

Figure S1: The asymmetric unit of $[\text{C}_8\text{H}_{10}\text{NO}]_2\text{HgBr}_4$ compound (expanded by symmetry to give complete metallic tetrahedron). Hydrogen bonds are represented by dashed lines.

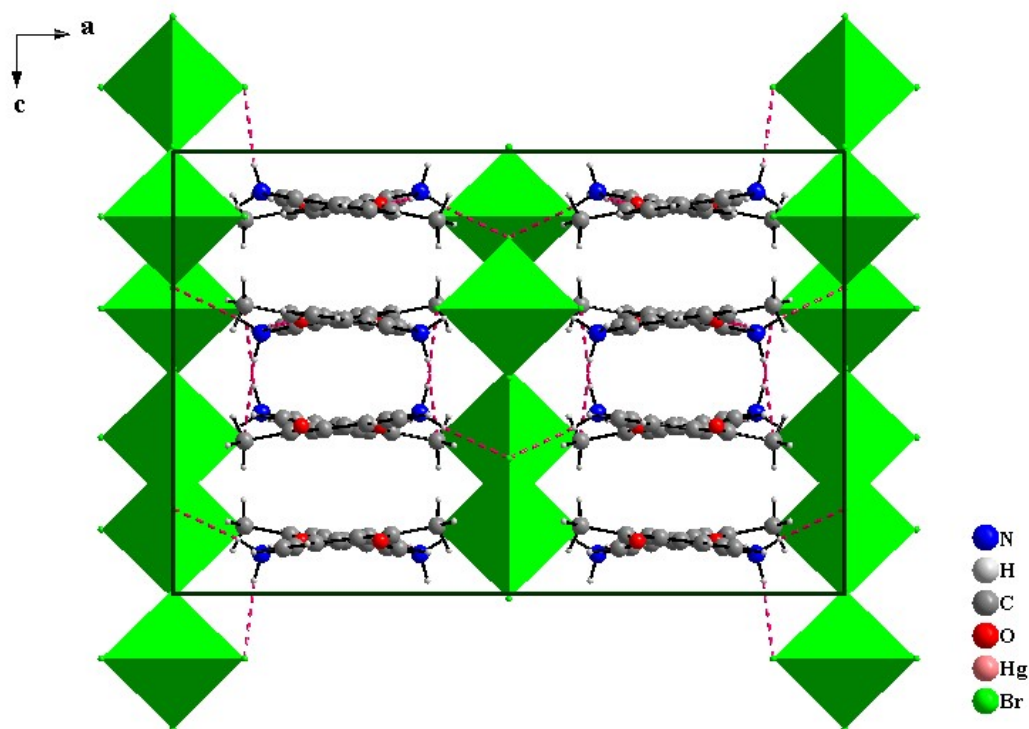


Figure S2: $[010]$ view showing alternation of organic and inorganic sheets in $[\text{C}_8\text{H}_{10}\text{NO}]_2\text{HgBr}_4$ sample.

