The Direct Reaction of the *t*Bu-DAB Ligand with $SeCl_4$: A Redox Route to Selenium-Nitrogen Heterocycles

Paul J. Ragogna, Jason L. Dutton, Jocelyn J. Tindale, and Micheal Jennings
Department of Chemistry
The University of Western Ontario, London, Ontario N6A 5V7, Canada

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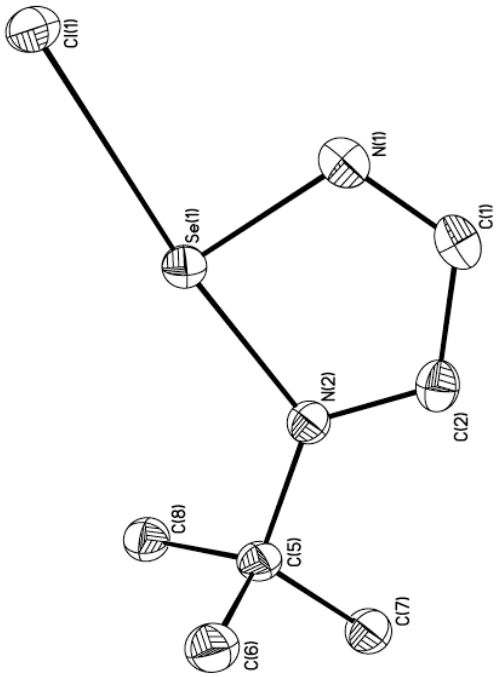

Figure S1: Solid state structure of compound **4Cl**. Ellipsoids are drawn to 50% probability, hydrogen atoms are removed for clarity and the full labeling is shown.

Table S1. Crystal data and structure refinement for Compound **4Cl**.

Identification code	05139b	
Empirical formula	C6 H11 Cl N2 Se	
Formula weight	225.58	
Temperature	150(2) K	
Wavelength	0.71073 ≈	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.1855(7) Å	a= 90°.
	b = 9.2467(7) Å	b= 104.012(4)°.
	c = 10.3396(6) Å	g = 90°.
Volume	852.07(10) $Å^3$	
Z	4	
Density (calculated)	1.758 Mg/m^3	
Absorption coefficient	4.649 mm^{-1}	
F(000)	448	
Crystal size	0.22 x 0.13 x 0.12 mm^3	
Theta range for data collection	3.00 to 28.27∞.	
Index ranges	-12<=h<=12, -12<=k<=11, -13<=l<=13	
Reflections collected	10131	
Independent reflections	2110 [R(int) = 0.060]	
Completeness to theta = 28.27∞	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6054 and 0.4210	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2110 / 0 / 91	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0682	
R indices (all data)	R1 = 0.0507, wR2 = 0.0738	
Largest diff. peak and hole	0.462 and -0.631 e.$≈^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (≈^{2}x 10^3) for **4Cl**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Se	111(1)	371(1)	2763(1)	20(1)
Cl	-2150(1)	-52(1)	3828(1)	25(1)
N(1)	-1177(3)	1280(3)	1408(2)	22(1)
C(2)	-495(3)	1800(3)	542(2)	23(1)
C(3)	1072(3)	1571(3)	754(2)	21(1)
N(4)	1653(2)	849(3)	1830(2)	18(1)
C(5)	3295(3)	530(3)	2372(3)	20(1)
C(6)	3887(3)	1671(3)	3430(2)	25(1)
C(7)	4110(3)	604(3)	1255(3)	26(1)
C(8)	3442(3)	-971(3)	2995(3)	24(1)

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Table S3. Bond lengths [Å] and angles [°] for **4Cl**.

