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Electronic Supplementary Information

Crystal structure, optical characterization, conduction and relaxation mechanisms in the new hybrid compound $(C_6H_9N_2)_2[Sb_2Cl_8]$

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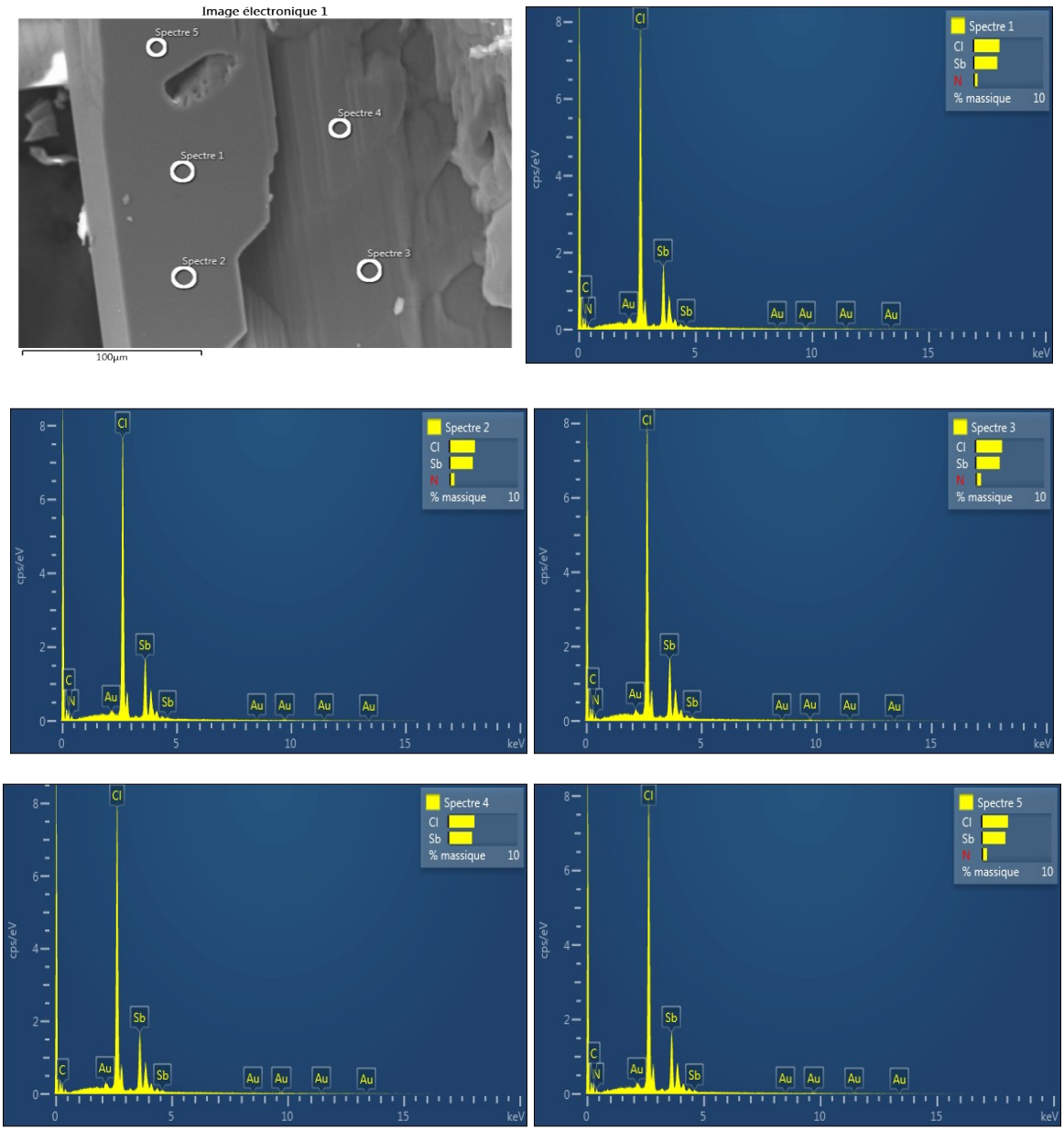

Figure S1: EDS profile of $(C_6H_9N_2)_2[Sb_2Cl_8]$ crystals for different crystals.