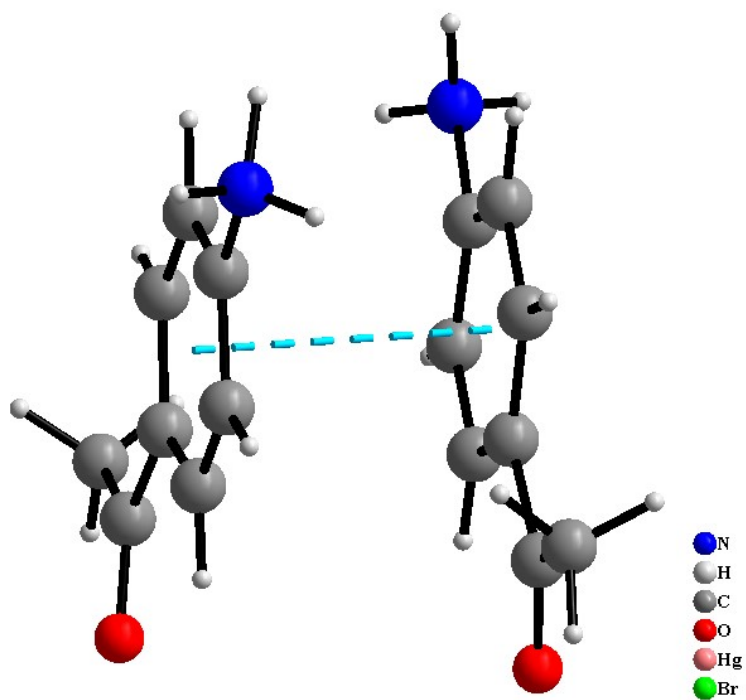
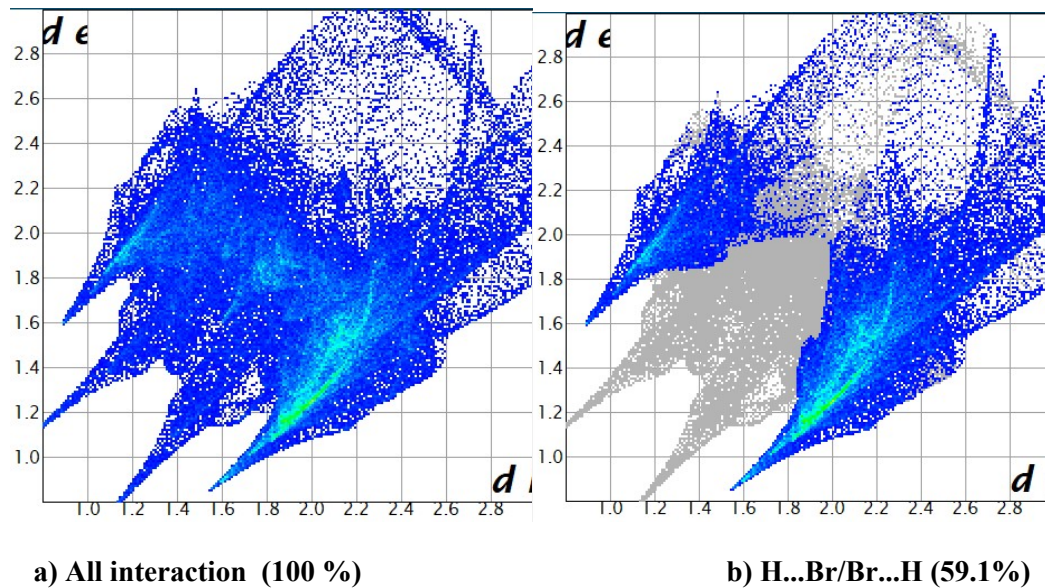
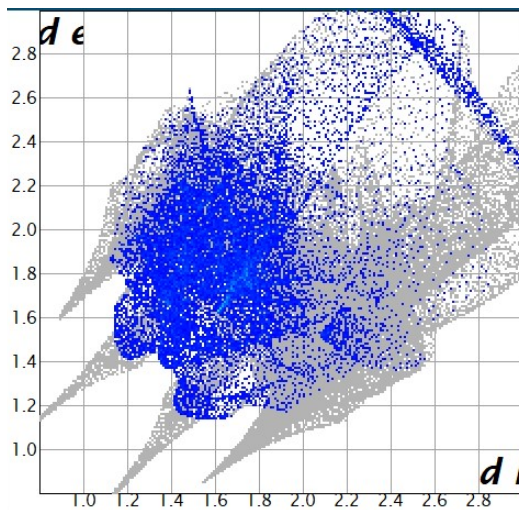
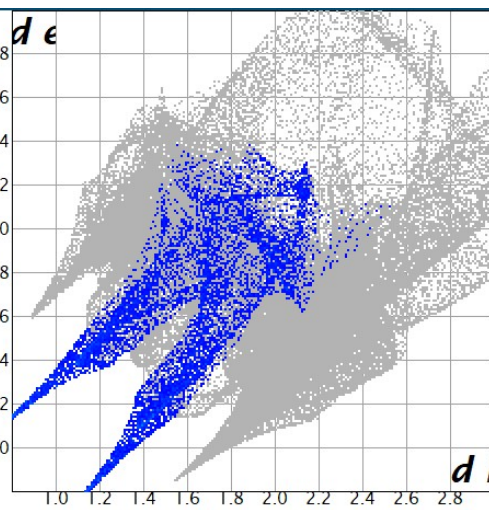


Figure S3: π - π interactions between the organic cations in the $[C_8H_{10}NO]_2HgBr_4$ compound.