Se-N(1)	1.807(2)
Se-N(4)	1.948(2)
Se-Cl	2.6051(8)
N(1)-C(2)	1.303(3)
C(2)-C(3)	1.418(4)
C(2)-H(2A)	0.9500
C(3)-N(4)	1.297(3)
C(3)-H(3A)	0.9500
N(4)-C(5)	1.505(3)
C(5)-C(8)	1.522(4)
C(5)-C(7)	1.522(4)
C(5)-C(6)	1.523(4)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
N(1)-Se-N(4)	85.91(10)
N(1)-Se-Cl	87.60(8)
N(4)-Se-Cl	173.31(7)
C(2)-N(1)-Se	111.8(2)
N(1)-C(2)-C(3)	118.5(2)
N(1)-C(2)-H(2A)	120.7
C(3)-C(2)-H(2A)	120.7
N(4)-C(3)-C(2)	113.7(2)
N(4)-C(3)-H(3A)	123.2
C(2)-C(3)-H(3A)	123.2
C(3)-N(4)-C(5)	126.0(2)
C(3)-N(4)-Se	110.10(19)
C(5)-N(4)-Se	123.64(16)

N(4)-C(5)-C(8)	108.4(2)
N(4)-C(5)-C(7)	109.9(2)
C(8)-C(5)-C(7)	110.6(2)
N(4)-C(5)-C(6)	106.4(2)
C(8)-C(5)-C(6)	110.4(2)
C(7)-C(5)-C(6)	111.0(2)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\approx^2$x 10^3) for **4Cl**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Se	17(1)	23(1)	20(1)	2(1)	5(1)	2(1)
Cl	19(1)	30(1)	26(1)	-1(1)	8(1)	-1(1)
N(1)	22(1)	21(1)	21(1)	-3(1)	3(1)	2(1)
C(2)	26(2)	21(2)	20(1)	1(1)	1(1)	4(1)
C(3)	26(2)	19(2)	18(1)	-1(1)	6(1)	-1(1)
N(4)	18(1)	19(1)	18(1)	-1(1)	5(1)	1(1)
C(5)	15(1)	24(2)	20(1)	0(1)	6(1)	1(1)
C(6)	22(2)	30(2)	24(1)	-2(1)	7(1)	-3(1)
C(7)	21(2)	36(2)	21(1)	0(1)	8(1)	1(1)
C(8)	21(2)	26(2)	26(2)	2(1)	7(1)	2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (≈^{2}x 10 ^{3}) for **4Cl**.

	x	y	z	U(eq)
H(2A)	-1035	2321	-215	27
H(3A)	1641	1914	163	25
H(6A)	3351	1598	4140	38
H(6B)	3729	2635	3026	38
H(6C)	4962	1516	3806	38
H(7A)	3710	-139	588	38
H(7B)	5184	437	1622	38
H(7C)	3960	1561	837	38
H(8A)	3060	-1693	2302	36
H(8B)	2862	-1015	3673	36
H(8C)	4501	-1170	3409	36

Table S6. Torsion angles [º] for **4Cl**.

N(4)-Se-N(1)-C(2)	-1.1(2)
Cl-Se-N(1)-C(2)	177.23(19)
Se-N(1)-C(2)-C(3)	1.1(3)
N(1)-C(2)-C(3)-N(4)	-0.3(4)
C(2)-C(3)-N(4)-C(5)	-175.3(2)
C(2)-C(3)-N(4)-Se	-0.6(3)
N(1)-Se-N(4)-C(3)	1.00(19)
Cl-Se-N(4)-C(3)	-13.1(7)
N(1)-Se-N(4)-C(5)	175.9(2)
Cl-Se-N(4)-C(5)	161.8(5)
C(3)-N(4)-C(5)-C(8)	-144.3(3)
Se-N(4)-C(5)-C(8)	41.7(3)
C(3)-N(4)-C(5)-C(7)	-23.3(4)
Se-N(4)-C(5)-C(7)	162.70(19)
C(3)-N(4)-C(5)-C(6)	97.0(3)
Se-N(4)-C(5)-C(6)	-77.0(2)

Symmetry transformations used to generate equivalent atoms:

