Investigation of structural, optical, and electrical conductivity study for $(CH_3NH_3)_3(SbCl_5)Cl$ compound

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Table S1. Anisotropic Displacement Parameters ($Å^2×10^3$) for $[(CH_6N)_3(SbCl_5)\cdot Cl]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb1	0.2543(8)	0.2658(9)	0.3602(9)	-0.0353(6)	0.0451(6)	-0.00135(6)
Cl1	0.54(4)	0.418(3)	0.429(4)	0.067(3)	0.131(3)	-0.0004(3)
Cl3	0.418(3)	0.389(3)	0.461(4)	-0.094(3)	0.068(3)	-0.00134(3)
Cl4	0.602(4)	0.716(5)	0.397(4)	-0.55(3)	0.080(3)	-0.0080(4)
Cl2	0.389(3)	0.459(4)	0.732(5)	-0.115(3)	0.022(3)	0.013(3)
N1	0.665(17)	0.41(13)	0.661(17)	-0.77(11)	0.257(13)	-0.004(11)
N2	0.456(12)	0.48(12)	0.49(14)	0.026(10)	0.13(10)	0.041(10)
N3	0.525(15)	0.517(14)	0.651(17)	0.015(12)	0.016(13)	0.009(11)
C2	0.73(2)	0.513(18)	0.65(2)	0.107(15)	0.071(18)	0.0118(15)
C1	0.65(2)	0.548(18)	0.61(2)	-0.156(14)	0.157(16)	-0.0019(14)
C4	0.61(2)	0.111(3)	0.58(2)	-0.01(2)	0.037(17)	0.09(2)
Cl6	0.413(3)	0.516(4)	0.499(4)	0.009(3)	0.070(3)	-0.0038(3)
Cl5	0.557(4)	0.49(4)	0.791(6)	0.051(4)	0.003(4)	0.0178(3)

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $[(CH_6N)_3(SbCl_5)\cdot Cl]$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Sb1	0.40447(2)	0.33225(2)	0.27808(2)	0.02925(5)
Cl1	0.38507(5)	0.28673(8)	0.44482(4)	0.04584(15)
Cl3	0.52337(5)	0.56235(7)	0.32623(4)	0.04213(15)
Cl4	0.44388(6)	0.40782(10)	0.11214(5)	0.05697(18)
Cl2	0.54978(5)	0.13059(8)	0.2877(5)	0.0529(18)
N1	0.6428(2)	0.3131(3)	0.50972(18)	0.0566(7)
N2	0.69391(17)	0.4488(3)	0.18574(15)	0.0470(5)
N3	0.4441(2)	0.8179(3)	0.15123(18)	0.0567(6)
C2	0.6433(3)	0.1453(3)	0.5440(2)	0.0630(9)
C1	0.7401(3)	0.3432(3)	0.1214(2)	0.0597(8)
C4	0.4092(3)	0.8806(5)	0.0633(2)	0.0768(10)
Cl6	0.81251(5)	0.33545(8)	0.37015(5)	0.04743(16)
Cl5	0.75931(6)	0.43345(9)	0.72255(6)	0.0620(2)

Table S3. Bond length (Å) and angles (°) of compound$[(CH_6N)_3(SbCl_5)\cdot Cl]$.

Bond distances (Å)	Bond angles (°)	Bond angles (°)
Sb1–Cl1= 2.5836(7)	Cl1–Sb1–Cl4= 172.56(2)	Cl2–Sb1– Cl1= 89.31(3)
Sb1–Cl3=2.4740(6)	Cl1–Sb1–Cl5^1= 87.23(2)	Cl2–Sb1– Cl5^1= 176.78(3)
Sb1–Cl4= 2.6790(7)	Cl3–Sb1–Cl1= 86.41(2)	
Sb1–Cl2= 2.4834(6)	Cl3–Sb1–Cl4= 86.22(2)	
Sb1–Cl5^1= 2.4834(6)	Cl3–Sb1–Cl2= 91.19(2)	
N1–C2= 1.445(3)	Cl3–Sb1–Cl5^1= 87.26(2)	
N2–C1= 1.464(3)	Cl4–Sb1– Cl5^1= 93.40(3)	
N3–C4= 1.452(4)	Cl2–Sb1– Cl1= 89.86(2)	