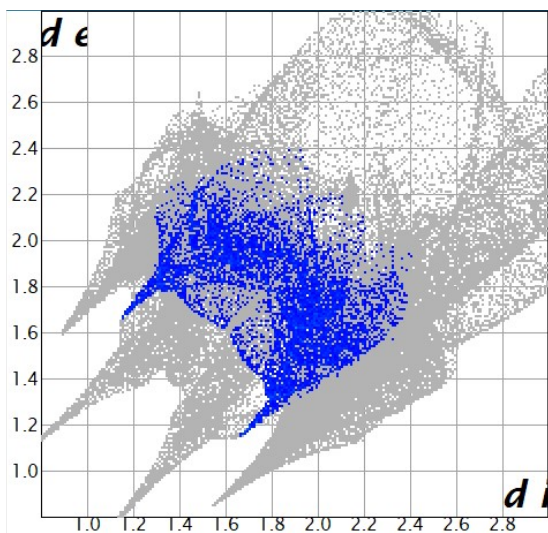




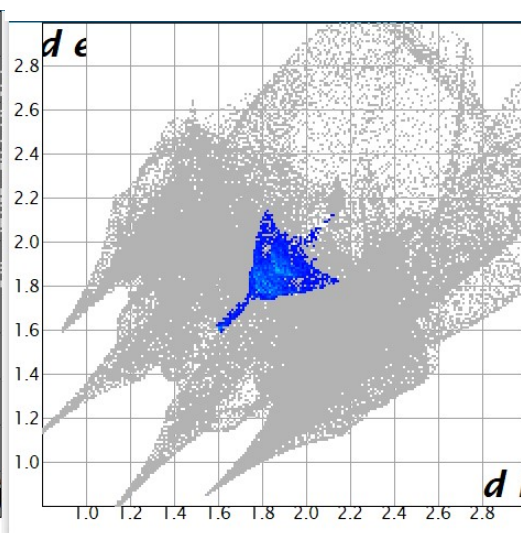
e) H...H/H...H (17.7%)



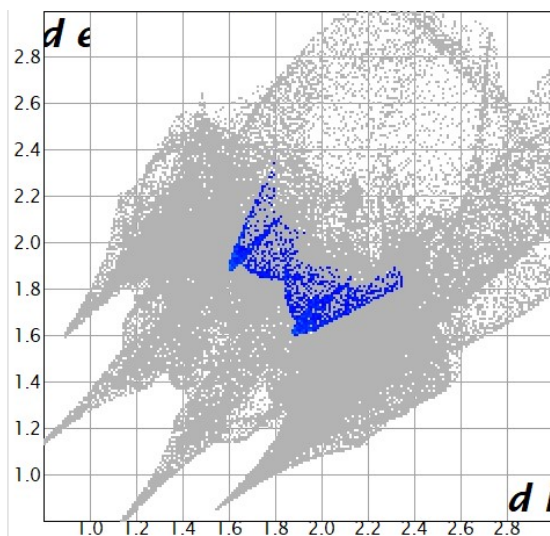
d) O...H/H...O (7.9%)



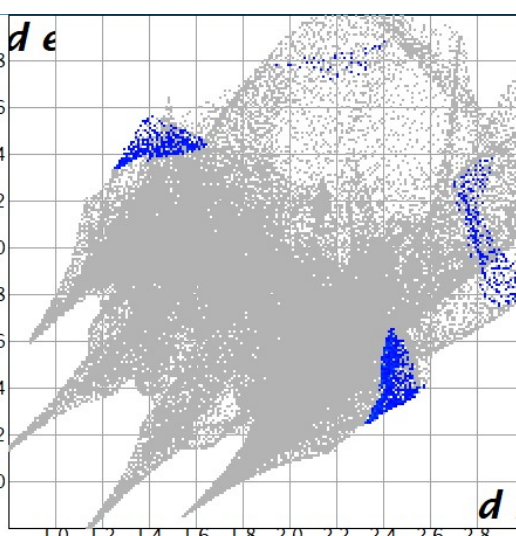
e) C...H/H...C (7.4%)



f) C...C/C...C (3.3%)



g) C...O/O...C (1.7%)



h) H...Hg/Hg...H (1.5%)