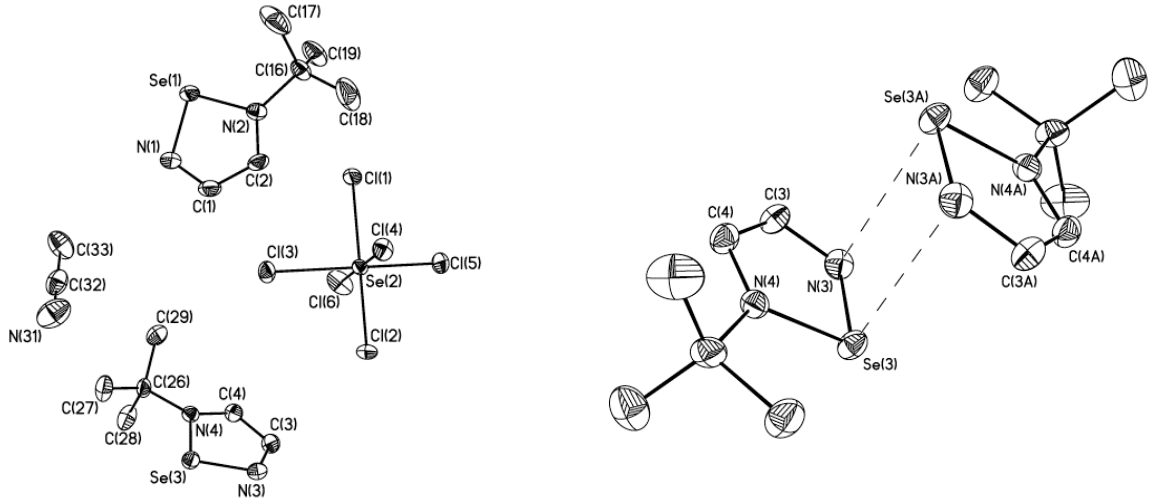

Figure S2: Solid state structure of **[4]$_2$[SeCl$_6$]** (right). Ellipsoids are drawn to 50% probability, hydrogen atoms are removed for clarity and the full labeling scheme is shown. Figure (left) highlights the elongated (3.714 Å) Se•••N secondary bonding interaction.

Table S7. Crystal data and structure refinement for **$[4]_2[SeCl_6]$**.

Identification code	05152
Empirical formula	C14 H25 Cl6 N5 Se3
Formula weight	712.97
Temperature	150(2) K
Wavelength	.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 14.5099(4) A alpha = 90 deg. b = 10.4455(2) A beta = 93.718(2) deg. c = 16.7518(7) A gamma = 90 deg.
Volume	2533.61(14) A^3
Z, Calculated density	4, 1.869 Mg/m^3
Absorption coefficient	5.000 mm^-1
F(000)	1392
Crystal size	0.38 x 0.30 x 0.28 mm
Theta range for data collection	2.65 to 25.02 deg.
Limiting indices	-17<=h<=17, -12<=k<=12, -19<=l<=19
Reflections collected / unique	8643 / 4477 [R(int) = 0.0379]
Completeness to theta = 25.02	99.8 %
Absorption correction	None
Max. and min. transmission	0.3401 and 0.2557
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4477 / 0 / 254
Goodness-of-fit on F^2	1.207
Final R indices [I>2sigma(I)]	R1 = 0.0532, wR2 = 0.1230
R indices (all data)	R1 = 0.0686, wR2 = 0.1276
Largest diff. peak and hole	.915 and -.724 e.A^-3