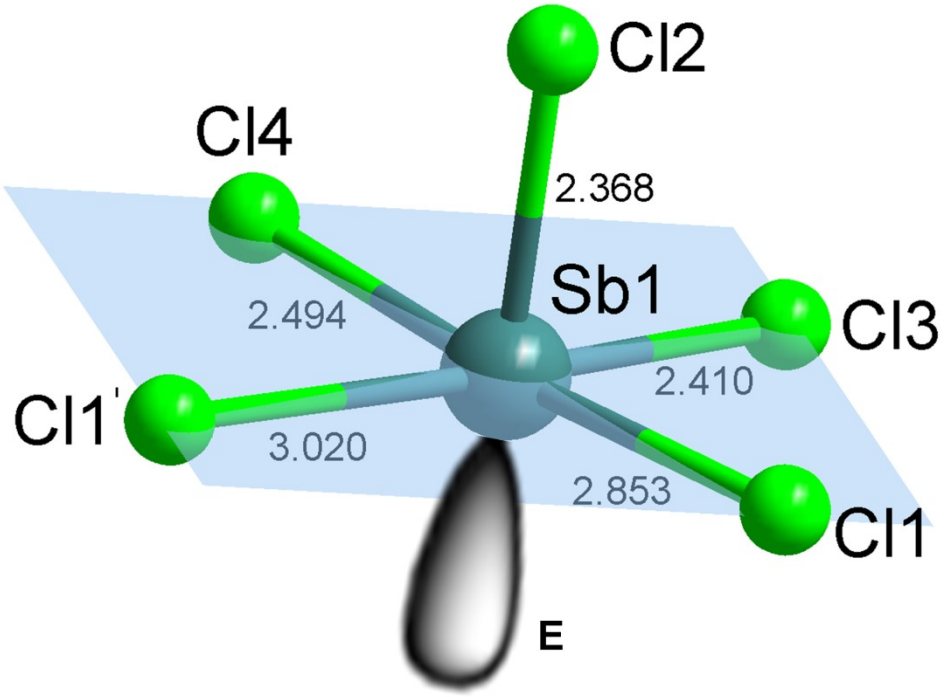

Figure S2: The coordination sphere around antimony atom in $(C_6H_9N_2)_2[Sb_2Cl_8]$ (symmetry code: [I] 1-x, -y, -z).