Figure S4 : The two-dimensional fingerprint plot for $[C_8H_{10}NO]_2HgBr_4$ showing contributions from different contacts a): all contacts, b): $H\cdots Br/Br\cdots H$, c): $H\cdots H$, d): $O\cdots H/H\cdots O$, e): $C\cdots H/H\cdots C$, f): $C\cdots C$, g): $C\cdots O/O\cdots C$, h): $H\cdots Hg/Hg\cdots H$

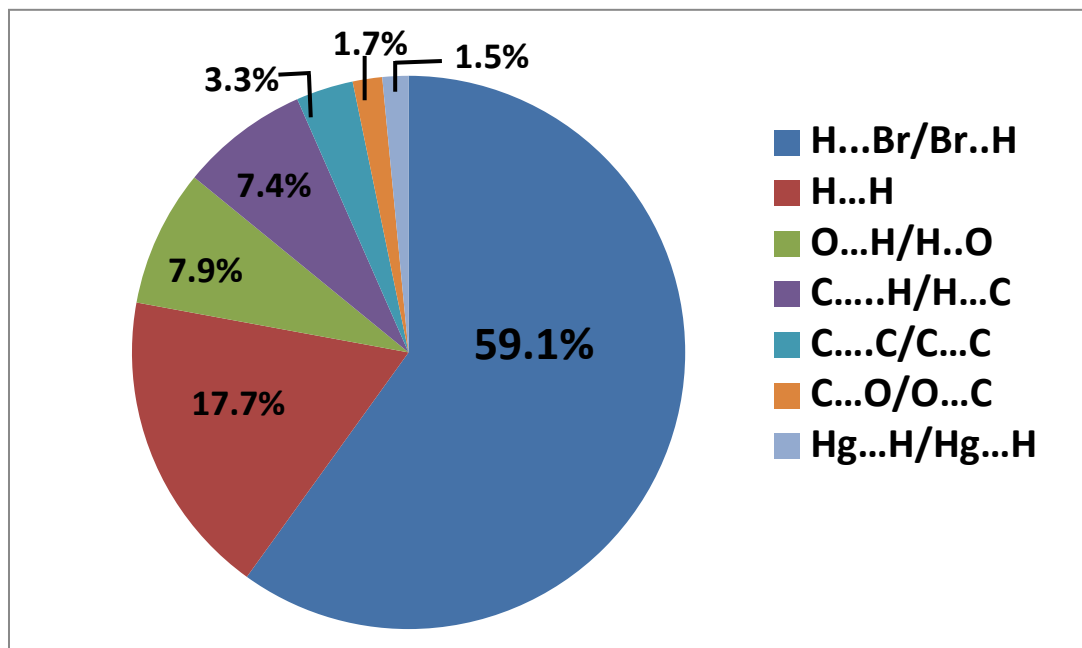


Figure S5: Relative contributions to the Hirshfeld surface areas for the various intermolecular contact