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **[4]$_2$[SeCl$_6$]**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	U11	U22	U33	U23	U13	U12
Cl(1)	17(1)	26(1)	72(2)	4(1)	2(1)	1(1)
Se(1)	15(1)	26(1)	35(1)	0(1)	0(1)	1(1)
N(1)	18(4)	29(4)	28(4)	-1(3)	2(3)	-2(3)
C(1)	16(4)	34(5)	38(6)	-2(4)	-1(4)	0(4)
Se(2)	16(1)	17(1)	22(1)	-2(1)	5(1)	-1(1)
Cl(2)	16(1)	33(1)	26(1)	-1(1)	1(1)	-2(1)
C(2)	15(4)	27(5)	36(5)	-3(4)	0(4)	6(3)
N(2)	18(4)	25(4)	23(4)	-5(3)	3(3)	0(3)
Cl(3)	29(1)	21(1)	44(1)	4(1)	15(1)	5(1)
Se(3)	20(1)	24(1)	23(1)	4(1)	6(1)	3(1)
N(3)	20(4)	27(4)	23(4)	-1(3)	-1(3)	0(3)
C(3)	26(4)	28(5)	21(5)	5(4)	4(4)	0(4)
Cl(4)	36(1)	24(1)	25(1)	-8(1)	-1(1)	1(1)
C(4)	25(4)	27(5)	17(5)	2(4)	0(4)	-1(4)
N(4)	18(3)	19(3)	23(4)	-3(3)	3(3)	0(3)
Cl(5)	32(1)	27(1)	35(1)	11(1)	4(1)	-2(1)
Cl(6)	48(2)	45(2)	34(1)	-20(1)	21(1)	-12(1)
C(16)	24(4)	24(4)	32(5)	-2(4)	9(4)	-6(4)
C(17)	76(8)	55(7)	39(7)	-5(6)	-8(6)	-38(6)
C(18)	50(7)	24(6)	116(12)	-9(6)	27(7)	-1(5)
C(19)	36(6)	37(6)	56(7)	-4(5)	20(5)	-13(5)
C(26)	25(4)	16(4)	32(5)	5(4)	6(4)	5(3)
C(27)	44(6)	27(5)	34(6)	8(4)	14(5)	11(4)
C(28)	51(6)	29(5)	33(6)	0(4)	-7(5)	10(5)
C(29)	27(5)	36(6)	71(8)	11(5)	4(5)	10(4)
N(31)	46(6)	74(7)	43(6)	-3(5)	6(5)	21(5)
C(32)	43(6)	31(5)	25(5)	-1(4)	-4(5)	6(4)
C(33)	50(6)	43(6)	36(6)	-5(5)	20(5)	-11(5)

Table S9. Bond lengths [Å] and angles [°] for **[4]$_2$[SeCl$_6$]**.

Cl(1)-Se(2)	2.511(2)
Se(1)-N(1)	1.780(7)
Se(1)-N(2)	1.880(7)
N(1)-C(1)	1.295(11)
C(1)-C(2)	1.400(12)
C(1)-H(13A)	.9500
Se(2)-Cl(5)	2.270(2)
Se(2)-Cl(2)	2.299(2)
Se(2)-Cl(6)	2.340(2)
Se(2)-Cl(4)	2.453(2)
Se(2)-Cl(3)	2.567(2)
C(2)-N(2)	1.289(10)
C(2)-H(14A)	.9500
N(2)-C(16)	1.514(10)
Se(3)-N(3)	1.766(7)
Se(3)-N(4)	1.852(7)
N(3)-C(3)	1.315(11)
C(3)-C(4)	1.416(12)
C(3)-H(23A)	.9500
C(4)-N(4)	1.298(10)
C(4)-H(24A)	.9500
N(4)-C(26)	1.524(10)
C(16)-C(19)	1.487(12)
C(16)-C(18)	1.489(13)
C(16)-C(17)	1.542(14)
C(17)-H(17A)	.9800
C(17)-H(17B)	.9800
C(17)-H(17C)	.9800
C(18)-H(18A)	.9800
C(18)-H(18B)	.9800
C(18)-H(18C)	.9800
C(19)-H(19A)	.9800
C(19)-H(19B)	.9800
C(19)-H(19C)	.9800
C(26)-C(29)	1.510(12)
C(26)-C(28)	1.512(12)
C(26)-C(27)	1.527(12)
C(27)-H(27A)	.9800
C(27)-H(27B)	.9800
C(27)-H(27C)	.9800
C(28)-H(28A)	.9800
C(28)-H(28B)	.9800
C(28)-H(28C)	.9800