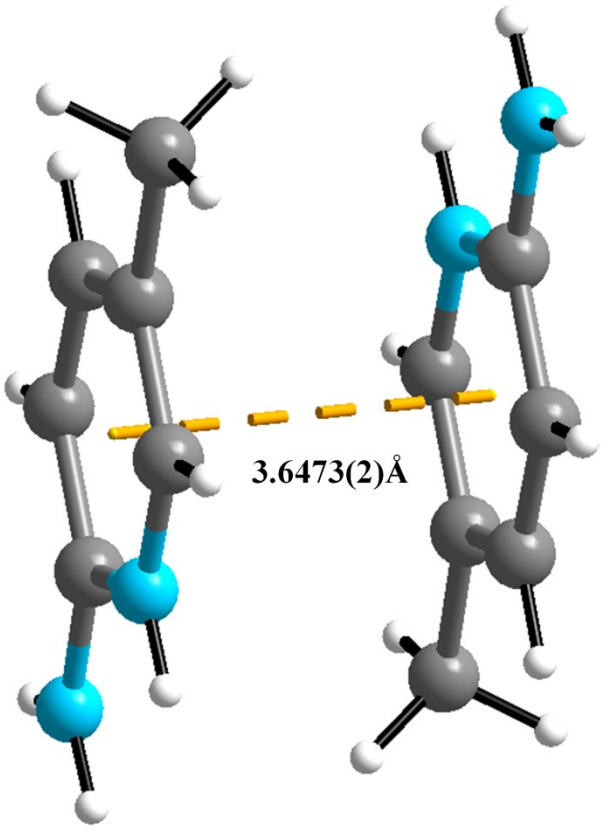

Figure S3: π-π interactions in the structure of $(C_6H_9N_2)_2[Sb_2Cl_8]$

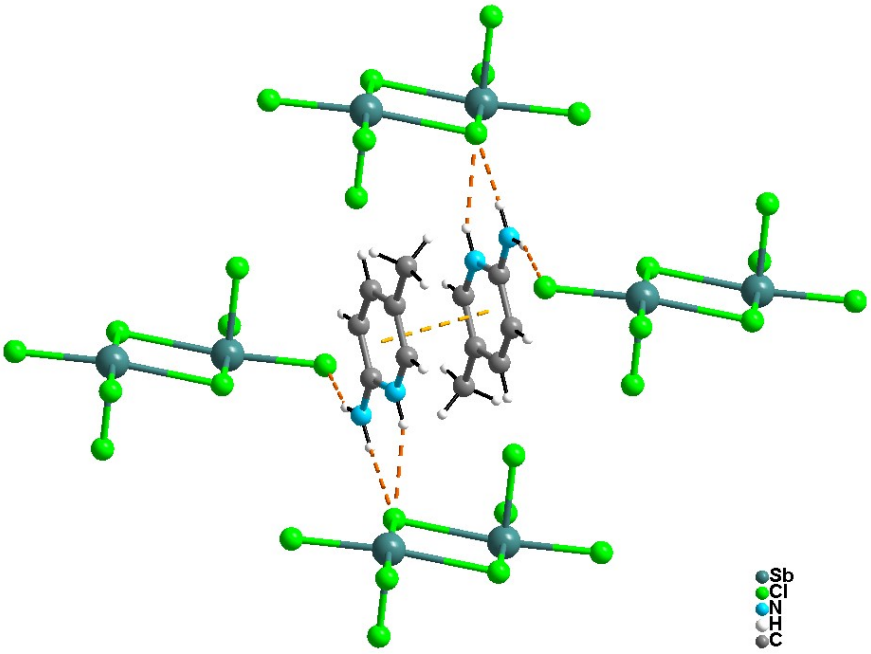

Figure S4: Hydrogen bonds established by the protonated amines

Table S1: Selected bond distances and angles (bond length in Å, bond angle in degrees).

Bond lengths (Å)		**Angle (°)**	
		$[Sb_2Cl_8]^{2-}$	
Sb1-Cl1	2.8527(8)	Cl1-Sb1-Cl2	84.39(3)
Sb1-Cl2	2.3677(8)	Cl1-Sb1-Cl3	89.81(3)
Sb1-Cl3	2.4097(8)	Cl1-Sb1-Cl4	172.89(3)
Sb1-Cl4	2.4942(8)	Cl1-Sb1-$Cl1^{I}$	88.001(22)
Sb1-$Cl1^{I}$	3.0196(9)	Cl2-Sb1-Cl3	92.69(3)
		Cl2-Sb1-Cl4	88.93(3)
		Cl2-Sb1-$Cl1^{I}$	84.247(25)
		Cl3-Sb1-Cl4	92.95(3)
		Cl3-Sb1-$Cl1^{I}$	176.395(23)
		Cl4-Sb1-$Cl1^{I}$	88.913(25)
		$[C_6H_9N_2]^{+}$	
N1-C5	1.337(3)	C5-N1-C6	123.3(2)
N1-C6	1.354(4)	C1-C2-C3	122.2(3)
N2-C5	1.332(4)	C1-C2-C6	122.2(3)
C1-C2	1.501(4)	C3-C2-C6	116.1(3)
C2-C3	1.397(4)	C2-C3-C4	122.5(3)
C2-C6	1.352(4)	C3-C4-C5	119.5(3)
C3-C4	1.355(4)	N1-C5-N2	119.0(3)
C4-C5	1.399(4)	N1-C5-C4	117.1(3)
		N2-C5-C4	123.8(3)
		N1-C6-C2	121.5(3)

Symmetry code: ^{I} 1-x, -y, -z

Table S2: Hydrogen bonding geometry (Å, °) in $(C_6H_9N_2)_2[Sb_2Cl_8]$.