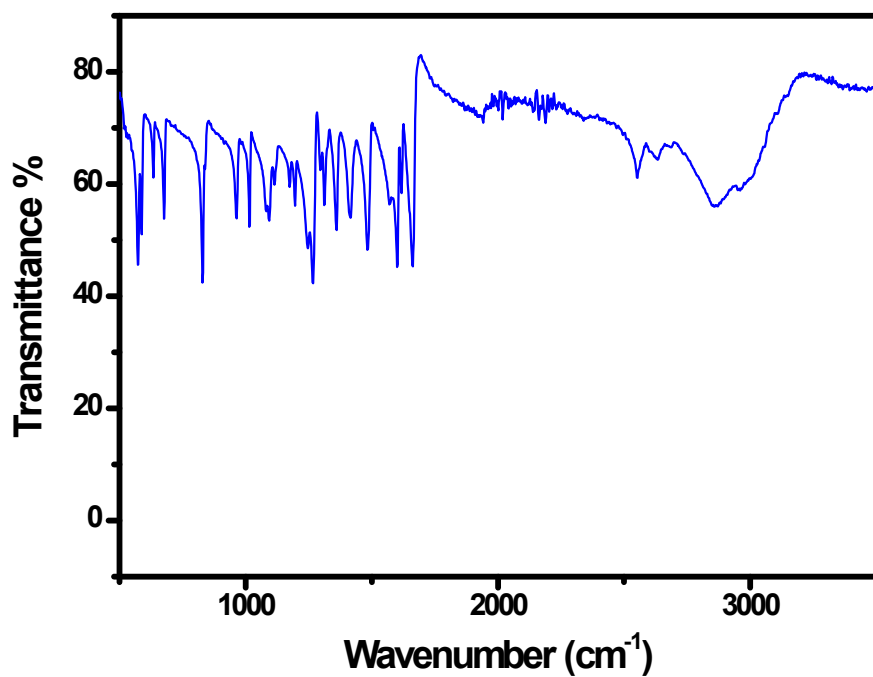


Figure S6: FT-IR spectrum of [C₈H₁₀NO]₂HgBr₄ compound measured at room temperature

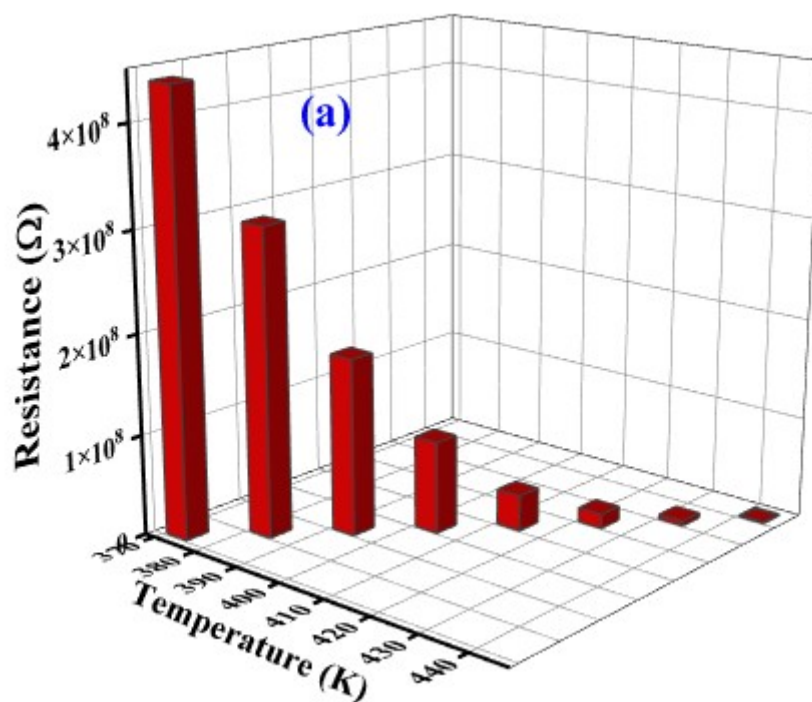


Figure S7: (a) the variation Resistance of [C₈H₁₀NO]₂HgBr₄ at different temperatures.