C(29)-H(29A)	.9800
C(29)-H(29B)	.9800
C(29)-H(29C)	.9800
N(31)-C(32)	1.144(12)
C(32)-C(33)	1.447(13)
C(33)-H(33A)	.9800
C(33)-H(33B)	.9800
C(33)-H(33C)	.9800
N(1)-Se(1)-N(2)	87.5(3)
C(1)-N(1)-Se(1)	110.7(6)
N(1)-C(1)-C(2)	118.0(7)
N(1)-C(1)-H(13A)	121.0
C(2)-C(1)-H(13A)	121.0
Cl(5)-Se(2)-Cl(2)	90.78(8)
Cl(5)-Se(2)-Cl(6)	90.37(10)
Cl(2)-Se(2)-Cl(6)	89.76(9)
Cl(5)-Se(2)-Cl(4)	90.09(8)
Cl(2)-Se(2)-Cl(4)	89.82(8)
Cl(6)-Se(2)-Cl(4)	179.38(9)
Cl(5)-Se(2)-Cl(1)	89.33(8)
Cl(2)-Se(2)-Cl(1)	179.73(10)
Cl(6)-Se(2)-Cl(1)	90.48(9)
Cl(4)-Se(2)-Cl(1)	89.93(9)
Cl(5)-Se(2)-Cl(3)	179.85(10)
Cl(2)-Se(2)-Cl(3)	89.17(8)
Cl(6)-Se(2)-Cl(3)	89.77(9)
Cl(4)-Se(2)-Cl(3)	89.76(8)
Cl(1)-Se(2)-Cl(3)	90.72(8)
N(2)-C(2)-C(1)	113.9(7)
N(2)-C(2)-H(14A)	123.0
C(1)-C(2)-H(14A)	123.0
C(2)-N(2)-C(16)	128.0(7)
C(2)-N(2)-Se(1)	109.9(6)
C(16)-N(2)-Se(1)	122.1(5)
N(3)-Se(3)-N(4)	88.4(3)
C(3)-N(3)-Se(3)	110.9(6)
N(3)-C(3)-C(4)	116.7(8)
N(3)-C(3)-H(23A)	121.7
C(4)-C(3)-H(23A)	121.7
N(4)-C(4)-C(3)	113.5(8)
N(4)-C(4)-H(24A)	123.2
C(3)-C(4)-H(24A)	123.2
C(4)-N(4)-C(26)	126.4(7)
C(4)-N(4)-Se(3)	110.5(6)
C(26)-N(4)-Se(3)	122.9(5)
C(19)-C(16)-C(18)	112.7(9)

C(19)-C(16)-N(2)	108.0(7)
C(18)-C(16)-N(2)	109.3(7)
C(19)-C(16)-C(17)	109.3(8)
C(18)-C(16)-C(17)	111.9(9)
N(2)-C(16)-C(17)	105.2(7)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(29)-C(26)-C(28)	114.0(8)
C(29)-C(26)-N(4)	109.0(7)
C(28)-C(26)-N(4)	106.3(7)
C(29)-C(26)-C(27)	109.1(8)
C(28)-C(26)-C(27)	111.3(8)
N(4)-C(26)-C(27)	106.8(7)
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5

H(29B)-C(29)-H(29C)	109.5
N(31)-C(32)-C(33)	179.6(12)
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5

Table S-10. Anisotropic displacement parameters (A^2 x 10^3) for **[4]$_2$[SeCl$_6$]**.
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
Cl(1)	17(1)	26(1)	72(2)	4(1)	2(1)	1(1)
Se(1)	15(1)	26(1)	35(1)	0(1)	0(1)	1(1)
N(1)	18(4)	29(4)	28(4)	-1(3)	2(3)	-2(3)
C(1)	16(4)	34(5)	38(6)	-2(4)	-1(4)	0(4)
Se(2)	16(1)	17(1)	22(1)	-2(1)	5(1)	-1(1)
Cl(2)	16(1)	33(1)	26(1)	-1(1)	1(1)	-2(1)
C(2)	15(4)	27(5)	36(5)	-3(4)	0(4)	6(3)
N(2)	18(4)	25(4)	23(4)	-5(3)	3(3)	0(3)
Cl(3)	29(1)	21(1)	44(1)	4(1)	15(1)	5(1)
Se(3)	20(1)	24(1)	23(1)	4(1)	6(1)	3(1)
N(3)	20(4)	27(4)	23(4)	-1(3)	-1(3)	0(3)
C(3)	26(4)	28(5)	21(5)	5(4)	4(4)	0(4)
Cl(4)	36(1)	24(1)	25(1)	-8(1)	-1(1)	1(1)
C(4)	25(4)	27(5)	17(5)	2(4)	0(4)	-1(4)
N(4)	18(3)	19(3)	23(4)	-3(3)	3(3)	0(3)
Cl(5)	32(1)	27(1)	35(1)	11(1)	4(1)	-2(1)
Cl(6)	48(2)	45(2)	34(1)	-20(1)	21(1)	-12(1)
C(16)	24(4)	24(4)	32(5)	-2(4)	9(4)	-6(4)
C(17)	76(8)	55(7)	39(7)	-5(6)	-8(6)	-38(6)
C(18)	50(7)	24(6)	116(12)	-9(6)	27(7)	-1(5)
C(19)	36(6)	37(6)	56(7)	-4(5)	20(5)	-13(5)
C(26)	25(4)	16(4)	32(5)	5(4)	6(4)	5(3)
C(27)	44(6)	27(5)	34(6)	8(4)	14(5)	11(4)
C(28)	51(6)	29(5)	33(6)	0(4)	-7(5)	10(5)
C(29)	27(5)	36(6)	71(8)	11(5)	4(5)	10(4)
N(31)	46(6)	74(7)	43(6)	-3(5)	6(5)	21(5)
C(32)	43(6)	31(5)	25(5)	-1(4)	-4(5)	6(4)
C(33)	50(6)	43(6)	36(6)	-5(5)	20(5)	-11(5)