D*—H···*A	***D*—H**	**H···*A***	***D*···*A***	***D*—H···*A***
N1-H1···Cl1	0.86	2.44	3.246(2)	156.3
N2-H2A···Cl1	0.86	2.65	3.402(3)	146.9
N2-H2B···Cl4^{I}	0.86	2.66	3.487(3)	162.6

Symmetry code: ^{I} x-1, y, z

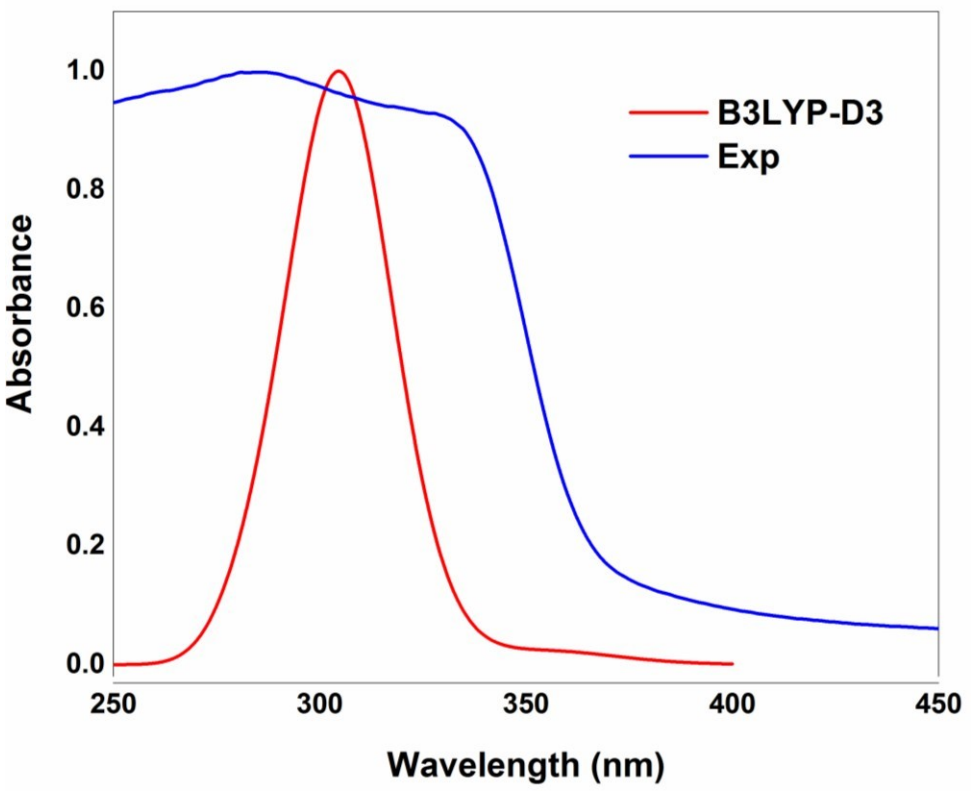

Figure S5: Absorption spectrum predicted with TD-B3LYP-D3/LanL2DZ method in HCl solvent, superimposed to the experimental spectrum.