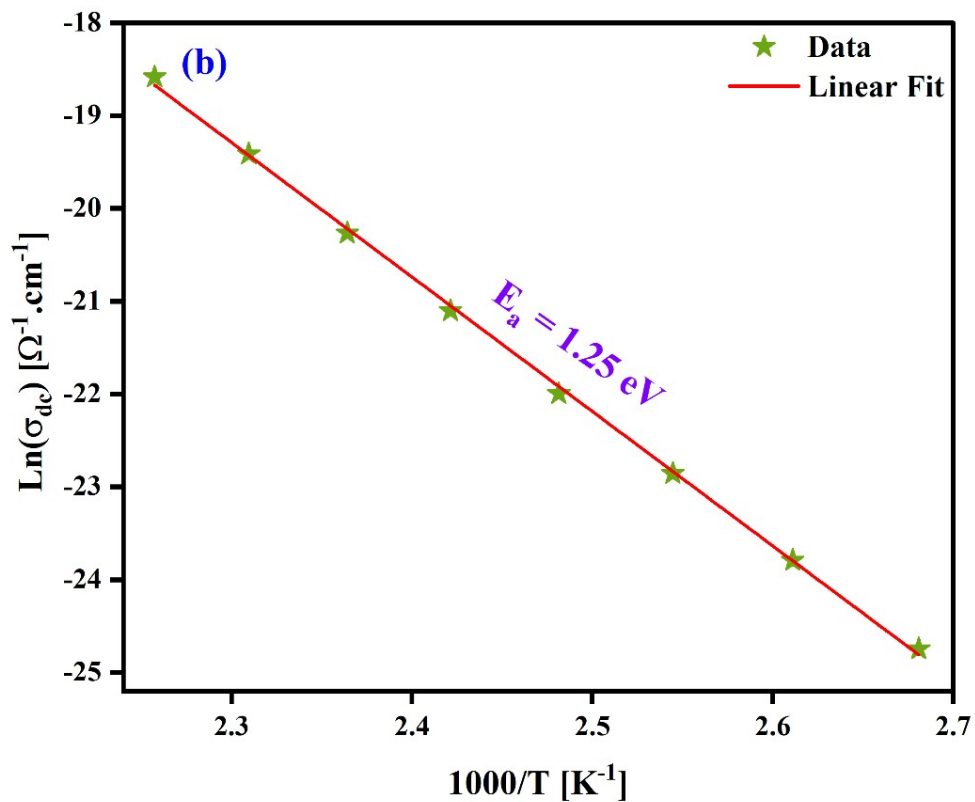


Figure S7 : (b) Arrhenius plots of dc conductivity for $[\text{C}_8\text{H}_{10}\text{NO}]_2\text{HgBr}_4$.

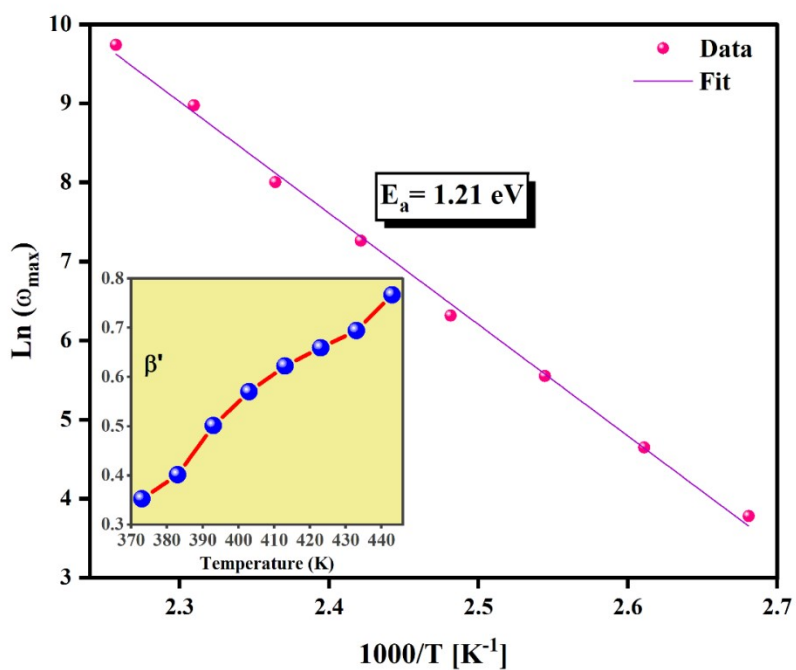


Figure S8: The variation of $\text{Ln}(\omega_{max})$ versus $1000/T$. (inset: Temperature dependence of β' value)

Table S1. Fractional atomic coordinates and equivalent isotropic temperature factors (Å²).