Table S11. Torsion angles [°] for **$[4]_2[SeCl_6]$**.

N(2)-Se(1)-N(1)-C(1)	-1.6(7)
Se(1)-N(1)-C(1)-C(2)	.5(11)
N(1)-C(1)-C(2)-N(2)	1.5(13)
C(1)-C(2)-N(2)-C(16)	176.1(8)
C(1)-C(2)-N(2)-Se(1)	-2.6(10)
N(1)-Se(1)-N(2)-C(2)	2.4(6)
N(1)-Se(1)-N(2)-C(16)	-176.4(7)
N(4)-Se(3)-N(3)-C(3)	-1.0(6)
Se(3)-N(3)-C(3)-C(4)	.0(9)
N(3)-C(3)-C(4)-N(4)	1.5(11)
C(3)-C(4)-N(4)-C(26)	-177.0(7)
C(3)-C(4)-N(4)-Se(3)	-2.2(9)
N(3)-Se(3)-N(4)-C(4)	1.8(6)
N(3)-Se(3)-N(4)-C(26)	176.9(6)
C(2)-N(2)-C(16)-C(19)	113.4(10)
Se(1)-N(2)-C(16)-C(19)	-68.0(9)
C(2)-N(2)-C(16)-C(18)	-9.6(13)
Se(1)-N(2)-C(16)-C(18)	169.1(8)
C(2)-N(2)-C(16)-C(17)	-129.9(10)
Se(1)-N(2)-C(16)-C(17)	48.7(9)
C(4)-N(4)-C(26)-C(29)	-48.2(11)
Se(3)-N(4)-C(26)-C(29)	137.6(7)
C(4)-N(4)-C(26)-C(28)	75.1(10)
Se(3)-N(4)-C(26)-C(28)	-99.2(8)
C(4)-N(4)-C(26)-C(27)	-166.0(8)
Se(3)-N(4)-C(26)-C(27)	19.8(9)

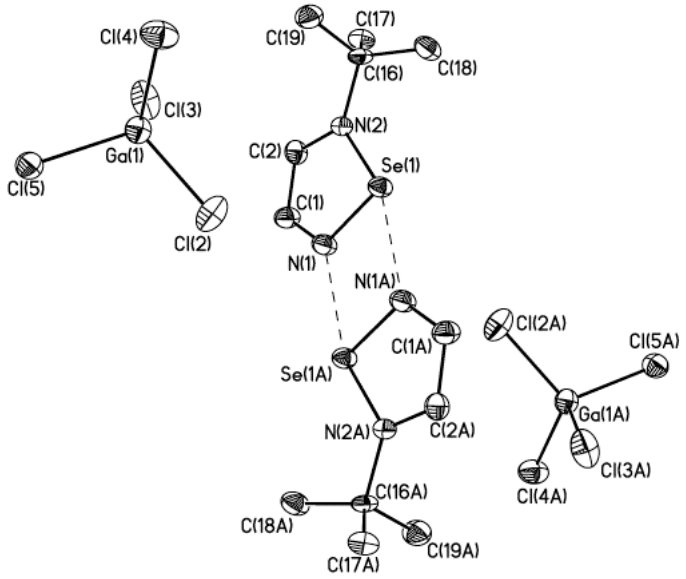

Figure S3: Solid state structure of **[4][$GaCl_4$]**. Ellipsoids are drawn to 50% probability, hydrogen atoms are removed for clarity and the full labeling scheme is shown.