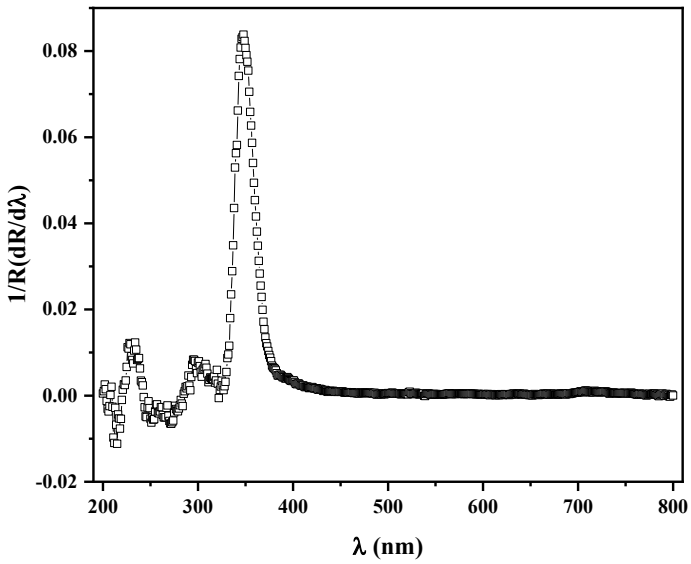

Figure S6: Variation of (1/R)(dR/dλ) as a function of wavelength.

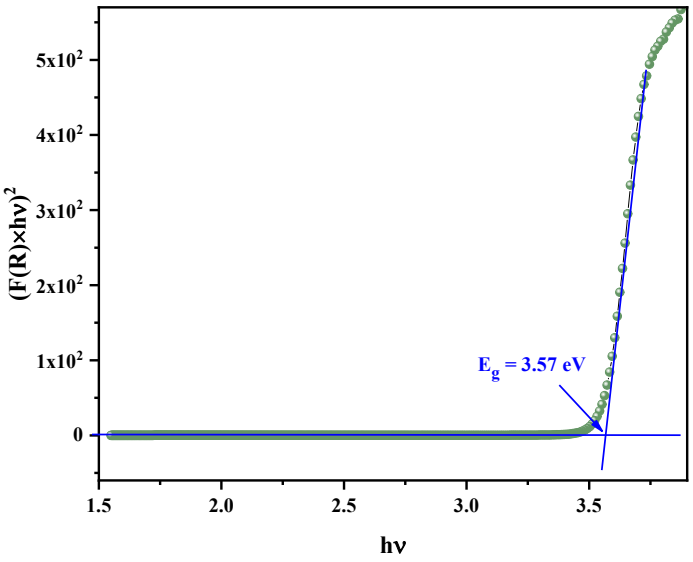

Figure S7: Tauc plot of $(C_6H_9N_2)_2[Sb_2Cl_8]$ compound.

Table S3: Absorption wavelength (λ), excitation energy (E), and oscillator strength (*f*) along with the percentage of the major contribution of each electronic transition calculated by using the TD-B3LYP/LanL2DZ method in HCl solvent.

No	E (cm^{-1})	λ (nm)	f (a.u)	Major contributions
1	3.38	356	0.0009	HOMO→LUMO (97%)
2	3.40	353	0.0001	HOMO→LUMO+1 (97%)
3	3.91	307	0.019	HOMO-1→LUMO (86%) ; HOMO-1→LUMO+1 (11%)
4	3.94	304	0.0227	HOMO-1→LUMO (10%) ; HOMO-1→LUMO+1 (87%)
5	4.15	289	0.0028	HOMO-2→LUMO (66%) ; HOMO-2→LUMO+1 (30%)
6	4.17	287	0.0059	HOMO-2→LUMO (27%) ; HOMO-2→LUMO+1 (63%)

Table S4: TD–DFT calculations of HOMO-LUMO energy gap, chemical potential (μ), electronegativity (χ), global hardness (η), global softness (ζ), electrophilicity index (ω).

Parameters	**Value**
E_{HOMO} (eV)	-6.71
E_{LUMO} (eV)	-2.67
$\Delta E_{HOMO\text{-}LUMO\ gap}$ (eV)	4.04
Global Electrophilicity index ω (eV)	11.00
Electronegativity χ (eV)	4.69
Chemical potential (μ)	-4.69
Global hardness (η) (eV)	2.02
Global softness (ζ) $(eV)^{-1}$	1.00