Atome	x	y	z	U_{eq}
Hg1	0.50000	0.25764(1)	0.64600(1)	0.02288(4)
Br1	0.39316(1)	0.17174(1)	0.64602(2)	0.02655(6)
Br2	0.50000	0.35170(2)	0.48913(2)	0.02194(7)
Br02	0.50000	0.35245(2)	0.80651(2)	0.02165(7)
N1	0.63189(9)	0.26326(1)	0.90983(1)	0.02055(4)
C2	0.68157(1)	0.32937(1)	0.89396(1)	0.01668(4)
C3	0.74428(1)	0.30375(1)	0.87978(2)	0.01917(4)
C4	0.7915(1)	0.36711(1)	0.86900(1)	0.01835(4)
C5	0.77506(1)	0.45514(1)	0.87280(1)	0.01602(4)
C6	0.71147(1)	0.47875(1)	0.88542(1)	0.01827(4)
C7	0.66392(1)	0.41645(1)	0.89640(1)	0.01910(4)
C8	0.82519(1)	0.52506(1)	0.86662(1)	0.01772(4)
C10	0.89316(1)	0.50129(1)	0.84616(2)	0.02334(4)
O9	0.80890(8)	0.60105(9)	0.88007(1)	0.02588(3)

Table S2. Principal intermolecular distances (Å) and angles (°).

	Distances (Å)		Angles (°)
Hg1-Br1	2.586(1)	Br1 ⁱ -Hg1-Br1	118.69(1)
Hg1-Br1 ⁱ	2.586(2)	Br2-Hg1-Br1	106.53(1)
Hg1-Br2	2.589(1)	Br1 ⁱ -Hg1-Br2	106.53(1)
Hg1-Br02	2.637(1)	Br1-Hg1-Br02	106.34(1)
N1-C2	1.465(3)	Br1 ⁱ -Hg1-Br02	106.34(1)
C2-C7	1.387(3)	Br2-Hg1-Br02	112.60(1)
C2-C3	1.378(3)	C7-C2-C3	121.99(2)
C3-C4	1.391(3)	C7-C2-N1	118.48(2)
C4-C5	1.395(3)	C3-C2-N1	119.50(2)
C5-C6	1.384(3)	C4-C3-C2	119.04(2)
C5-C8	1.500(3)	C3-C4-C5	120.00(2)
C6-C7	1.385(3)	C4-C5-C6	119.55(2)
C8-O9	1.229(2)	C4-C5-C8	121.36(2)
C8-C10	1.488(3)	C6-C5-C8	119.06(2)
		C5-C6-C7	121.13(2)
		C2-C7-C6	118.27(2)
		O9-C8-C10	121.57(2)
		O9-C8-C5	118.61(2)
		C10-C8-C5	119.81(2)

Symmetry code: ⁱ -x, y, z

Table S3. Assignments of the most important observed bands in IR spectra of $[\text{C}_8\text{H}_{10}\text{NO}]_2\text{HgBr}_4$ at room temperature.

$[\text{C}_8\text{H}_{10}\text{NO}]_2\text{ZnBr}_4$ Attribution	
IR	Attribution
2968	$\nu_{\text{as}}\text{CH}_3$
2852.93	$\nu_{\text{s}}\text{CH}_3$
1660.89	$\nu(\text{C}=\text{O})$
1619.35	$\delta_{\text{as}} \text{NH}_3$
1618.29	C=C stretching vibrations
1600.12	C=C stretching vibrations
1571.91	C=C stretching vibrations
1482.89	C=C stretching vibrations
1414.16	C=C stretching vibrations
1483.53	$\delta_{\text{as}} \text{NH}_3$
1313.65	C-H in-plane bending
1173.68	C-H in-plane bending
963.97	C-H out-of-plane bending
830	C-H out-of-plane bending
1091.13	$\rho(\text{NH}_3)$.
634.15	C-C-C in plane bending
572.73	C-C-C in plane bending
463.34	C-C-C out-of-plane bending

Table S4. Electrical parameters obtained from the fit of Nyquist plots using the Zview software for $[\text{C}_8\text{H}_{10}\text{NO}]_2\text{HgBr}_4$.

T(K)	R ($10^6 \cdot \Omega$)	C ($10^{-11} \cdot \text{F}$)	Q($10^{-10} \cdot \text{F}$)	α
373	439	3.27	0.848	0.6821
383	306	3.28	1.18	0.65305
393	176	3.30	1.78	0.61743
403	91.80	3.32	3.22	0.56864
413	35.80	3.30	3.87	0.57336
423	14.30	3.29	5.04	0.56793
433	4.84	3.29	8.78	0.5442
443	1.17	3.26	7.18	0.59239