Table S12. Crystal data and structure refinement for **[4][$GaCl_4$]**.

Identification code	06038b
Empirical formula	C6 H11 Cl4 Ga N2 Se
Formula weight	401.65
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.7117(5) Å alpha = 90°. b = 9.9671(4) Å beta = 99.724(2)°. c = 11.0754(4) Å gamma = 90°.
Volume	1383.08(9) A^3
Z, Calculated density	4, 1.929 Mg/m^3
Absorption coefficient	5.361 mm^-1
F(000)	776
Crystal size	0.52 x 0.48 x 0.20 mm
Theta range for data collection	2.61 to 27.55 °.
Limiting indices	-16<=h<=16, -12<=k<=12, -14<=l<=14
Reflections collected / unique	6048 / 3174 [R(int) = 0.0429]
Completeness to theta = 27.55	99.3 %
Absorption correction	None
Max. and min. transmission	0.4136 and 0.1652
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3174 / 0 / 128
Goodness-of-fit on F^2	1.015
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0900
R indices (all data)	R1 = 0.0567, wR2 = 0.0968
Extinction coefficient	.0100(7)
Largest diff. peak and hole	.816 and -.883 e.A^-3

Table S 13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **[4][GaCl$_4$]**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ga(1)	7826(1)	-4403(1)	3354(1)	26(1)
Cl(2)	9112(1)	-3356(1)	4488(1)	46(1)
Cl(3)	7203(1)	-3260(1)	1721(1)	42(1)
Cl(4)	6517(1)	-4760(1)	4352(1)	37(1)
Cl(5)	8400(1)	-6324(1)	2788(1)	30(1)
Se(1)	8626(1)	420(1)	4776(1)	22(1)
N(1)	9548(2)	-43(3)	3797(3)	25(1)
C(1)	9079(3)	-174(4)	2665(3)	27(1)
C(2)	7965(3)	84(4)	2416(3)	25(1)
N(2)	7573(2)	422(3)	3400(3)	19(1)
C(16)	6414(3)	702(3)	3425(3)	21(1)
C(17)	5979(3)	1577(4)	2349(3)	28(1)
C(18)	6347(3)	1407(4)	4623(3)	30(1)
C(19)	5857(3)	-644(4)	3346(4)	32(1)

Table S14. Bond lengths [Å] and angles [°] for **[4][GaCl$_4$]**.

Ga(1)-Cl(2)	2.1549(11)
Ga(1)-Cl(3)	2.1708(11)
Ga(1)-Cl(4)	2.1762(10)
Ga(1)-Cl(5)	2.1793(10)
Se(1)-N(1)	1.787(3)
Se(1)-N(2)	1.851(3)
N(1)-C(1)	1.301(4)
C(1)-C(2)	1.420(5)
C(1)-H(13A)	.9500
C(2)-N(2)	1.317(4)
C(2)-H(14A)	.9500
N(2)-C(16)	1.504(4)
C(16)-C(17)	1.504(5)
C(16)-C(19)	1.513(5)
C(16)-C(18)	1.517(5)
C(17)-H(17A)	.9800
C(17)-H(17B)	.9800
C(17)-H(17C)	.9800
C(18)-H(18A)	.9800

