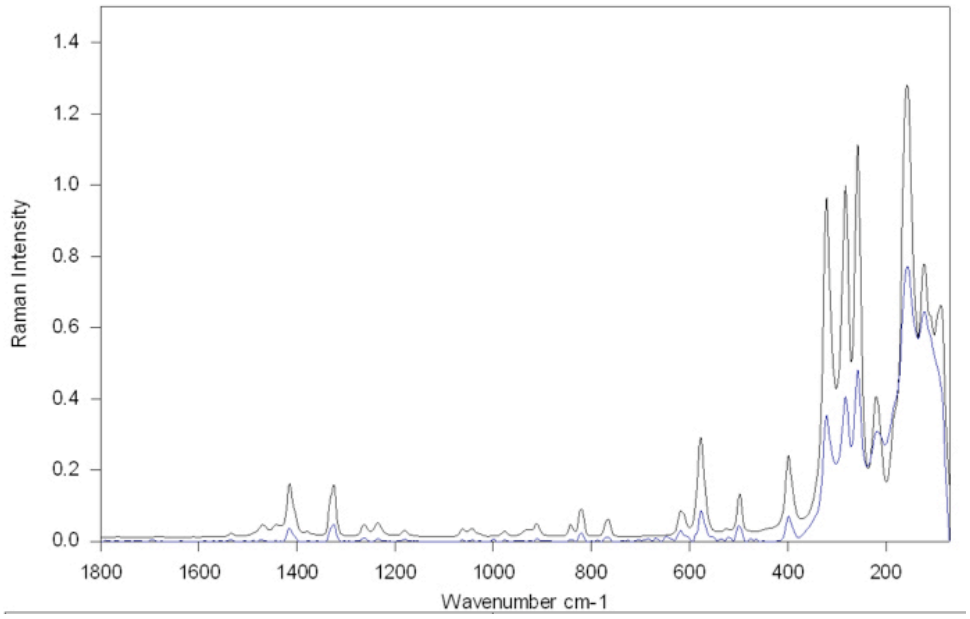

Figure S-11. FT-Raman spectrum of $[5]_2[SeCl_6]$ prepared from *tert*-butyl DAB and $SeCl_4$ (grey) overlayed with $[5]_2[SeCl_6]$ prepared from the reaction of 5Cl with $SeCl_4$ (blue).

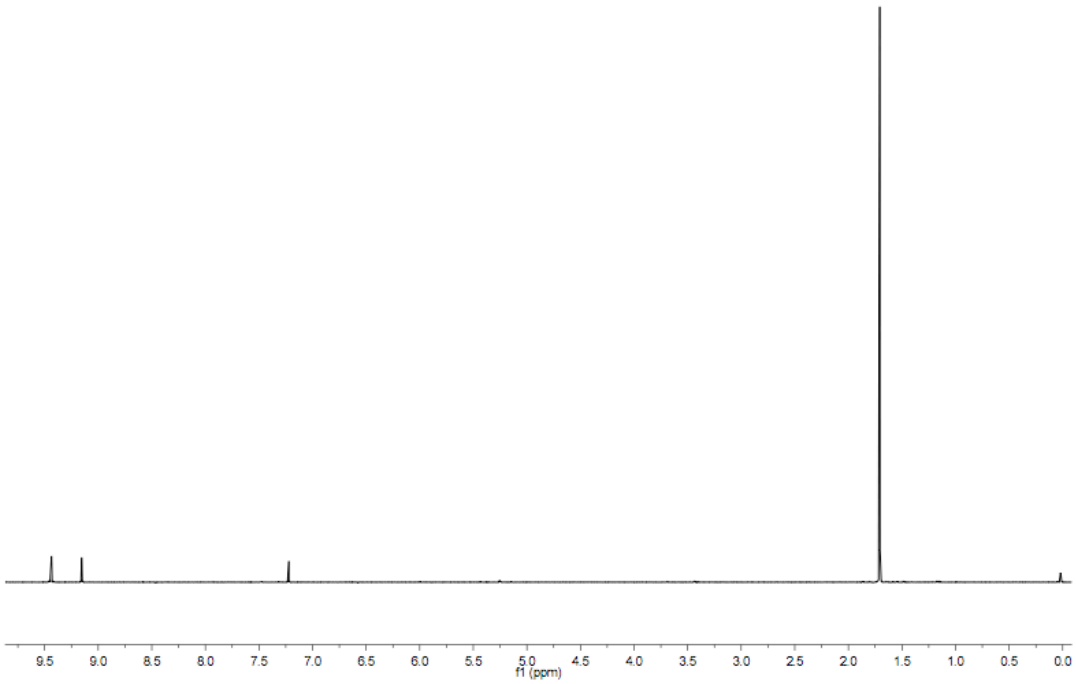

Figure S-12. Proton-NMR spectrum of **5I**.