C(18)-H(18B)	.9800
C(18)-H(18C)	.9800
C(19)-H(19A)	.9800
C(19)-H(19B)	.9800
C(19)-H(19C)	.9800
Cl(2)-Ga(1)-Cl(3)	111.42(5)
Cl(2)-Ga(1)-Cl(4)	110.66(4)
Cl(3)-Ga(1)-Cl(4)	107.88(4)
Cl(2)-Ga(1)-Cl(5)	109.58(4)
Cl(3)-Ga(1)-Cl(5)	108.30(4)
Cl(4)-Ga(1)-Cl(5)	108.94(4)
N(1)-Se(1)-N(2)	87.59(13)
C(1)-N(1)-Se(1)	111.7(2)
N(1)-C(1)-C(2)	116.7(3)
N(1)-C(1)-H(13A)	121.7
C(2)-C(1)-H(13A)	121.7
N(2)-C(2)-C(1)	113.0(3)
N(2)-C(2)-H(14A)	123.5
C(1)-C(2)-H(14A)	123.5
C(2)-N(2)-C(16)	124.8(3)
C(2)-N(2)-Se(1)	111.1(2)
C(16)-N(2)-Se(1)	124.1(2)
C(17)-C(16)-N(2)	108.9(3)
C(17)-C(16)-C(19)	111.2(3)
N(2)-C(16)-C(19)	106.6(3)
C(17)-C(16)-C(18)	110.9(3)
N(2)-C(16)-C(18)	107.6(3)
C(19)-C(16)-C(18)	111.5(3)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

Table S 15. Anisotropic displacement parameters (A^2 x 10^3) for **[4][GaCl$_4$]**. 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
Ga(1)	29(1)	27(1)	23(1)	1(1)	5(1)	-1(1)
Cl(2)	48(1)	41(1)	48(1)	-9(1)	0(1)	-15(1)
Cl(3)	64(1)	35(1)	26(1)	6(1)	11(1)	14(1)
Cl(4)	28(1)	57(1)	27(1)	5(1)	7(1)	3(1)
Cl(5)	28(1)	26(1)	38(1)	1(1)	8(1)	-1(1)
Se(1)	18(1)	31(1)	18(1)	1(1)	4(1)	1(1)
N(1)	19(2)	32(2)	24(2)	0(1)	4(1)	3(1)
C(1)	20(2)	37(2)	23(2)	-1(2)	4(2)	-2(2)
C(2)	27(2)	32(2)	16(2)	-2(2)	6(2)	1(2)
N(2)	16(2)	21(2)	21(2)	1(1)	3(1)	0(1)
C(16)	11(2)	30(2)	23(2)	1(1)	1(1)	0(1)
C(17)	20(2)	32(2)	31(2)	4(2)	3(2)	3(2)
C(18)	24(2)	44(2)	22(2)	-3(2)	4(2)	9(2)
C(19)	25(2)	27(2)	46(3)	0(2)	7(2)	-4(2)

Table S 16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **[4][GaCl$_4$]**.

	x	y	z	U(eq)
H(13A)	9463	-429	2036	32
H(14A)	7546	19	1622	30
H(17A)	6029	1102	1587	42
H(17B)	6394	2409	2387	42
H(17C)	5230	1790	2374	42
H(18A)	6634	820	5309	45
H(18B)	5599	1617	4659	45
H(18C)	6762	2240	4674	45
H(19A)	5910	-1070	2561	49
H(19B)	5103	-515	3407	49
H(19C)	6195	-1219	4018	49

Table S17. Torsion angles [deg] for **[4][$GaCl_4$]**.

N(2)-Se(1)-N(1)-C(1)	-1.0(3)
Se(1)-N(1)-C(1)-C(2)	.8(4)
N(1)-C(1)-C(2)-N(2)	-.1(5)
C(1)-C(2)-N(2)-C(16)	-177.6(3)
C(1)-C(2)-N(2)-Se(1)	-.7(4)
N(1)-Se(1)-N(2)-C(2)	1.0(2)
N(1)-Se(1)-N(2)-C(16)	177.9(3)
C(2)-N(2)-C(16)-C(17)	-44.7(4)
Se(1)-N(2)-C(16)-C(17)	138.8(2)
C(2)-N(2)-C(16)-C(19)	75.4(4)
Se(1)-N(2)-C(16)-C(19)	-101.2(3)
C(2)-N(2)-C(16)-C(18)	-165.0(3)
Se(1)-N(2)-C(16)-C(18)	18.5(4)